# **The American Ceramic Society**

# 49th International Conference & Exposition on Advanced Ceramics and Composites

# **ABSTRACT BOOK**

# January 26–31, 2025 Daytona Beach, Florida

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# Introduction

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# How to Use the Abstract Book

Refer to the Table of Contents to determine page numbers on which specific session abstracts begin. At the beginning of each session are headings that list session title, location and session chair. Starting times for presentations and paper numbers precede each paper title. The Author Index lists each author and the page number on which their abstract can be found.

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### Monday, January 27, 2025

### **Plenary Session**

#### Plenary and Award Talks

#### Room: Coquina D/E

Session Chairs: Amjad Almansour, NASA Glenn Research Center; Jie Zhang, Institute of Metal Research, Chinese Academy of Sciences; Young-Wook Kim, WORLDEX Industry and Trading Co. LTD

#### 8:50 AM

#### (ICACC-PLEN-001-2025) James L. Mueller Memorial Award: The Enduring Legacy of Mullite the Quintessential Engineering Ceramic

S. H. Risbud\*1

1. University of California, Davis, Materials Science and Engineering, USA

Ever since its discovery on the Island of Mull in Scotland, Mullite has enjoyed a rich reputation as an engineering ceramic with widespread applications ranging from high temperature refractories to space shuttle tiles. Research on the Silica-Alumina phase equilibrium diagram date back to the classic work of Bowen and Greig in 1924 followed by many re-evaluations over the past 6 to 7 decades by Aramaki and Roy, Davis and Pask, Aksay and Pask and other ceramic researchers worldwide. Standard melt quenching, diffusion couple heating and sol-gel techniques have been used among others for studying stable and metastable phase equilibria, liquidus-solidus curves, and liquid-liquid immiscibility domes. The time temperature processing parameters are at the heart of the formation of mullite both in the metastable condition as well as the lowest energy stable phase. Clearly, time-temperature-pressure all influence the morphology, structure and properties of mullite. Most phase diagrams of the mullite phase shown on the silica-alumina system are at one atmosphere pressure though high-pressure studies have been reported. While mullite is a dominant phase in modern aluminosilicate ceramics like refractories its presence has been observed in pottery dating back millennia. And in recent times mullite is finding applications in space, electronics and photonics.

#### 9:30 AM

#### (ICACC-PLEN-002-2025) 2025 Mrityunjay Singh Bridge Building Award: Nanocarbon added ceramics: Current status and future trends

#### C. Balazsi\*1

1. ELKH Centre for Energy Research, Hungary

The plenary lecture will give a comprehensive view on innovative developments made in the field of nanocarbons e.g. carbon black, carbon nanotubes, graphene added ceramics highlighting the key issues related to integration technology and improvements in the mechanical, tribological or functional properties as a result. Among non-oxide ceramics the silicon nitride based ceramics are wellknown as low density materials with high strength and toughness. Silicon nitride, known as a typical dielectric material, is an ideal candidate for several structural applications, even at high temperatures. The addition of graphene or carbon nanotubes to silicon nitride to create ceramic nanocomposites gives rise to promising applications in a wide range of fields such as electronics, biomedical aids, membranes, flexible wearable sensors and actuators, energy systems. The presentation will show how the use of different reinforcing phases and sintering methods influence the microstructure and as a result, mechanical properties, electrical, thermal conductivity and tribological properties of the final silicon nitride nanocomposites. The prospective future applications will be also discussed.

#### 10:40 AM

# (ICACC-PLEN-003-2025) Plenary: Nanoparticles engineering toward NT and ET applications

U. Paik\*1; T. Song1; J. Park1; G. Lee1; J. Kim1; I. Kim1; M. Woo1

1. Hanyang University, Department of Energy Engineering, Republic of Korea

The importance of nanoparticle engineering in the fields of semiconductor fabrication and Li-ion battery (LiB) applications will be discussed as follows: (1) Semiconductor: Molybdenum (Mo) is a promising candidate for replacing tungsten in sub-3nm logic and 3D memory devices due to its low resistivity and superior gap-filling ability. However, during the chemical mechanical planarization (CMP) process, the instability of nanoparticles in a suspension and high dissolution rate of Mo films hinder its practical use. This presentation will discuss the importance of nanoparticle engineering in CMP, highlighting its potential to improve CMP performances, increase yield, and enhance compatibility with sub-3nm devices. (2) LiBs: The roll-to-roll dry coating process is a promising method for fabricating high-energy density, low-cost Li-ion batteries. Compared to conventional wet processing, it reduces manufacturing time and cost and offers environmental benefits by avoiding toxic solvents. However, thick dry electrodes increase charge transfer resistance  $(R_{ct})$  and Li-ion migration resistance  $(R_{ion})$  due to microstructural inhomogeneity. By systematically manipulating the variables of microstructural evolution, a high-thickness dry electrode with a homogeneous structure, featuring 1) uniform component distribution and 2) crack-free particles, could be achieved.

#### 11:20 AM

#### (ICACC-PLEN-004-2025) Plenary: 2D Ceramics - Nanoscale Bricks that Will Shape the Future Technology

Y. Gogotsi\*1

1. Drexel University, USA

Materials define the progress of humanity as access to new materials enables new tools and technologies. In the Silicon Age, electronic and computer technologies greatly accelerated the technical progress, changing our life. What is next? The age of nanomaterials. The era of assembly of new materials, structures and devices from nanoscale building blocks providing any imaginable, but impossible in conventional materials, combinations of properties and functions. Assembly from nanoparticles will allow integration of electronics, energy harvesting and storage in the same device, creating self-powered internet of things and wearable internet, at the same time minimizing the waste during manufacturing. Numerous 2D materials, including oxides, graphene, and carbides/nitrides (MXenes) are available nowadays and thousands more coming. They provide very attractive building blocks, because they can be assembled into dense structures, just like bricks in the wall. 2D transition metal carbides and nitrides (MXenes) have been expanding rapidly since their discovery at Drexel University in 2011 but have already become the fastest growing family of materials. This presentation will describe the state of the art in manufacturing those new 2D materials, their delamination into single-layer flakes and assembly into films. MXene-based composite films offer high strength and unique functional properties.

### 14th Global Young Investigator Forum

#### **GYIF- Energy Harvesting for Sustainable Systems** Room: Coquina G

Session Chairs: Meelad Ranaiefar, NASA Glenn Research Center; Bin Ouyang, Florida State University

#### 1:30 PM

#### (ICACC-GYIF-001-2025) Spatial tailoring of ceramics via additive manufacturing for material-efficient processing (Invited)

D. Oropeza\*1

1. University of California at Santa Barbara, USA

Over the past 30 years we have seen significant growth, evolution, and implementation of additive manufacturing processes from the laboratory to the factory floor, with demonstrated capability to attain highly complex parts at low production volumes and have demonstrated reduction in component lead times. For ceramics, the formation of high-density, geometrically complex features via additive manufacturing is still a challenge and the fabrication of multi-material spatially-tailored components is of great interest. This talk will discuss ongoing projects at the Materials and Manufacturing for Aerospace and Extremes Laboratory (MMAX Lab) at UCSB related to the use of additive manufacturing for efficient deposition of ceramic materials for spatially-tailored functionality. I will highlight two projects, demonstrating methods for generating spatially-tailored microstructure and composition. First, I'll present work on the control of microstructure and deformation of ceramics via reactive binder jet additive manufacturing. Second, I'll showcase work on the exploration of nanoparticle material jetting fundamentals for multi-material ceramic components. This presentation aims to provide a perspective on the possibilities for spatial tailoring of ceramics and the current state-of-the-art in processing science for compositional control.

#### 2:00 PM

## (ICACC-GYIF-003-2025) Design and integration challenges in sustainable sodium-zinc batteries (Invited)

F. D'Isanto\*1; A. Baggio1; M. Salvo1; D. Basso2; D. Gaia2; F. Smeacetto1

- 1. Politecnico di Torino, Department of Applied Science and Technology, Italy
- 2. FZSoNick SA, Switzerland

The excessive demand of non-renewable energy sources due to the increasing electricity consumed in everyday life are guiding research to the development of emerging, more efficient and sustainable energy devices, which can store energy and convert it for utility-scale energy-storage applications. Since their high energy and power density, sodium-zinc molten salt batteries could be one of the best solutions for the intermediate/high temperature (300°-600°C) energy storage request for stationary applications. The Na batteries require hermetic and corrosion resistant seals to provide containment for the molten materials. The definition of suitable joining materials and the development of a reliable joining process are of tremendous importance because they have to guarantee a long lifetime and safe operation. The key issues to be focused on for this application are the corrosive environment (Na liquid, vapor, and molten salts) and the long-term durability. In the framework of the SOLSTICE project (www.solstice-battery.eu), different joining materials are considered (glasses, glass-ceramics, commercial adhesives) as potential candidates for ensuring a proper sealing between the cell components and an appropriate separation between the cathode and anode compartments. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 963599.

#### 2:30 PM

#### (ICACC-GYIF-007-2025) Ceramic Microchannel Array to Enhance Heat Transfer and Mechanical Strength in High Temperature Heat Exchanger (Invited)

X. Li\*1; C. Wilson<sup>2</sup>; O. Brandt<sup>3</sup>; R. Orta Guerra<sup>3</sup>; R. Trice<sup>3</sup>; J. P. Youngblood<sup>3</sup>

- 1. The University of Tennessee Knoxville Tickle College of Engineering, Mechanical Aerospace and Biomedical Engineering, USA
- 2. Massachusetts Institute of Technology, Mechanical Engineering, USA
- 3. Purdue University, Department of Materials Engineering, USA

The efficiency of a heat engine can be significantly improved in a high-temperature conditions. However, such extreme operating conditions pose a severe challenge. Recently developed superalloys and ceramics can survive high-temperatures and high-pressure loads. However, using these materials in a traditional heat exchanger design requires high cost and large volume. This work proposes a high power density ceramic heat exchanger enabled by a multiscale porous design. By optimizing the design of centimeter-scale macrochannels and micrometer-scale microchannels, significant improvement to heat transfer and structural strength is predicted, with a negligible pressure drop penalty. An optimized design is expected to achieve high power density, light weight, low cost along with less than 2% pressure drop penalty. Furthermore, the heat exchanger design is customizable for different applications in hybrid and electric aerospace applications, as well as terrestrial power generation such as nuclear power generation and concentrated solar power generation, promising more than 2.5x thermal performance compared to state-of-the-art solutions. By utilizing commercially available superalloy and ceramic materials, the proposed solution brings the benefits of low cost, scalable fabrication, low pressure drop and high structural strength.

### GYIF- Energy Harvesting for Sustainable Systems/ Sustainable Careers

Room: Coquina G

Session Chairs: Dong Liu, University of Oxford; Anna Schneller, University of Augsburg

#### 3:20 PM

#### (ICACC-GYIF-004-2025) Halide perovskite soft semiconductors for sustainable technologies: from THz anharmonic lattice dynamics to outstanding optoelectronic properties (Invited) Y. Guo<sup>\*1</sup>

1. University of Nebraska-Lincoln, USA

Lead halide perovskites (LHPs) have emerged as a promising class of solution processable semiconductors, showing outstanding performance in optoelectronic applications including photovoltaics, solid-state lighting, and photodetection. Many of these properties originate from their soft, anharmonic structural dynamics. In this talk, we will discuss recent advances in understanding phonon anharmonicity of halide perovskites and explore its implications on the functional behaviors of these materials. On the optoelectronic side, we show the large amplitude highly anharmonic lattice displacement produces local polar fluctuations, dynamically stabilizing band edge charge carriers inside a crystalline lattice akin to solvation of excited fluorophore in polar liquids. We further examine the generality of this dynamic carrier relaxation behavior by tuning the halide mass. On the structural side, we show that soft bonding leads to easy formation and coherent switching of ferroelastic twin domains across the LHP family. These twin domain walls produce finite internal reflections and steer photon recycling optically. We suggest LHP twin domain walls be used as optical guides of internal energy transport, introducing a novel device component with non-volatile on-off switching and tunable positioning, enabled by their soft lattice.

## Abstracts

#### 3:50 PM

#### (ICACC-GYIF-005-2025) Application of Oxygen Transport Membranes to improve the sustainability of energy-intensive industrial processes (Invited)

P. Fedeli\*<sup>1</sup>; S. De La Pierre<sup>2</sup>; F. Da Prato<sup>2</sup>; A. Cavaliere<sup>1</sup>; A. Cammi<sup>1</sup>;

- V. Marzaroli<sup>1</sup>; E. Malgrati<sup>1</sup>; A. Benelli<sup>2</sup>; F. Smeacetto<sup>2</sup>; M. Ferraris<sup>2</sup>; F. Drago<sup>1</sup>
- 1. Ricerca sul Sistema Energetico RSE SpA, Italy
- 2. Politecnico di Torino, DISAT, Italy

To increase the sustainability of the industrial sector, the efficiency of many energy-intensive processes must be improved. The replacement of traditional air-fired combustion with oxy-fired processes can lead to significant energy savings and a decrease of hazardous emissions, but large quantities of pure oxygen  $(O_2)$  are required. Oxygen Transport Membranes (OTMs) are considered a promising solution to produce pure O<sub>2</sub> from air with high efficiency. This work describes the development of a proof-of-concept OTM module for O<sub>2</sub> separation, consisting of a planar membrane component made of the ceramic material La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-8</sub> and housed in a metallic frame. The main technological challenge, this work is focused on, is the development of junction layers able to join the ceramic membrane and the metal together, providing gas tightness, adequate mechanical strength and both thermo-mechanical and chemical stability at the high operating temperatures (T > 750 °C). We will show that a proper design of the sealing regions and a precise control of thickness and uniformity of the sealant, which can be achieved by a fine optimization of additive manufacturing techniques, are crucial to obtain gas-tight joints. Possible solutions to achieve a reasonable long-term stability of the junctions at high temperature will be also discussed.

#### 4:20 PM

#### (ICACC-GYIF-006-2025) Developing New Ceramic-Based Solutions through a Company-University Network: Advanced Ceramics and Coating Research Line at Leonardo Innovation Labs (Invited) **WITHDRAWN**

A. De Zanet<sup>\*1</sup>; A. Kumar<sup>1</sup>

1. Leonardo SpA, Leonardo Innovation Labs - Materials, Italy

The aerospace sector faces major challenges, such as improving aviation sustainability, which significantly impacts global greenhouse gas emissions, and developing innovative products for space exploration and defense. Overcoming these challenges requires a multidisciplinary approach, with material science and engineering playing a crucial role in creating advanced materials that improve both environmental and technological sustainability. To address these challenges, Leonardo has established a dedicated Materials research area within its Innovation Labs - technology hubs designed to enhance company's agility by accelerating research validation and its transfer into new products and services. The Leonardo Innovation Labs focus on advanced solutions across several fields like quantum computing and materials science, leveraging in-house expertise and fostering collaborations with company divisions, other firms, research centers, and universities. This presentation outlines the Advanced Ceramics and Coating Research Line within the Materials Labs, focusing on solutions for aerospace challenges, from erosion resistance to the manufacturing of components for harsh environments. It highlights the Labs' collaborative approach, emphasizing knowledge exchange and resource sharing between industry and academia.

### Special Focused Session on Diversity Entrepreneurship and Commercialization

#### **Special Focused Session On Diversity, Entrepreneurship, and Commercialization** Room: Coquina H

Session Chairs: Surojit Gupta, University of North Dakota; Valerie Wiesner, NASA Langley Research Center

#### 1:30 PM

#### (ICACC-DIV-001-2025) Sustainable bone replacement material: Additive manufacturing of TCP-HAP-Wollastonite composite for tissue engineering applications

M. V. Sudandaradoss\*1; G. Rajan2

- 1. Anna University, Ceramic Technology, India
- 2. Alagappa College of Technology, Anna Uiversity., Ceramic Technology, India

Additive manufacturing (AM) has emerged as a transformative technology, enabling the layer-by-layer construction of three-dimensional objects directly from digital models. Among its diverse applications, ceramic additive manufacturing holds considerable promise across various sectors, including medical, aerospace, and academia. This research specifically focuses on the utilization of Direct Ink Writing (DIW) or robocasting techniques for bio ceramic applications, particularly tri-calcium phosphate (TCP), hydroxyapatite (HAP) and wollastonite as a bone replacement material in Tissue Engineering (TE). Despite advancements in AM technologies, challenges persist in optimizing printability, necessitating thorough investigations into factors such as powder-to-binder and binder-water ratios, rheological properties, and alternative binder materials. The invention introduces a novel bone replacement material that is both cost-effective and sustainable, showcasing enhanced mechanical properties. This composite material is primarily composed of TCP, HAP, and wollastonite. A significant aspect of this development is the synthesis of HAP from orange peels, which exemplifies an environmentally friendly approach and aligns with the project's motto, GREEN PRINT HEALTH. This innovation not only minimizes waste but also effectively reduces overall production costs.

#### 2:10 PM

#### (ICACC-DIV-002-2025) Investigating composites and ceramic materials for energy storage and conversion through multipronged R&D approaches

W. Tang\*1

1. Underwriters Laboratories Inc, Electrochemical Safety Research Institute, USA

Although battery cells and electrification technologies have become ubiquitous, the complete understanding of their hazards is still lacking. Hence, it is necessary to investigate the potential risks of future pre-commercialized battery chemistries during the whole design process. The materials-level research and development (R&D) at the Electrochemical Safety Research Institute (ESRI) is studying new chemistries and novel systematic engineering methods related to energy storage and conversion with early-technology readiness level (TRL) through a safety lens. This presentation will describe several on-going projects, which are investigating composites and ceramic materials for current and future lithium chemistries, sodium and magnesium battery technologies, and green hydrogen generation, as well as our database to document best practices of in-house processes associated with cell fabrication and destructive physical analysis. The Director of Research (Novel Materials & New Energy Forms), Dr. Wan Si TANG, will be presenting this talk for ESRI, under UL Research Institutes. At ESRI, we are advancing safer energy storage through science.

#### 2:50 PM

#### (ICACC-DIV-003-2025) Nanomaterials by Design: Tailored Morphology for Today's Energy and Environmental Challenges E. Moretti<sup>\*1</sup>

1. Ca' Foscari University of Venice, Department of Molecular Sciences and Nanosystems, Italy

Nowadays, one of the main technological challenges that we are facing is the ability to provide a sustainable supply of clean energy and, among all renewable sources, solar energy displays the greatest potential. Recently, the development of novel synthetic strategies has led to the preparation of nanostructured materials displaying unique properties compared to the bulk counterpart systems, with controlled and tunable morphologies able to enhance the activity and selectivity of a catalytic process. In particular, nanostructured materials synthesized via the bottom-up approach present an opportunity for future generation manufacturing of devices. This talk will focus on the importance of tuning the morphological features of a catalyst as a strategy to the photocatalytic activity, focusing on how rationally designing inorganic materials at the nanoscale can lead to morphologies and structures suitable to enhance the catalytic performance of industrially and environmentally important processes. The talk will discuss some energy and environmental applications that can be addressed by multi-component oxide systems synthesized via the bottom-up approach, highlighting their structure-reactivity relationship. Photocatalytic H<sub>2</sub> production and purification and drugs degradation will be presented as a successful case history.

#### 3:40 PM

#### (ICACC-DIV-004-2025) The State of Selective Laser Melting for Infrastructure Development Using In-Situ Materials In Terrestrial & Space Systems (Invited)

M. Feehan\*1

1. Space Copy Inc., Canada

Selective Laser Melting (SLM) has emerged as a transformative technology for additive manufacturing, particularly in the processing of ceramic-like materials such as terrestrial sands, basalts, and lunar regolith. The ability to fabricate intricate structures using indigenous materials enables significant advancements in sustainable construction in off-world environments like the Moon. This review outlines the current state of SLM in advanced ceramics, including its adaptation for in-situ resource utilization (ISRU) on the lunar surface, utilizing materials that bear similar mineralogical recognizance to Silicate prevalent materials commonly applied for ceramics manufacturing of precision tooling and complex geometries. SLM's use in processing these diverse materials enables advancements in aerospace, construction, defense, and energy storage, aligning with global trends in the development of advanced ceramics. This processing method, as researched by Space Copy Inc., demonstrates that in remote environments, SLM is used to process ceramic-like materials such as sands and basalts for high-strength components, leveraging the mechanical behavior of porous ceramics and advanced coatings for applications ranging from protective materials to energy storage systems, paving the way for commercialization of extreme construction.

#### 4:10 PM

#### (ICACC-DIV-005-2025) Solid-State Batteries for Air and Space: Pushing Boundaries with Materials Science (Invited)

Y. Lin\*1

1. NASA Langley Research Center, Advanced Materials and Processing Branch, USA

NASA SABERS (Solid-State Architecture Batteries for Enhanced Rechargeability and Safety) project aims to demonstrate the feasibility of safe and high energy density solid-state batteries for future electric aviation. Compared to the current state-of-the-art batteries that use highly flammable liquid electrolytes, SABERS batteries use solid-state electrolytes that are intrinsically safe. However, significant challenges emerge with the battery reactions to be conducted with only solid components, while still needing to meet all of the stringent performance requirements. Our team started a few years ago with fundamental materials chemistry concepts, but has now grown into a versatile research hub that is ready to take on many facets of challenges in solid-state batteries and energy storage for applications in air and space. This presentation intends to provide an overview of the recent NASA solid-state battery research. We will discuss not only the challenges, achievements, and excitements, but also the failures and lessons learned throughout the SABERS project toward fulfilling and balancing the scientific explorations, the project milestones, and the commercialization interests.

#### 4:40 PM

#### (ICACC-DIV-006-2025) Interdisciplinary Research and Education for Microelectronics Workforce (Invited)

A. Kumar<sup>\*1</sup>

1. University of South Florida, Mechanical Engineering, USA

As evident from the 2022 CHIPS and Science Act and the 2020 National AI Initiative Act, there is an acute need for talented and trained workforce in semiconductor manufacturing and Artificial Intelligence (AI)/Machine Learning (ML) areas. Recent NSF NRT (National Research Traineeship) grant has provided support to develop and implement a comprehensive and experiential learningbased education, research, training, and skills development program in semiconductor design, manufacturing, and packaging. This talk will provide interdisciplinary semiconductor concepts and emerging technologies that will be integrated in existing courses with novel experiential lab training in Class 1000 cleanroom environment. Students will be involved with industrial partners to define research problems using a convergence approach to design and develop application-driven semiconductor systems and devices. This program is innovatively designed such that the students on completion will gain essential competencies, namely, transdisciplinary knowledge, communication, teamwork, experimental & computational skills, informed decision making, entrepreneurship skills, project management, ethics, leadership, and safe and sustainable manufacturing. Students with entrepreneurial interest will have the opportunity to complete NSF I-Corps site training. This work is supported by NSF National Research Traineeship (NRT) Grant no. 2347019.

#### 5:10 PM

## (ICACC-DIV-007-2025) From College to C-suite: Mentorship in DE&I Initiatives (Invited)

E. Deena\*1

1. Case Western Reserve University, USA

Executing successful DE&I initiatives striving to reach representative parity with the population's demographics require intentionality in recruiting and growing diverse talent. Early and mid-career mentorship built around creating a culture that celebrates diversity and leverages it as a strength can contribute to retaining and growing diverse talent and strengthening existing leadership. Pairing an incoming diverse workforce with existing leadership provides mentees with the professional development and networks needed to accelerate their career while providing executive mentors with the fresh perspectives and innovative thinking that gives a diverse workplace its strategic advantage. Mentorship programs integrated into DE&I strategies contribute directly to creating an inclusive environment by providing personal experiences from underrepresented individuals proven to foster community and allyship that leads to higher employee retention and engagement. Mentorship programs are also a powerful tool in increasing representation in management, strengthening organizations from top to bottom.

## Abstracts

#### 5:40 PM

#### (ICACC-DIV-008-2025) Turning Challenges into Profits: Navigating Business Success Amidst Adversity

A. Dodson\*1

1. Strayer University, USA

Join Anthony Dodson in this empowering presentation as he shares insights on "Turning Challenges into Profits." Learn practical tips and techniques for identifying untapped potential in any circumstance and transforming hurdles into opportunities for growth and success. Discover the power of adaptability and resilience, and explore new possibilities to turn passions into profitable ventures. Be inspired to see beyond obstacles, embrace change, and harness unique skills to carve a path towards financial prosperity and personal fulfillment. Equip your team with the tools to confidently navigate challenges and thrive in any situation, transforming adversity into a catalyst for business triumph.

### FS2 Protective ceramics- Fundamental challenges and new developments

#### FS 2: Protective Ceramics- Fundamental challenges and new developments

#### Room: Coquina D

Session Chair: Kristopher Behler, DEVCOM-Army Research Lab

#### 1:30 PM

#### (ICACC-FS2-001-2025) Impact performance and cratering behavior of boron carbide ceramics

K. Muly\*1; J. Moreno1; K. Ramesh1; J. LaSalvia2; S. Satapathy2

- 1. Johns Hopkins University, USA
- 2. DEVCOM Army Research Laboratory, USA

Three different polycrystalline boron carbide materials were subjected to impact at velocities between 1 and 4 km/s, using a sphere-on-plate impact configuration. The three materials have different composition and microstructure, including different mesoscale defect distributions. The lower velocity impact regime provides insight into the cratering of the boron carbide plates, while the higher velocity impact regime provides information on the penetration of the ceramic plates. Using high-speed optical visualization together with quantitative image analyses, the evolution of the crater radius and ejecta cone angle with time for each impact velocity. These metrics provide insight into the cratering mechanism in these materials. The high-velocity regime penetration experiments were backed with large metallic blocks that allow estimation of the residual energies after penetration. Finally, flash x-ray methods together with quantitative image analysis were used to visualize ejecta distributions inside the ejecta cloud during the cratering process. Put together, these metrics allow us to develop an understanding of how the fragmentation and cratering processes develop in the boron carbide variants, as well as providing insight into the time dependencies of different mechanisms involved in ceramic cratering.

#### 1:50 PM

#### (ICACC-FS2-002-2025) Behavior of silicon carbide under laser shock loading

K. Muly\*1; A. Mirzaei1; K. Ramesh1

1. Johns Hopkins University, USA

Laser shock micro flyer experiments are used to investigate the dynamic behavior and spall strength of silicon carbide. Commercially available single crystal 4H silicon carbide is studied, together with a commercial hot-pressed polycrystalline silicon carbide. Some of the polycrystalline samples is heat treated to a range of temperatures in order to understand the role of temperature, and potentially microstructural evolution, on the dynamic behavior of the material. The polycrystalline materials are characterized prior to dynamic loading, using XRD and EBSD to quantify the initial microstructural characteristics of the sample. After testing the same characterization methods are performed in order to assess any impact-induced (or heating-induced) changes in the microstructure. Postmortem SEM fractography is performed to understand the dynamic failure mechanisms in both single crystal and polycrystalline materials.

#### 2:10 PM

#### (ICACC-FS2-003-2025) Plastic deformation of cubic-boron nitride under shock wave impacts

A. Qadir\*1; C. Schimpf1; M. Mykhaylo1; T. Schlothauer2; K. Keller2; G. Heide2; D. Rafaia<sup>1</sup>

- 1. Technische Universitat Bergakademie Freiberg, Institute of Materials Science, Germany
- 2. Technische Universitat Bergakademie Freiberg, Institute of Mineralogy, Germany

Cubic boron nitride (cBN) is a super-hard material possessing a high thermal and chemical stability, which predestines it for applications in special cutting tools. As for other super-hard materials, less is still known about the plastic deformation of cBN. This study was an attempt to find out more about this phenomenon by presenting evidence of the plastic deformation in cBN subjected to the shock wave impact. The changes in the crystal structure and microstructure of the shock-wave compacted cBN were elucidated with the aid of X-ray diffraction (XRD), transmission electron microscopy (TEM), and high-resolution TEM (HRTEM) imaging. The intricate microstructural features in cBN are nanotwins, stacking faults, dislocations, and shear bands-analogous phenomena, which are observed in the face-centered cubic (fcc) metals undergoing plastic deformation. The observed mechanisms of plastic deformation in cBN contribute to a discourse in materials science discussing the plasticity of ultrahard covalently bonded materials.

#### 2:30 PM

#### (ICACC-FS2-004-2025) Modeling frictional properties with neural networks

I. Garcia-Suarez\*

1. Ecole Polytechnique Federale de Lausanne, Civil Engineering, Switzerland

The potential application of neural networks to model frictional properties in various materials (including ceramics) is discussed. Traditional methods of predicting friction and wear rely on empirical laws and physical theories, often limited by their complexity and accuracy. Leveraging neural networks may allow capturing the intricate patterns inherent in interface behavior without resolving all the meso and microstructural details. I will discuss methodologies and potential applications in fields that involve friction and wear in ceramic interfaces as, e.g., machining and biomedical implants.

#### 3:10 PM

#### (ICACC-FS2-005-2025) Carbon Reinforced Boron sub-Oxide Nanocomposite (CaRBON)

J. Kenny\*1

1. AWE plc, Non Nuclear Components, United Kingdom

It was possible to make a nanocomposite of Boron Suboxide (B<sub>6</sub>O) and Boron Carbide  $(B_4C)$  formed via the reaction of the  $B_6O$  with carbon (C) deriving from reduced Graphene Oxide (rGO). This material could be potentially useful for neutron moderation and absorption applications, through to armour applications. This nanocomposite was formed by blending the B<sub>6</sub>O with rGO in aqueous suspension before filtering and consolidating it via Spark Plasma Sintering (SPS). It was shown that the pure B<sub>6</sub>O sintered at 1850 °C, densified to ~95% of the samples theoretical density (TD), exhibited

a comparable hardness to near-fully dense  $B_4C$  made through similar methods (~35 GPa at ~95% of TD for  $B_6O$ , compared to ~32.5 GPa at >98.5% TD). In 1 wt.% GO additions, it was possible to detect  $B_6O$  and  $B_4C$  using X-Ray Diffraction when the composite was sintered at 1570 °C for 15 mins. After 30 mins of sintering, the sample almost completely transformed to  $B_4C$ , thereby proving the hypothesis of the study. Furthermore, it was possible to prove that none of the significant indicators of shock induced amorphisation were present in any of the CaRBON samples. During neutron irradiation testing, the samples were exposed to a neutron fluence of  $39.6 \pm 3.41$  n/cm<sup>2</sup> with energies of  $13.7 \pm \sim 1.5$  MeV. By the end of the test, all samples had a radioactivity of 0.2 mSv. Post irradiation analysis revealed no signs of radiation-induced damage across the tested samples.

#### 3:50 PM

#### (ICACC-FS2-007-2025) Synthesis and Simulation of Microstructural Evolution in Reaction-Infiltrated Diamond-SiC Composites WITHDRAWN

A. A. DiGiovanni\*1; M. Guziewski1

1. US Army Research Laboratory, Ceramic and Transparent Materials, USA

Reaction-infiltrated ceramic composites are advantageous because they can be made in complex near-net shapes, often at lower temperatures and cost than traditional sintering, for applications demanding rigorous structural, thermal, and/or wear resistance. The addition of granular diamond to those formulas, can further improve the wear and thermal management properties of such composites. Careful examination and simulation of liquid silicon infiltration and reaction at the grain-scale and its influence on bulk density were performed using coarse grit diamond powders in carbide composites. Diamond-packed silicon carbide tubes were infiltrated with molten silicon at temperatures below 1500°C and evaluated using x-ray computed microtomography (XCT) before and after infiltration. Analogues of the powder compacts were simulated with LAMMPS discrete element code to create the packings. A custom Python script implements infiltration and growth at the microscale, differentiating between diamond, non-diamond carbon, silicon, and silicon carbide phases. Comparisons between experimental observations and modeling are presented and discussed. Distribution Statement A: Approved for public release: distribution is unlimited.

### FS6 Innovative material processing for diverse resource circulation loops

# FS 6- Novel products and materials oriented toward easy disassembly and circulation design

Room: Ballroom 5

Session Chairs: Sonia Fiorilli, Politecnico di Torino; Olivier Guillon, Forschungszentrum Juelich

#### 1:30 PM

(ICACC-FS6001-2025) Development of Circular Manufacturing Technology Using Photochemical Reaction Processes (Invited) T. Tsuchiya\*<sup>1</sup>

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Conventional manufacturing was based on the premise of mass production and mass consumption. In recent years, in order to solve environmental problems, it has become essential to build innovative resource recycling cycles, in addition to recycling electronic materials and components used in a variety of products, such as solar panels, organic EL displays, smartphones, and lighting. In this talk, we will discuss research and development from three perspectives in order to develop a circular manufacturing process for electronic components and devices. Firstly, we will report on the development of functional ceramic films that achieve high durability and high functionality for various components and devices. We will also introduce on-demand repair technology for ITO transparent conductive film wiring defects in large-area displays, etc. Furthermore, we will report on research and development of optimally designed components that enable environmentally efficient remanufacturing.

# FS 6- Recovery of critical/valuable materials from exhausted complex products I

Room: Ballroom 5

Session Chairs: Olivier Guillon, Forschungszentrum Juelich; Sonia Fiorilli, Politecnico di Torino

#### 2:00 PM

# (ICACC-FS6002-2025) Separation technology for resource circulation of renewable energy devices

C. Tokoro\*1

1. Waseda University, Japan

Devices to create and store renewable energy, such as lithium-ion batteries, solar panels, and wind turbine blades, are in increasing demand to promote carbon neutrality. However, to improve energy efficiency and extend the service life of these devices, they are made of multi-materials that are tightly bonded, joined, and encapsulated due to their high functionality, lightweight, high strength, and high secrecy. As a result, it is more difficult to disassemble and separate them for resource circulation after use. There is concern that recycling will be more costly and energy-intensive than ever before. In this presentation, I will introduce the results of our study on physical separation technologies for low-cost and energy-saving disassembly of these renewable energy devices.

## Abstracts

#### 2:20 PM

## (ICACC-FS6003-2025) Towards recycling of thiophosphate-based all-solid-state batteries

K. Wissel\*1; O. Clemens1

1. Universitat Stuttgart, Germany

As the importance of all-solid-state batteries (ASSBs) continues to grow, the need for sustainable recovery and recycling strategies becomes increasingly urgent. However, relatively few studies have addressed the recycling of ASSBs. In contrast, for conventional lithium-ion batteries a wide array of recycling approaches, including pyrometallurgical, hydrometallurgical, and direct recycling methods, has been established. These methods typically focus on recovering valuable critical elements or regenerating active cathode materials. For ASSBs, however, the recycling process must also account for the solid electrolytes, adding significant complexity. The need to process mixtures of active electrode materials, solid electrolytes, binders, and other battery components underscores the importance of developing effective component separation strategies. Given the potential for solution-processing of thiophosphate electrolytes, direct recycling strategies involving dissolution, precipitation, and recrystallization show promise for separating these electrolytes from insoluble components. In contrast, pyrometallurgical and hydrometallurgical processes are impractical for thiophosphate electrolytes due to their degradation in the presence of water or O<sub>2</sub>. This contribution discusses the feasibility of a dissolution-based separation process and the associated challenges.

#### 2:40 PM

(ICACC-FS6004-2025) Separation of lithium iron phosphate-type cathode materials from lithium-ion batteries by electrical pulsed discharge and their direct recycling

T. Kurihara\*1; A. Narita2; C. Tokoro2

- 1. Waseda University, Department of Resources and Environmental Engineering, Graduate School of Creative Science and Engineering, Japan
- 2. Waseda University, Faculty of Science and Engineering, Japan

Lithium iron phosphate (LFP)-type secondary batteries are rapidly growing in demand due to their cost and safety benefits, raising the need to develop recycling processes. Developing direct recycling methods that recover and regenerate cathode active materials (CAMs) without destroying the structure is essential because current metallurgical methods lack benefits due to the low price of raw materials. CAMs are typically recovered from aluminum foils through chemical or thermal treatment, which generate harmful wastewater or require high energy. In contrast, the pulsed discharge method shows potential for solving the problems. Applying a high voltage causes separation between conductors and non-conductors at their interface instantaneously. We have also reported the recovery of lithium nickel-manganese-cobalt oxide-type cathode materials using this method. In this study, we separated LFP-type cathode materials by pulsed discharge. When the 10.0 kV pulse was discharged on virgin sheets without electrolytes, 100% of the cathode materials were separated. Cathode materials from spent cells were also separated 100 % as a maximum, depending on the applied voltage. The XRD analysis showed that the crystal structures of both CAMs were maintained even after the pulsed discharge. The assembly of cells using recovered CAMs will also be reported.

# FS 6- Recovery of critical/valuable materials from exhausted complex products II

Room: Ballroom 5

Session Chairs: Kerstin Wissel, Universitat Stuttgart; Chiharu Tokoro, Waseda University

#### 3:20 PM

## (ICACC-FS6005-2025) Resource Recycling Technology Initiatives at AIST (Invited)

A. Endo<sup>\*1</sup>

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

In 2009, Dr. Johan Rockström introduced the concept of "Planetary Boundaries," which identifies critical thresholds where human activities impact the Earth's stability. Particularly, the emission of CO<sub>2</sub>, nitrogen compounds and phosphorus, are pressing issues. Moreover, stringent waste regulations, especially in Europe, are becoming a global trend, highlighting the increasing importance of material reuse. From the perspective of the SDGs, it is essential to establish a circular economy that addresses these issues while achieving economic development. At the Resource Recycling Technology Research Lab in AIST, we aim to establish a resource-circulating society that balances industrial development with environmental conservation. Our focus is on developing functional material recycling technologies to regenerate post-use waste, such as plastics, metals, and composite materials into valuable resources. We are also working on carbon, nitrogen, phosphorus recycling technologies to reprocess emissions like carbon dioxide, nitrogen compounds, and phosphates, which are byproducts of production and disposal processes. Furthermore, in cooperation with AIST Solutions, we aim to implement these technologies in society through collaboration with industrial partners. In the presentation, the latest results of these activities will be introduced.

#### 3:50 PM

#### (ICACC-FS6006-2025) The recycling process of lithium-ion secondary batteries for implementation of high-voltage electric pulsed discharge method (Invited)

- A. Narita\*1; Z. Zhou2; H. Xiong2; T. Kurihara2; C. Tokoro1
- 1. Waseda Universiity, Faculty of Science and Engineering, Japan
- 2. Waseda University, Graduate School of Creative Science and Engineering, Japan

Nickel-manganese-cobalt oxide (NMC)-type lithium-ion batteries (LiBs) have a high market share. Developing the recycling technology of NMC-type cathode active materials (CAMs) is essential for the sustainability of the supply of elements. Although pyrometallurgy and hydrometallurgy with acid or alkali leaching are the current mainstream methods, further reduction of energy consumption and environmental impact are still needed. We have reported that more than 95% of CAMs can be recovered quickly while saving energy by discharging high-voltage electric pulses directly onto NMC-based cathode sheets. This method is effective for cathode sheets with a relatively large area, such as batteries for automotive. After the recovery, 1 - 2% of contaminated aluminum can be reduced without a chemical process only by sieving. On the other hand, the electric disintegration method, which is discharged in water, can also be applied to batteries covered by resin or metal and have various shapes, such as small electric devices. In such cases, although discharge and deactivation can be performed more safely, it is necessary to consider another recycling process using water. It is essential not only to develop individual technologies but also to design the total process from disassembly, which is necessary to implement the electric pulsed discharge method for LiB recycling.

#### 4:20 PM

# (ICACC-FS6007-2025) Innovative approaches to pyrometallurgical recycling strategies for lithium-ion batteries waste management (Invited)

A. Zanoletti\*2; E. Bontempi1

- 1. Universita degli Studi di Brescia, DIMI, Italy
- 2. Universita degli Studi di Brescia, Italy

Projections indicate global waste battery production will reach 2 million metric tons by 2030. The imperative for technological innovations become evident in response to this challenge and to mitigate the potential scarcity of strategic metals. This study introduces a recently patented technology for managing waste lithium-ion batteries in alignment with the principles of the circular economy. The innovative technology relies on microwave utilization, serving as a replacement for traditional pyrometallurgical methods in the recovery processes of the black mass. Some examples of the treatments are presented and discussed. The newly developed pyrometallurgical processes, that have been patented, have the potential to be energy-efficient, especially when utilizing microwave technologies.

#### 4:50 PM

#### (ICACC-FS6008-2025) Sustainable Ceramics – Solid Oxide Cells on their Way to Circular Economy (Invited)

O. Guillon\*1; S. Sarner1; N. H. Menzler1

1. Forschungszentrum Julich GmbH, IMD-2, Germany

SOC are set to undergo significant global growth in the coming years. As a pioneering effort, we developed and tested a recycling concept for one widely established type of SOCs-the fuel electrode-supported cell design. Studies have highlighted that the most critical step in reprocessing the main weight fraction of the cell (over 85 wt% in our case) is the separation of perovskite components, which are used for oxygen electrodes and contact materials. A scalable method that minimizes safety risks (e.g., harmful dust release) while producing high-purity products is wet chemical separation using acids. After leaching, the solid residues - nickel oxide, stabilized zirconia, and doped ceria - can be directly reprocessed, replacing pristine, expansive raw materials with recycled powders. While small changes in microstructure evolution and chemical composition may occur, it was confirmed that recycled cells containing 50 wt% recycled substrates perform on par with their non-recycled counterparts. This closed-loop process is able to preserve materials with a high yield (up to 97 %). For open-loop recovery of the dissolved perovskite fraction (less than 15 wt% in our case), several established recovery methods can be applied. Implementing these recycling methods may provide a direct, energy-saving way to handle SOC waste ceramics, contributing to more efficient and sustainable SOC production.

#### 5:20 PM

# (ICACC-FS6009-2025) Recovery of critical and valuable raw materials from End-of-Life Solid Oxide Cell for close and open-loop recycling

S. Fiorilli\*1; S. Saffirio<sup>1</sup>; S. Anelli<sup>1</sup>; S. Fiore<sup>2</sup>; M. Bruno<sup>2</sup>; C. Gerbaldi<sup>1</sup>; M. Rath<sup>3</sup>; F. Smeacetto<sup>1</sup>

- 1. Politecnico di Torino, Department of Applied Science and Technology, Italy
- 2. Politecnico di Torino, Department of Environment, Land and Infrastructure Engineering, Politecnico di Torino, Italy
- 3. Elcogen, Estonia

Solid oxide cells (SOCs) provide a mature alternative to conventional power-generation sources to achieve carbon neutrality goals. Given these perspectives, the SOC market will significantly increase in the next few years, with a consequent heavy demand for critical and high-cost raw materials for cell manufacturing, including yttria, zirconia, Ni, La, and Co. In this context, the engineering of efficient, scalable and cost-effective end-of-life (EoL) strategies for recovering and recycling materials from dismantled/scrap cells is crucial to envisage the full deployment and the sustainability of SOC technologies. Although the awareness regarding the need for circular solutions has progressively increased in the last few years, there is still minimal coverage in the literature on SOC disassembling and recycling. In this contribution, the authors present engineered strategies for the efficient and selective recovery of ceramics from exhausted and scrap SOC electrodes. The recovered materials have been comprehensively characterised and their physicochemical features benchmarked against commercial precursors, envisaging their re-use (min. 30% wt.) in novel SOC cell components (close loop). Open-loop recycling pathways, including the synthesis of Ni-rich layered cathodes for Li-ion batteries and the development of formulations for 3D printing, are also presented.

### <u>S1 Mechanical Behavior and Performance</u> of Ceramics & Composites

# **S1-** Mechanical Testing, and Fracture Mechanics of Ceramics and Composites

Room: Coquina E

Session Chairs: Michael Jenkins, Bothell Engineering and Science Technologies; Jonathan Salem, NASA Glenn Research Center

#### 1:30 PM

## (ICACC-S1-001-2025) Failure Location Effects on Slow Crack Growth Parameters (Invited)

J. Salem\*

1. NASA Glenn Research Center, Materials and Structures, USA

As part of an optical component development program for the Roman Space Telescope, the slow crack growth (SCG) parameters of a glass were measured using constant stress rate testing of beams in bending. Failures occurred on the faces, bevels, and sides of the test specimens, thereby providing an opportunity to examine the effects of failure location on SCG parameter estimates. Censoring of the data by location did not have a statistically significant effect on the slow crack growth parameter estimates. Linear and nonlinear fits were also made to various strength estimators. Nonlinear fits gave slightly lower estimates of the parameters. The main influence on parameter estimates was a low strength, infrequent flaw population. Exponential model parameters were estimated via swarm optimization.

#### 2:00 PM

## (ICACC-S1-002-2025) On the Brittleness of Ceramics and Glasses (Invited)

G. D. Quinn<sup>\*1</sup>

1. National Institute of Standards and Technology, Materials Measurement Sciences Division, USA

Twenty-nine years ago, J. Quinn and I proposed a new brittleness parameter based on our studies of hardness and fracture around indentations. The hardness of a brittle material is a measure of a material's resistance to deformation, densification, displacement, and fracture. Fracture is not simply an interference in measuring Vickers or Knoop hardness, but is an intrinsic part of the hardness response. Deformation is predominant at low loads, whereas fracture is more a factor at high loads. Hardness versus load curves sometimes exhibit dramatic transition points that previously had been overlooked. The transitions correspond to extensive micro-fracturing and are directly related to the new brittleness parameter  $B = H_c E/K_{Ic}$ that we proposed in 1996. B is related to the ratio of the energies of fracture and deformation. Differences in the balance of deformation and fracture processes give rise to a cube/square size scaling phenomenon leading to a critical length for behavioral transitions. Such transitions had been noted by Puttick, Mouginot, Atkin and

Mai, and Lawn and Marshall. The critical length could be a specimen size, a crack size, or an indentation size. This energy balance determines whether a body behaves elastically (brittle), elastic-plastically, or plastically (ductile). This presentation reviews the progress in the utilization and interpretation of the Quinn and Quinn brittleness parameter B over the last 29 years.

#### 2:30 PM

## (ICACC-S1-003-2025) A novel strength testing method for ceramics fabricated by additive manufacturing (Invited)

M. Schwentenwein\*1; M. Staudacher2; U. Scheithauer3; T. Lube2

- 1. Lithoz GmbH, Austria
- 2. Montanuniversitat Leoben Department Werkstoffwissenschaft, Austria
- 3. Fraunhofer IKTS, Shaping, Germany

Because of the layer-by-layer printing process components fabricated by additive manufacturing typically exhibit textured surfaces. The geometry and periodicity of this texture typically depends on the printing parameters and printing orientation. Therefore, the strength of ceramic 3D-printed components may depend on the orientation in which tensile stresses act with respect to the printing direction. In order to provide reliable material data for the design of components, the strength characteristics have to be assessed routinely for various processing conditions. Such investigations are laborious and costly if standardized strength specimens and methods for ceramics are used. Thus, a novel test specimen was designed and investigated. It allows manufacturing of a sample set of sufficient size (comprising 48 cantilevers) for statistical strength evaluation within one single part. In this work a round robin using this new methodology was conducted. In total, 48 specimens (each having 48 cantilevers) were manufactured by four partners in three specimen configurations. Thermal post-processing and testing was conducted at a single partner to minimize other influences. Ultimately, the geometry and strength of more than 2300 cantilevers were analyzed. This yielded plenty of data to assess the geometrical consistency as well as differences in strength for and between each partner.

#### 3:20 PM

# (ICACC-S1-004-2025) Microscale mechanical properties of silicon nitride ceramics determined by microcantilever bending tests (Invited)

T. Ohji\*1; J. Tatami1

1. Yokohama National University, Japan

This paper presents recent works on microscale mechanical properties of silicon nitride  $(Si_3N_4)$  determined by microcantilever bending test. We first focus on deformation behaviors and fracture strength of Si<sub>3</sub>N<sub>4</sub> single crystals.  $\beta$ -Si<sub>3</sub>N<sub>4</sub> single crystals are plastically deformed at room temperature under high bending stress, and the yield stress depends on the crystal orientation. The critical resolved share stress of the primary slip system is determined to be below 1.5 GPa from the yield stress. Next, we address microscale mechanical properties of Si<sub>3</sub>N<sub>4</sub> polycrystalline ceramics. Emphasis is placed on their grain-boundary strength or toughness in conjunction with intergranular glassy film (IGF) which is determined by processing parameters such as sintering additives. Assessment is made on two cases of fractures at the IGF-grain interface and that within the IGF, and in each of the cases, effects of rare earth oxide additives are discussed. Finally, we shed light on microscale property-degradation behaviors of Si<sub>3</sub>N<sub>4</sub> ceramics. The variation of the microscale properties appears in very short periods compared to the macroscale approaches, demonstrating the advantage in terms of rapid assessment of time-dependent degradation behaviors This work was supported by JST, CREST Grant Number JPMJCR2192, Japan.

#### 3:50 PM

#### (ICACC-S1-005-2025) Investigation of fracture toughness, slow crack growth and crack healing in sapphire using chevron notched microcantilevers (Invited)

R. I. Todd\*1; J. Jiang1; S. Wang2; F. Giuliani2

- 1. University of Oxford, Department of Materials, United Kingdom
- 2. Imperial College London, Department of Materials, United Kingdom

The condition for crack propagation in ceramics and glasses is most often characterised in terms of the stress intensity factor required for fast fracture in inert conditions, K<sub>c</sub>. In real applications, however, components are often expected to survive for long periods of time in reactive environments, so slow crack growth in a range of conditions is of more practical importance, as well as being of greater scientific significance. However, the few literature reports on the subject show wide discrepancies, partly because of the difficulty of investigating the slow crack growth rates of relevance using macroscopic specimens. In this talk, slow crack growth in sapphire is investigated using microcantilevers three orders of magnitude smaller than conventional specimens. Chevron notches were used to obtain stable crack growth and specimens loaded in vacuum and in air with 54% relative humidity were compared. Reproducible results with crack growth rates down to 2 10-8 m s<sup>-1</sup> were obtained and the stress intensity factor required to advance cracks on the a-plane of sapphire was reduced by 38% in air compared to the value in vacuum. Unloading a partially cracked specimen in vacuum resulted in healing along the full length of the crack but the toughness of the healed interface was progressively degraded compared with the pristine material in repeated cycling.

#### 4:20 PM

#### (ICACC-S1-006-2025) Revision of ASTM C1424 "Monotonic Compressive Strength of Advanced Ceramics at Ambient Temperature" Based on Recent Tests Using High-Speed Imaging (Invited)

M. G. Jenkins\*1; J. Swab2; J. E. Gallego1

- 1. Bothell Engineering and Science Technologies, USA
- 2. Army Research Laboratory, USA

ASTM C1424 "Monotonic Compressive Strength of Advanced Ceramics at Ambient Temperature" was first approved and published in 1999. This test method was derived from extensive work completed successfully in the 1980s at the Army Materials Technology Laboratory, Watertown, MA. Several dumb bell test specimen geometries are included in the ASTM test method along recommendations for end caps, alignment, strain measurement and interpretation of test results. In the early 2020's, extensive compression testing various ceramics and glasses using dumb bell test specimens and high speed video resulted in numerous and sometimes extensive revision of ASTM C1424 that have made extensive improvements to an already sound ASTM standard. The revised standard removes references to right circular cylinder test specimens, provides guidance on interpretation of test results, includes references to recent compression test results for Al<sub>2</sub>O<sub>3</sub>, B<sub>4</sub>C and WC, describes the utility of high-speed imaging for validating test results.

#### 4:50 PM

# (ICACC-S1-007-2025) High temperature fracture mechanics of Si containing ternary and quaternary transition metal diborides

A. Hirle\*<sup>1</sup>; A. Bahr<sup>1</sup>; R. Hahn<sup>1</sup>; T. Wojcik<sup>1</sup>; S. Kolozsvári<sup>2</sup>; P. Polcik<sup>2</sup>; J. Ramm<sup>3</sup>; C. Jerg<sup>3</sup>; H. Riedl<sup>4</sup>

- 1. Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria, Austria
- 2. Plansee Composite Materials GmbH, Germany
- 3. Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein
- 4. TU Wien, Institute of Materials Science and Technology, Austria

To improve the limited oxidation resistance of transition metal diboride (TMB) ceramics, alloying with Si-based phases is a powerful approach. Especially for TiB<sub>2</sub>, CrB<sub>2</sub>, or HfB<sub>2</sub>-based bulk

ceramics and thin films, the addition of Si and disilicides has been proven to be favorably effective by forming highly dense and protective SiO<sub>2</sub> scales. In more detail, alloying of TaSi<sub>2</sub> and MoSi<sub>2</sub> into TiB<sub>2</sub> thin films reduces the amount of Si needed to provide excellent oxidation resistance at 1200 °C and minorly influences mechanical properties. For so-called quaternary TiB<sub>2</sub> based coatings, hardness values of 36 GPa (TaSi<sub>2</sub>) and 27 GPa (MoSi<sub>2</sub>) compared to 38 GPa for the binary TiB<sub>2</sub> have been achieved. In contrast to the oxidation resistance, the fracture characteristics of these Si alloyed TMBs are rather unexplored. In the present study, we aim to unravel the fracture resistance of these Si containing TMBs at elevated temperatures and small scales. Therefore, a set of Ti-TM-Si-B $_{2\pm z}$  coatings was deposited by non-reactive DC magnetron sputtering using different composite targets TiB<sub>2</sub>, TiB<sub>2</sub>/TiSi<sub>2</sub>, TiB<sub>2</sub>/TaSi<sub>2</sub> and TiB<sub>2</sub>/MoSi<sub>2</sub>. After detailed structural and chemical analysis using XRD, SEM, TEM and ERDA/RBS, the fracture characteristics, in particular, K<sub>IC</sub>, of these coatings have been determined using in-situ micromechanical testing techniques at different temperatures up to 850 °C.

#### 5:10 PM

# (ICACC-S1-008-2025) Hard and Electrically Conductive Ceramic Engineered For Toughness

J. Zimmermann\*1

1. Corning Incorporated, USA

This paper investigates the development of composite ceramic materials designed to optimize hardness, toughness, and machinability for use in abrasive wear applications. Traditional solutions for high abrasive resistance applications have primarily relied on metal bonded carbides or ceramic carbide monoliths. However, an application gap exists due to the unsuitability of these traditional materials, namely the soft metal erosion witnessed in cemented carbides and the inherent brittleness of monolithic ceramics. Our research presents the development of innovative carbide and boride composite materials aiming to bridge this application gap. The high hardness ceramic solution with high toughness potential are engineered to have sufficient electrical conductivity to enable electron discharge machining (EDM). The paper will provide a detailed exploration of these composite materials, their development, and their potential impact on abrasive wear applications.

#### 5:30 PM

#### (ICACC-S1-009-2025) Mechanical properties of Zirconia-Yttria-Tantala (YTZ) Ceramics in tetragonal compositions

M. Galeano Camacho\*1; J. Muñoz Saldaña1; H. Ageorges2

- 1. Cinvestav, Materials, Mexico
- 2. Universite de Limoges, Science et Technique, France

 $ZrO_2$  stabilized with 7-8 wt.% Y  $P_2$ , v1.SZ) forms a non-transform-able tetragonal phase (t') wie av sed in thermal barrier coatings for its excellent high-tempera up aracture toughness. However, 7YSZ has reached its thermodynamic limit due to intrinsic oxygen vacancies. As an alternative, the agonal compositions within a narrow range formed by equicomposition additions of trivalent and pentavalent cations in solid solution with  $ZrO_2$  have been proposed. This study gradu in solid solution with ZrO<sub>2</sub> have been proposed. This study evaluates the effects of milling and solid-state reaction parameters on the phase stability of the ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub>-Ta<sub>2</sub>O<sub>5</sub> (YTZ) system to select the best composition for the deposition of thermal barrier coatings by plasma spraying. Five YTZ compositions within the t'-phase zone were prepared by solid-state reaction using powder mixtures of ZrO<sub>2</sub>-(x) YO<sub>1.5</sub>-(x)TaO<sub>2.5</sub>, where x=15.4%, 16%, 16.6%, 17.2%, and 17.8%. The precursors were preheated, milled in stoichiometric proportions, pressed, and calcined at 1500°C. Highly dense ceramics with over 95% t'-phase were obtained by sintering. SEM observations showed that increasing yttria and tantala content leads to coarse grained microstructure. The elastic modulus, measured by nanoindentation, increases with equicomposition, consistent with hardness values. Pop-ins observed in load-displacement curves suggest a combination of ferroelasticity and microcrack formation under applied load.

#### 5:50 PM

## (ICACC-S1-010-2025) Local deformation in glassy solids in the elastic regime

W. Dmowski\*1; T. Iwashita2;; C. J. Benmore3; T. Egami1

- 1. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science and Eng., USA
- 2. Oita Daigaku, Japan
- 3. Argonne National Lab, X-ray Science Division, USA

We used high energy x-ray diffraction to measure deformation strains in glassy materials using pair distribution function (PDF). We performed measurements in-situ during elastic deformation. Because of induced structural anisotropy by applied axial stress we used spherical harmonics expansion to obtain isotropic and anisotropic components of the scattering function S(Q) from the diffraction data. Using Bessel transformation, components of S(Q), were converted into isotropic and anisotropic pair distribution function. From the PDF we obtained r-dependent strains. In disordered materials every atom has a distinctive atomic environment and thus the response of every atom to the macroscopic stress can be different resulting in non-affine displacements of the atoms. However, there is a different range of non-affine strains in metallic and covalent systems. In metallic systems local relaxation easily accommodates strain and local displacement is compatible with average strain. In covalent systems strong local bonding inhibits local displacements and strain is accommodated by rotation of local units. Thus local deformation is not compatible with average strain. Interestingly beyond few molecular units deformation in covalent systems looks similar to metallic. We present data for metallic, oxide and polymeric glasses. Supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division.

### <u>S2 Advanced Ceramic Coatings for</u> <u>Structural/Environmental & Functional</u> <u>Applications</u>

#### **S2- Environmental Barrier Coatings I**

Room: Coquina C

Session Chair: Peter Mechnich, DLR - German Aerospace Center

#### 1:30 PM

#### (ICACC-S2-001-2025) Design of Environmental barrier coatings based on high-throughput method and co-doping synergistic effect (Invited)

Y. h. Wang<sup>1</sup>; J. Zhang<sup>\*1</sup>; J. Wang<sup>1</sup>

1. Institute of Metal Research Chinese Academy of Sciences, Shenyang National Laboratory for Materials Science, China

Coordinated optimization of the thermal cycling durability and hermetic property has become a chief concern in designing reliable environmental barrier coatings (EBCs) for Si-based ceramics. The Si bond layer of the existing EBCs is easy to melt and be corroded by water vapor in higher temperature oxidation and water vapor corrosion environment, which leads to the failure of EBCs. The current work focuses on the design and screening of multi-Re-Si Bond Coat. The combinatorial material chips of the Si-Gd-Yb systems have been synthesized by magnetron sputtering method to obtain massive sample patches covering the broad compositional range. With the combined high-throughput mechanical, oxidation and water vapor recession tests, the effects of co-doped rare earth elements on the melting point and high-temperature water-oxygen corrosion resistance of the multi-rare earth elements modified Si bond were studied. This work provides an efficient method and new perspective for the design and optimization of the composition of co-doping bond coats, and filtrates specific composition range worth for further investigation.

## Abstracts

#### 2:00 PM

# (ICACC-S2-002-2025) Suspension plasma sprayed ytterbium disilicate coatings: Phase stability and microstructural evolution in extreme environments

E. B. Owusu\*<sup>2</sup>; A. R. Romero<sup>2</sup>; A. Lynam<sup>2</sup>; B. Zhang<sup>2</sup>; O. Gavalda-Diaz<sup>1</sup>; T. Hussain<sup>2</sup>

- 1. Imperial College London, United Kingdom
- 2. University of Nottingham, United Kingdom

Suspension plasma spray (SPS) technique offers the prospect to tailor the microstructure of thermal sprayed coatings. In this research, we explored this capability to manufacture ytterbium disilicate environmental barrier coatings via the SPS route with the aim of improving the performance against steam and molten calcium-magnesiumaluminium-silicate (CMAS) corrosion. Sample exposed to steam with 1 m/s velocity at 1350 °C for 96 h experienced some degree of silica volatilisation without material erosion. CMAS degradation tests for 5 and 240 mins at 1300 °C on the coatings showed that the large aspect ratio of the splats facilitated reaction between CMAS and ytterbium monosilicate to form a dense layer that slowed further CMAS infiltration. The coating developed no cracks after further CMAS tests at prolonged times of 96 h and 250 h, and increased temperature of 1350 °C, although it infiltrated completely. However, when it was exposed to an environment containing both steam and CMAS at 1350 °C for 96 h, a new phase (ytterbium alumina garnet, YbAG), no silica-volatilised layer and 54-µm CMAS interaction zone were observed. These outcomes suggest that SPS has the potential to manufacture EBCs with improved resistance to steam and CMAS degradations.

#### 2:20 PM

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# (ICACC-S2-003-2025) Evaluation of Co-Substitution of $Y_2Si_2O_7$ for Tailoring Thermal Expansion and Phase Stability for Environmental Barrier Coatings

- C. Brockman\*3; J. L. Stokes1; R. I. Webster1; A. S. Almansour2; P. Sarin3
- 1. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA
- 2. NASA Glenn Research Center, Ceramic and Polymer Composites Branch, USA
- 3. Oklahoma State University, Materials Science and Engineering, USA

Environmental barrier coatings (EBCs) enable the use of ceramic matrix composites (CMCs) in turbine engine components by protecting the CMC from oxidation and recession in extreme environments. Rare earth (RE) disilicates have been used as an EBC topcoat layer to slow the degradation of underlying EBC layers. Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> is a promising material, but the presence of polymorphs at high temperatures limits its usage. A method to stabilize Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> has been investigated, through the substitution with another RE material, scandium. Compositions of  $(Y_xSc_{1-x})_2Si_2O_7$  systems with increasing Sc content at the RE site were synthesized at 1100°C. X-ray diffraction (XRD) was used to confirm the alpha-phase of Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, and beta-phase for each (Y<sub>x</sub>Sc<sub>1-x</sub>)<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> system (6, 13, 21 mol% Sc) after synthesis. Results from high temperature XRD will be presented to elucidate the phase stability, phase transformation and anisotropic thermal expansion properties of each (Y<sub>x</sub>Sc<sub>1-x</sub>)<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> system as a function of composition and temperature. Thermal expansion tensors of each system will be calculated, and expansion will be modeled in three dimensions.

#### S2- Environmental Barrier Coatings II

#### Room: Coquina C

Session Chair: Douglas Wolfe, Pennsylvania State University

#### 3:20 PM

#### (ICACC-S2-005-2025) Environmental Barrier Coating Processing with the Plasma Spray- Physical Vapor Deposition (PS-PVD) Facility at NASA Glenn Research Center

B. J. Harder\*<sup>1</sup>; L. C. Hoffman<sup>1</sup>; J. R. Colmenares<sup>2</sup>

- 1. NASA Glenn Research Center, Environmental Effects and Coatings, USA
- 2. Berkshire Community College, Engineering, USA

Improved fuel efficiency and reduced emissions are driving the use of Si-based ceramics such as silicon carbide into the hot section of gas turbine engines. However, in these extreme conditions, silicon carbide does not have sufficient durability without an environmental barrier coating (EBC). Advanced EBCs are necessary for operation beyond 3000°F, and new application methods and chemistries are required to achieve these capabilities. Coatings were prepared utilizing NASA GRC's Plasma Spray-Physical Vapor Deposition (PS-PVD) facility. Composition and microstructure were optimized based on target coating layer requirements. Materials such as Yb-silicate, hafnium oxide, and mullite were considered for multilayer architectures. The PS-PVD facility can generate lamellar or columnar structures as well as deposit a range of compositions by changing processing parameters. Steam oxidation was performed at high temperature in 90%  $H_2O/O_2$  to determine durability of these coating systems and thermally grown oxide (TGO) kinetics are shown at various temperatures.

#### 3:40 PM

# (ICACC-S2-006-2025) The Effect of Testing Parameters on Degradation Mechanisms for Environmental Barrier Coatings

B. Kowalski<sup>\*1</sup>; J. L. Stokes<sup>1</sup>

1. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA

Greater gas turbine engine efficiency is a major goal in aeronautics research often pursued through increased engine operating temperatures. However, it is necessary to replace the current hot-stage alloy components with more thermally robust parts such as silicon-based ceramics. Unfortunately, these materials are susceptible to the effects of oxidation, water vapor, and (Calcium-Magnesium-Alumino-Silicate) CMAS interaction, among other issues at high temperature. To mitigate these effects, environmental barrier coating (EBC) materials are employed to help control the rate of degradation to the underlying composite. Since these materials are a critical technology for operation, they must be durable in the corrosive turbine environment. This presentation will explore the degradation of EBCs by water vapor and CMAS and the ways in which the parameters of each test and subsequent analysis can affect the outcome. These testing parameters will be discussed within the context of promising EBC materials.

#### 4:00 PM

#### (ICACC-S2-007-2025) Synergistic effects of coating variables on the steam oxidation of modified silicon/ytterbium disilicate environmental barrier coatings

K. Lee\*1; J. Stuckner1; A. Garg1; R. I. Webster1; L. Wilson1

1. NASA Glenn Research Center, USA

Environmental barrier coatings (EBCs) are an enabler for SiC/ SiC ceramic matrix composites (CMCs) in gas turbines. One of the most critical EBC failure modes is steam oxidation-induced failure. Long steam oxidation life, therefore, is a key to the reliability of CMC components. The chemistry of the EBC and underlying CMC substrate has a significant impact on the steam oxidation resistance of the current state-of-the-art EBC (Gen 2 EBC: Si/Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>). NASA has developed chemically modified Gen 2 EBCs (Mod Gen 2 EBCs) that reduce the parabolic steam oxidation rate constant of the Gen 2 EBC by more than tenfold. This study investigates the synergistic effects of three EBC variables (EBC chemistry, substate chemistry, post-spray annealing) on the steam oxidation kinetics of Mod Gen 2 EBCs. Aluminum and boron in the SiO<sub>2</sub> oxide scale were the key elements having an overarching influence on EBC oxidation kinetics. Complex interactions among the three EBC variables dictated the concentration of aluminum and boron in the SiO<sub>2</sub> oxide scale and thus the EBC oxidation kinetics.

#### 4:20 PM

# (ICACC-S2-008-2025) SiO $_2$ activity measurements in the Gd $_2O_3\text{-}SiO_2$ system via Knudsen Effusion Mass Spectrometry (KEMS)

R. I. Webster\*1; B. Kowalski1; N. Jacobson2

- 1. NASA Glenn Research Center, USA
- 2. HX5 Sierra, LLC, USA

Environmental barrier coatings (EBCs) are required for the use of silicon carbide (SiC)-based ceramic matrix composites (CMCs) in gas turbine engines, as they protect the SiO<sub>2</sub> thermally grown oxide (TGO) formed at the CMC/coating interface from volatilization in a combustion environment. Current-generation EBCs consist of a silicon bond coat and a rare earth (RE) silicate topcoat. The RE silicate topcoat is exposed to high-velocity steam during engine operation, and SiO<sub>2</sub> within the coating can preferentially volatilize to form Si(OH)<sub>4</sub> gas species, albeit at a lesser degree than SiO<sub>2</sub> alone. Therefore, it is of interest to investigate the stability of these materials in steam as a function of their RE. In this study, SiO<sub>2</sub> activity, which can be related to the partial pressure of Si(OH)<sub>4</sub>, was measured across the Gd<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> phase diagram, which includes Gd<sub>2</sub>SiO<sub>5</sub>, Gd<sub>933</sub>(SiO<sub>4</sub>)<sub>6</sub>O<sub>2</sub>, and Gd<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> as line compounds, via Knudsen Effusion Mass Spectrometry (KEMS). Values obtained for the  $Gd_2O_3$ -SiO<sub>2</sub> system were compared to those of other RE<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> systems and contextualized in terms of EBC viability.

### <u>S3 22th Intl Symp on Solid Oxide Cells</u> <u>Materials Science & Technology</u>

#### S3- System design and demonstration

Room: Ballroom 4

Session Chair: Scott Barnett, Northwestern University

#### 1:30 PM

## (ICACC-S3-001-2025) Status and progress of SOE development in EU (Invited)

M. Kusnezoff<sup>\*1</sup>; S. Megel<sup>1</sup>; N. Trofimenko<sup>1</sup>; S. Mosch<sup>1</sup>; S. Rothe<sup>1</sup>; A. Michaelis<sup>1</sup>

1. Fraunhofer IKTS, Germany

Solid oxide electrolysis is the most efficient technology for hydrogen production. The presentation provides an overview on progress of SOE stack and cell development in EU. Based on published data the update on SOE stack and system performance will be provided. Especially, the performance and degradation issues for electrolysis and co-electrolysis operation will be addressed and conclusions about limitations for existing stack and cell concepts made. The overview of factors limiting the performance and the corresponding degradation mechanisms affecting durability will be provided.

#### 2:00 PM

#### (ICACC-S3-002-2025) Zero-Electricity Electrolytic Solid Oxide Cells for Industrial Decarbonization and H<sub>2</sub> Generation (Invited) B. Blackburn<sup>\*1</sup>

1. Utility Global, USA

An overview will be provided for our eXERO<sup>TM</sup> Solid Oxide Cell (SOC) technology platform, which unlike conventional electrolysis is driven by the inherent energy in process gas streams rather than externally provided electricity. Like other SOC technologies, such as solid oxide fuel cells (SOFCs), the eXERO<sup>TM</sup> cells operate at elevated temperature (~700-900 °C) and are capable of robust processing and conversion of industrial off gas streams (e.g., steel mill Blast Furnace Gas, or BFG) into  $H_2$  and other useful byproducts (e.g., syngas). A gas-tight membrane is the key to ultra-high purity hydrogen (>99%) without additional gas processing or cleanup. This mixed ionic electronic conducting (MIEC) electrolyte provides an internal circuit for transportation of charged species to the anode and cathode where a chemical potential difference drives oxidation and reduction reactions. A simple example is the introduction of pure carbon monoxide at the anode and steam at the cathode, which electrochemically react to form high-purity CO<sub>2</sub> and H<sub>2</sub>. During the presentation the basis of performance will be discussed from the standpoint of thermodynamics and reaction kinetics. An update will also be provided on the commercialization status of the eXERO<sup>TM</sup> technology and various demonstration projects, such as deployment of a reactor at an operating steel mill for the conversion of BFG to H<sub>2</sub>.

#### 2:30 PM

#### (ICACC-S3-003-2025) Recent Developments on Hydrogen Production Using Solid Oxide Electrolysis at GENVIA (Invited)

F. Monaco<sup>\*1</sup>; R. Tchakalov<sup>1</sup>; M. Delgado<sup>1</sup>; J. Poncelet<sup>1</sup>; M. Dessinges<sup>1</sup>; P. Tochon<sup>2</sup>

- 1. Genvia SAS, R&D Technological Group, France
- 2. Genvia SAS, R&D, France

Hydrogen production is seen by numerous experts as a potential great energetic vector for decarbonization, particularly for industry. In this context, high temperature electrolysis based on Solid Oxid Cells (SOC) has attracted great interest thanks to the high electrical efficiency. To accelerate the transition, large-scale systems will be required, in agreement with international and EU roadmaps. This is the background of Genvia's creation, a Clean Hydrogen Technology Venture, that aims to enable individual organizations, industries and nations to meet their goals for decarbonization by accelerating affordable clean hydrogen, energy storage and fuel applications at scale. By providing cost-effective and high-performance SOEC and SOFC technologies, Genvia will support heavy industry to decarbonize processes and achieve emissions targets, as well as energy providers to offer decarbonized electricity to consumers where and when they need it. Starting from 15 years of R&D from the French Atomic and Alternative Energies Commission (CEA), Genvia has created an extraordinary ecosystem to design, manufacture and operate high-performance electrolyzers, based on a proprietary stack technology that offers improved efficiency over competing approaches. The status of manufacturing and technological development at Genvia will be presented, as well as the remaining challenges.

#### S3- Electrolysis and applications I

Room: Ballroom 4 Session Chair: Mihails Kusnezoff, Fraunhofer IKTS

#### 3:20 PM

#### (ICACC-S3-004-2025) Commercialising large scale SOEC for Power-to-X applications (Invited)

S. D. Ebbesen\*1; P. Blennow2; A. Mai1; M. Hultqvist1; P. Moses1

- 1. Topsoe, Power to X, Denmark
- 2. Topsoe A/S, Denmark

Topsoe is a leading global provider of solutions for the energy transition. Power-to-X (P2X) will inevitably play an increasingly crucial role in our path towards a sustainable and carbon-neutral future. P2X bridges the gap between renewable electricity sources, and the fuel tanks of zero-emission transportation, as well as sustainable chemicals. The core technology of P2X is electrolysis, of which SOEC has shown to be the most energy-efficient and allows for efficient integration with downstream processes. Topsoe is among the few companies globally possessing solutions that span from electrolysers to downstream processes. Topsoe has advanced the Topsoe Stack Platform to a level enabling large-scale commercialisation. The stack is a designed for H<sub>2</sub> production, with the capability to produce CO also. The stacks are integrated in an industrial Concept Core containing 12 stacks. To scale up production, Topsoe is building a factory in Denmark to produce electrolysis stacks and modules with an initial annual production capacity of 500MW and be operational in 2025. Additionally, pending final investment decision, Topsoe has announced plans to build its second SOEC factory in USA.2 Our concepts applying SOEC for hydrogen production, and integration with downstream synthesis will be presented. Additionally, we will present results from our SOEC Demo Cores, and will give the latest status of our manufacturing plants.

#### 3:50 PM

#### (ICACC-S3-005-2025) Dynamic Response Evaluation of Grid-integrated High Temperature Steam Electrolysis for Grid Support (Invited)

T. O. Olowu\*<sup>1</sup>; J. L. Hartvigsen<sup>1</sup>; A. Shigrekar<sup>1</sup>; J. W. Lambrechtsen<sup>1</sup>; M. J. Casteel<sup>1</sup>

1. Idaho National Laboratory Research Library, Hydrogen and Thermal Systems, USA

With increasing penetration of distributed energy resources, the use of flexible loads such as High Temperature Steam Electrolysis (HTSE) to provide grid support have become very essential. Idaho National Laboratory has developed a range of HTSE test facilities aimed at assessing the dynamic operation of solid oxide electrolysis technology across the full TRL spectrum-from individual button cells to pre-commercial, sub-megawatt systems. To evaluate the ability of the HTSE systems to provide grid support, several dynamic operations of a 100kW HTSE test facility are presented. The system was ramped at different rates to evaluate its dynamic response to different grid power command and dynamics. The impacts of the dynamic operation of the HTSE on grid's power quality such as voltage and frequency at the point of grid interconnection (POGI) was also evaluated. Dynamic measurements taken from the grid at the POGI and the HTSE operational data show that the test stand is capable of responding to different power command setpoints based on the grid operational requirements. Although the HTSE has some ramp constraints, this is mainly due to the thermal inertia of its balance of plant and not the power electronic converters or the solid oxide electrolysis stacks. The HTSE system performance shows that it can be effectively used to improve the steady state dynamics of the power grid.

#### 4:20 PM

# (ICACC-S3-007-2025) Hydrogen Production at intermediate Temperatures and Protonic Ceramic Cells (Invited)

R. Costa\*1

1. German Aerospace Center, DLR, Institute of Engineering Thermodynamics, Germany

Hydrogen production at intermediate temperature is especially attractive for integration into industrial processes where excess heat in the form of steam is available. Protonic Ceremic Cells (PCC) are by nature and design especially suited for operation at temperature between 500°C and 600°C. In this contribution, we evaluate the production of hydrogen by proton conducting ceramic cell electrolysis (PCCEL) and compare with state-of-the-art (SOEL) to highlight the merits and key challenges of PCC technologies in terms of performance, durability and efficiency. In a 2nd part we report on the proof of concept and development of a PCC technolgy with a metal supported architecture based on a Fe-Cr porous substrate. Key aspects considering specific materials properties, characteristics of protonic ceramics for a succesful engineering are exposed and discussed. Performance in PCCEL operation are presented and discussed as well as improvement routes for on-going and future developments.

### <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

#### S6- All-solid-state batteries I

Room: Coquina B

Session Chairs: Palani Balaya, National University of Singapore; Valerie Pralong, CNRS ENSICAEN

#### 1:30 PM

## (ICACC-S6-003-2025) Toward high-energy lithium/sodium metal batteries with highly concentrated electrolytes (Invited)

Y. Ugata\*1; N. Yabuuchi1

1. Yokohama National University, Japan

Highly concentrated electrolytes (HCEs) typically containing electrolyte salts of over 3 mol L<sup>-1</sup> are effective in improving the electrochemical reversibility of lithium/sodium metal batteries. However, the insufficient wettability of HCEs to conventional polyolefin separators remains a critical issue to be addressed. Here, we present effective strategies to address the electrolyte wettability issue and to achieve stable cycling of lithium/sodium metal batteries under practical conditions. A functional polyolefin separator coated on both sides with a meta-aramid resin is one of the efficient approaches to improve the electrolyte wettability because polar functional groups offer a better affinity between the polyolefin separator and HCE. The combined use of HCE and aramid-coated polyolefin separator enables reversible lithium deposition/stripping cycling with high Coulombic efficiency of ~99% at practical areal capacity of 4 mA h cm<sup>-2</sup> and stable operation of high-energy lithium metal batteries with a high-loading pure Ni layered oxide positive electrode (~20 mg cm<sup>-2</sup>). Moreover, this approach is successfully applied to HCEs for sodium battery applications. These strategies would be one of the promising routes to realize practical high-energy lithium/ sodium metal batteries.

#### 2:00 PM

#### (ICACC-S6-021-2025) Towards the design of Li-metal solid polymer batteries and advances in battery technology in Singapore (Invited)

D. Fam\*1; N. Ding1; S. Goh1; D. Safanama1

1. Institute of Materials Research and Engineering, Singapore

The development of Li-metal solid polymer batteries represents a promising frontier in energy storage technology, primarily due to their potential for high energy densities. The integration of solid polymer electrolytes (SPEs) with Li-metal batteries is essential for achieving compatibility with high-voltage cathode materials, such as NMC and NCA. However, commercial SPEs, particularly polyethylene oxide (PEO), exhibit poor ionic conductivity below their melting point; operational temperatures must be elevated above their melting point. Furthermore, PEO oxidisesat voltages >4 V, making them unsuitable for high voltage cathodes. Our recent work has elucidated the bottleneck hindering room-temperature operation of PEO-based SPEs, leading to the design of a novel solid polymer electrolyte that demonstrates enhanced stability with NMC and practical ionic conductivities in its solid-state. This new electrolyte exhibits an unusually high lithium ion transference number exceeding 0.7, facilitating efficient ion transport. We have successfully fabricated NMC-Li metal cells that demonstrate stable cycling performance, indicating the feasibility of this approach for next-generation battery systems. This talk will detail our findings and the implications for the future of Li metal SPBs, emphasizing the critical interplay between material design and electrochemical performance.

#### 2:30 PM

#### (ICACC-S6-001-2025) Achieving Extreme High Ion-Current Densities in Tailored Materials, Structures, and Interfaces (Invited)

E. D. Wachsman<sup>\*1</sup>

1. University of Maryland, USA

Oxide-based solid-state batteries have the potential to be a transformational and intrinsically safe energy storage solution due to their non-flammable ceramic electrolyte that enables the use of high-capacity metal anodes and high voltage cathodes for higher energy density over a much wider operating temperature range. However, their progress has been limited due to electrode/electrolyte interfacial issues. In particular for metal anodes concerns over dendrite formation/propagation and the requirement for elevated temperature and high stack pressure are still prevalent. To eliminate these concerns a rational design of tailored materials, 3D structures, and interfaces in metal anodes will be presented. These 3D porous structures enabled critical current densities (CCDs) of 100 mA/cm<sup>2</sup> and cumulative Li-metal cycling of over 18.5 Ah/cm<sup>2</sup> at room temperature with no applied pressure. More recently due to the concern over Li availability we developed higher conductivity NASICON and demonstrated similar stable cycling of Na-metal in 3D structured NASICON achieving CCDs of 30 mA/cm<sup>2</sup> at room temperature with no applied pressure. These new solid-state compositions integrated into surface modified 3D structures enable previously unheard-of metal-anode cycling rates. Their development and progress toward full cells using these tailored materials, structures, and interfaces will be presented.

#### S6- All-solid-state batteries II

Room: Coquina B

Session Chairs: Valerie Pralong, CNRS ENSICAEN; Mahalingam Balasubramanian, Oak Ridge National Lab

#### 3:20 PM

## (ICACC-S6-004-2025) Next Generation Batteries for Electric Aviation and Space (Invited)

D. Dornbusch\*1; Y. Lin2; W. H. Huddleston1; V. Yamakov2; R. P. Viggiano1

- 1. NASA Glenn Research Center, Materials, Chemistry, and Physics Branch, USA
- 2. NASA Langley Research Center, USA

Energy storage plays a critical part in the success of future NASA missions that desire batteries with higher energy density, higher power, and most critically improved safety. These performance requirements stretch beyond that of electric automobile markets and are required for enabling widespread adoption of electric aviation. One approach to improve the safety and energy is the transition to non-volatile solid-state electrolytes (SSE) which promise many advantages over traditional flammable liquid electrolytes and may also be an enabling technology for next generation chemistries such as lithium-sulfur (Li-S). However, significant manufacturing challenges must be overcome before the adoption of such technology. Furthermore, design and development of novel cathode composites through integration of experiment and a particle dynamics model will be discussed [2] [3]. Beyond aeronautics, unique challenges and requirements exist for energy storage for space applications, which can cover extreme temperatures and material scarcity for in-situ derived materials.

#### 3:50 PM

#### (ICACC-S6-005-2025) Three-Dimensionally Interconnected Polymer/Ceramic Composite Polymer Electrolytes for Solid-State Batteries (Invited)

R. Sahore<sup>\*1</sup>; K. Owensby<sup>1</sup>; B. L. Armstrong<sup>1</sup>; J. Ock<sup>1</sup>; A. Ullman<sup>1</sup>; S. Kalnaus<sup>2</sup>; X. C. Chen<sup>1</sup>

- 1. Oak Ridge National Laboratory Physical Sciences Directorate, USA
- 2. Oak Ridge National Laboratory Computing and Computational Sciences Directorate, USA

Polymer-ceramic composite electrolytes (CPEs) aim to combine the advantages of both polymer & ceramic electrolytes. In the conventional CPE design, where the ceramic electrolyte particles are dispersed in the polymer matrix, the advantages of the ceramic phase are not fully utilized primarily due to large interfacial impedance of the polymer/ceramic interface. A three-dimensionally interconnected CPE, in which the ceramic electrolyte phase is interconnected or continuous, can potentially overcome these issues. Despite several literature reports on the fabrication and testing of such CPEs, an in-depth, systematic understanding of the role of the ceramic scaffold's architecture, polymer chemistry, and the associated polymer/ ceramic interfaces, on their electrochemical properties is still incomplete. In this work, we utilize a tunable platform of partial sintering to prepare randomly interconnected scaffolds. The scaffolds are infiltrated with cross-linkable polymer electrolyte precursors to obtain the CPEs. Due to the bi-continuous ceramic and polymer phases, the CPE presents improved transference number, reduced Li<sup>+</sup> concentration gradients, compared to neat polymer. However, despite the interconnectedness of ceramic, the high impedance polymer/ ceramic interface at the surface is a bottleneck. The polymer phase also dictates the limiting current density of the CPE.

## Abstracts

#### 4:20 PM

## (ICACC-S6-006-2025) Lithium Metal and Alloy Anodes for Solid-State Batteries (Invited)

#### M. McDowell\*1

#### 1. Georgia Institute of Technology, USA

Solid-state batteries offer the promise of improved energy density and safety compared to lithium-ion batteries, but electrochemo-mechanical degradation of materials can play an outsized role in limiting their performance. Here, I will present my group's work on understanding structural evolution in solid-state batteries with both lithium metal and alloy-based anodes. Using X-ray tomography and cryo-FIB we show that lithium metal anode-free solid-state batteries are intrinsically limited by current concentrations at the end of stripping due to localized lithium depletion. This causes accelerated short circuiting compared to lithium-excess cells. The beneficial influence of metal interfacial layers on controlling lithium evolution and mitigating contact loss from localized lithium depletion will be introduced. In the second part of the talk, alloybased anodes for solid-state batteries are investigated. We show that alloy foils such as aluminum and tin exhibit improved interfacial stability and better long-term cycling in solid-state batteries compared to liquid-cell batteries due to reduced solid-electrolyte interphase formation. A new design for multiphase aluminum foil alloy anodes is introduced. Taken together, these findings show the promise of both lithium metal and alloy anodes for solid-state batteries.

#### 4:50 PM

#### (ICACC-S6-007-2025) Addressing Interfacial Challenges in Liquid and Solid-State Symmetric Na-ion Cells

- P. Balaya\*1; S. Dwivedi1; S. Vasudevan1
- 1. National University of Singapore, Department of Mechanical Engineering, Singapore

The long-term cycling of the solid-state Na-ion cells is still challenging due to electrode-electrolyte interfacial hurdles compared to liquid-based cells. These challenges include undesirable reactions such as SEI, formation of unwanted phases, active material degradation etc. To learn more, we conducted a series of experiments on fresh and post-cycled liquid (NVP-cathode||1M NaBF4 in TEG||NVP-anode) and solid-state (NVP-catholyte||PEO-NaTFSI/ NZSP-MS||NVP-anolyte) symmetric full cells to identify the major stumbling block causing capacity loss and increased polarization during cycling of both the cells. These tests involved examining the structural integrity and electrochemical properties using FTIR, TEM, XPS, and EIS measurements. We further analysed the EIS data using Distribution of Relaxation Times method to delineate the impedance contributions of various cell components. This study has provided valuable insights into understanding the primary limiting factors of solid-state cells. Overcoming these challenges could facilitate the widespread adoption of all-solid-state batteries.

#### 5:10 PM

## (ICACC-S6-008-2025) Microstructure based modelling ceramic composite cathodes for all-solid-state lithium-ion batteries

F. Al-Jaljouli<sup>\*1</sup>; O. Guillon<sup>1</sup>; R. Muecke<sup>1</sup>; P. Kaghazchi<sup>1</sup>; C. Roitzheim<sup>1</sup>; Y. Sohn<sup>1</sup>; M. Finsterbusch<sup>1</sup>

1. Forschungzentrum Jülich, IMD-2, Germany

The transition to solid-state lithium-ion batteries enhances safety and energy density but introduces a substantial mechanical stress, potentially leading to capacity degradation. This study addresses the often-overlooked residual mechanical stress from manufacturing and its coupling with delithiation-induced stress in composite cathodes (consisting of different cathode active material – CAM – and Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> – LLZO). We introduced a "chemo-thermal mechanical stress" model, integrating thermal and chemical stresses to provide a more realistic model. Thermal stress mitigates induced stress in  $LiCoO_2$  but exacerbates it in  $Li_{0.5}NCM955$  and  $Li_{0.1}NCM955$ . We studied the impact of microstructural parameters, including the solid volume fraction of CAM and porosity on stress distribution. Mechanical stress inversely relates to both. The effect of composite grain's morphology on the chemo-thermal stress was also investigated. We propose a composite of hexagonal  $LiCoO_2$  with fiber-shaped LLZO to lower stress and enhance composite cathode durability.

### S7 19th Intl Symp on Functional Nanomaterials & Thin Films for Sustainable Energy Harvesting

# S7- Nanomaterials for energy conversion, storage and catalysis-I

Room: Flagler C

Session Chair: Muhammet Toprak, KTH Royal Institute of Technology

#### 1:30 PM

## (ICACC-S7-001-2025) Functional 2D material thin films for sustainable energy application (Invited)

- V. Brune<sup>1</sup>; T. Fischer<sup>2</sup>; S. Mathur<sup>\*2</sup>
- 1. University of Cologne, Chemistry, Germany
- 2. University of Cologne, Institute of Inorganic Chemistry, Germany

Chalcogenide-based 2D materials are crucial for sustainable energy storage and conversion in applications such as batteries, capacitors, solar harvesting, and (photo-)electrocatalysis. As the energy landscape evolves, innovative technologies are needed to develop long-term sustainable systems. Harnessing next-generation energy sources like solar, wind, tidal, and wave energy can support energy security and reduce environmental and health impacts, despite their intermittent nature. Targeted chemical synthesis plays a key role in enhancing the functional performance of materials. Atomic-level preorganization of nanostructured chalcogenide-based 2D thin films, using specially designed molecular compounds with pre-formed bonds, offers significant potential for improving energy conversion and storage efficiency. Unique synthetic approaches utilizing molecular building blocks, such as established air-stable precursor classes  $[M{X(C_2H_4)_2NMe}x]$  (where M = Mo<sup>IV</sup>, W<sup>IV</sup>, Ti<sup>IV</sup>,  $Zr^{IV}$ ,  $Hf^{IV}$ ,  $Nb^{IV}$ ,  $Sn^{IV}$ , x = 2;  $M = Ge^{II}$ ,  $Sn^{II}$ ,  $Ni^{II}$ , x = 1; X = S, Se), enable reliable processing of layered 2D van der Waals materials with tunable properties, driving advancements in next-generation chalcogenide-based materials.

#### 2:00 PM

#### (ICACC-S7-002-2025) Nano-materials for Green Energy:-A Sustainable Approach

M. Kaur\*1

1. Guru Kashi University, Agriculture, India

The climate crisis and the pressing need to reduce anthropogenic carbon dioxide emissions underline the need for renewable energy technology including catalytic and electrochemical conversion and storage devices such as fuel cells or water electrolysers for hydrogen production. Such devices are strongly dependent on novel nanomaterials. For example, a major obstacle that currently limits the performance of technologically important proton exchange membrane fuel cells is the sluggish oxygen reduction reaction (ORR) at fuel cell cathodes. Novel Pt-Ni alloy nanoparticles with octahedral shape are regarded as outstanding catalysts for the ORR. The atomic-scale structural and compositional analysis of Pt-Ni alloy nanoparticles with octahedral shapes, crucial for their activity and stability in catalysing the oxygen reduction reaction in proton exchange membrane (PEM) fuel cells, involves several advanced analytical techniques. Here are some methods commonly used for such analysis: Transmission Electron Microscopy, X-ray Diffraction, X-ray Photoelectron Spectroscopy and X-ray Scattering. By employing these advanced techniques in combination, researchers can achieve a comprehensive understanding of the atomic-scale elemental distribution. Moreover, this knowledge is essential for optimizing their catalytic activity and stability in PEM fuel cells, contributing to the development of more efficient renewable energy technologies.

#### 2:20 PM

## (ICACC-S7-003-2025) Photoluminescence and Raman studies of rare earth doped ZnO nanoparticles

S. karidas<sup>1</sup>; V. Priya<sup>1</sup>; G. Sriramulu<sup>1</sup>; K. Kumari\*<sup>1</sup>

1. Osmania University, PHYSICS, India

ZnO nanoparticles and Nd, Ce, Gd doped ZnO nanoparticles were prepared with Co-precipitation method. The solution was thoroughly mixed with magnetic stirrer, white precipitate was formed. Then the powder was kept in hot air oven, to make it dry. The grinded nano particles were sintered conventionally at 600°C for 2hours. Then characterised with XRD. From RAMAN spectra for undoped and Nd, Ce, Gd doped ZnO nanoparticles shows peaks at 434 cm<sup>-1</sup> corresponding to E<sub>2</sub>H mode which is the characteristic of the wurtzite lattice and indicates good crystallinity. For all the particles E<sub>2</sub>H mode decreased gradually with increasing rare earth concentration, which may be attributed to the lattice distortion in Zinc Oxide matrix and indicates that as the concentration increases crystallinity of the particles decreases. From the PL spectra of undoped and Nd, Ce, Gd doped nanoparticles it can be inferred that more defects are created in doped particles. The intensity of sharp Ultra Violet emission decreases for Nd,Ce, Gd doped ZnO nanoparticles. For Ce doped at some concentration like x = 0.01, 0.1, 0.05, broad peak intensity in visible region decreases than PL intensity of undoped ZnO nanoparticles. For Nd, Gd doped ZnO nanoparticles at all concentrations PL intensity is more than undoped ZnO nanoparticles. Hence Nd, Gd, Ce doped nanoparticles can be used as photocatalysts for the photodegradation of organic dyes.

#### 2:40 PM

#### (ICACC-S7-004-2025) Designing Efficient Bifunctional Photocatalysts: Insights from Two-Dimensional Noble-Metal Chalcogenides for Water Splitting

M. Boujnah\*1; M. Cruz Jáuregui3; J. Muñiz Soria2; J. Muñoz Saldaña1

- 1. Centro de Investigacion y de Estudios Avanzados Unidad Queretaro, Mexico
- 2. Universidad Nacional Autonoma de Mexico Instituto de Energias Renovables, Mexico
- Centro de Nanociencias y Nanotecnología (CNyN), Universidad Nacional Autónoma de México (UNAM), Mexico

The search for efficient and stable bifunctional photocatalyst capable of facilitating both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) is crucial to advance practical applications of water splitting under alkaline conditions. Janus and non-Janus monolayers is one of the transformations of the 2D materials viz present an exceptional opportunity to control and manipulate their physical properties. This study discusses two-dimensional noble-metal chalcogenide (NMC) materials of the form  $A_2B$  (where A = Ag, Au and B = S, Se) through first-principles calculations. Ab initio molecular dynamics simulations demonstrate that these monolayers exhibit excellent dynamic and mechanical stability. We examine a combination of Janus and non-Janus monolayers of NMCs and their heterobilayers. The band gap values of  $\alpha$  or  $\beta$  phases calculated at the HSE06 level is between 1.35 and 3.70 eV. A high optical absorption around  $4.5 \times 10^5$  cm<sup>-1</sup> and high anisotropic carrier mobility ~105 cm2 V-1s-1 was observed, in which indicate that they may shine in the next generation of electronic and

optoelectronic devices. Consequently, these heterostructures show promise as efficient photocatalysts for both HER and OER, thereby enhancing photocatalytic activity for water splitting.

#### S7- Nanomaterials for thermoelectrics,

#### **photocatalysis, electrocatalysis, and solar hydrogen** Room: Flagler C

Session Chair: Andreu Cabot, Catalonia Institute for Energy Research

#### 3:20 PM

(ICACC-S7-005-2025) Green Chemical Syntheses, Processing and Characterization of Nanostructured Thermoelectric Materials (Invited)

M. S. Toprak\*1

1. KTH Royal Institute of Technology, Dept. of Applied Physics, Sweden

There is an increasing interest to develop thermoelectric (TE) films from pre-made nanoparticles to enable conformally deposited films for waste-heat harvesting from any surface that radiates heat. A pre-requisite for these efforts to succeed is to have a set of well-defined, large-scale and highly reproducible quality of n- and p-type TE materials. TE materials in bulk scale are generally produced through energetic routes, such as solid-state reactions in sealed quartz ampoules for up to few days. Development of energy effective and scalable synthetic techniques are required for a broader use of TE materials technologies. We have been developed solution-based, green synthetic methods, with drastically reduced reaction times from days and hours to few minutes. Several TE materials operational at various temperature regimes have been synthesized by the optimization of the developed technique, enabled by the use of Microwave-assisted heating. In this presentation, a review of the materials developed will be presented, including their synthesis, structural characterization and finally processing into hybrid films using all solution-based strategies. Electronic transport characteristics were evaluated under a temperature gradient. The presented methods, and the developed materials, enable large scale production and integration of TE materials with rather promising qualities.

#### 3:50 PM

#### (ICACC-S7-006-2025) From Materials Synthesis through Green-Chemistry to Thermoelectric Device Engineering: A Multifaceted Approach for TEGs Development (Invited)

B. Hamawandi<sup>1</sup>; J. F. Serrano Claumarchirant\*<sup>1</sup>; A. B. Ergül<sup>1</sup>; M. S. Toprak<sup>1</sup>

1. Kungliga Tekniska Hogskolan, Applied Physics, Sweden

The demand for portable electronic devices has increased enormously in recent years by the integration into flexible substrates, which are easy to integrate into clothes. Wearable electronic devices are used in various applications, including pressure sensors and supercapacitors. The main problem in all cases is the need for a power supply, typically in the form of batteries and supercapacitors, which need to be recharged. Thermoelectric (TE) materials and devices can harvest thermal energy and transform it into useful electrical energy, allowing the operation of these devices without the need for batteries. The development of wearable, flexible TE generators (TEGs) has been an active subject of study in recent years, as it integrates ceramic-based TEGs and printed flexible TE devices. However, most of these TEGs exhibit low flexibility or contain heavy and toxic metals, limiting their practical use. This work demonstrates the synthesis of TE materials using Green Chemistry methods, enabling the integration of TE materials into polymer matrices, which were then formulated into inks for direct ink printing or additive manufacturing. Moreover, the ability to fabricate both p-type and n-type modules through the aforementioned techniques allows for the design and simulation of TEGs to optimize and predict their performance by COMSOL Multiphysics.

## Abstracts

#### 4:20 PM

#### (ICACC-S7-007-2025) Thermoelectric Performance Improvement in Hybrid Thermoelectric Materials via Magneto-Ordering Engineering (Invited)

S. Ballikaya\*1; E. Yetimoglu1; N. Özer1; A. Yusuf1; M. Boroglu1; I. Boz2

- 1. Istanbul Universitesi-Cerrahpasa, Engineering Sciences, Turkey
- 2. Bandirma Onyedi Eylul Universitesi, Turkey

In this work, we reported the structural and thermoelectric properties of Fe<sub>3</sub>O<sub>4</sub> magnetic nano particle incorporated PANI (Polyaniline) prepared by dip coating process. Structural analyses were performed using PXRD and particle analysis spectra, while the thermoelectric properties were measured through Seebeck coefficient and electrical conductivity measurements in the range of room temperature to 400 K. It was observed that the intense peaks seen in the PXRD analysis reflected the crystalline structure of magnetic nano Fe3O4 particles (MNP) rather than the PANI crystal structure. The Seebeck coefficient was positive for all samples, indicating that the p-type conduction mechanism was dominant. The Seebeck coefficient varied between 18-32  $\mu$ V/K in the range of room temperature to 400 K, while the electrical conductivity ranged between 2-30 S/cm. Although there was no significant change in the Seebeck coefficient with the addition of magnetic nanoparticles (MNP), the electrical conductivity improved by approximately 15 times. This improvement was attributed to the alignment of magnetic nanoparticles with the magnetic field, which opened the polymer chains. The structural and transport properties demonstrated that the MNP addition enhanced the performance of hybrid TE compounds.

#### 4:50 PM

#### (ICACC-S7-008-2025) Enhancing Wearable Device Autonomy Using Hybrid Thermoelectric and Piezoelectric Energy Harvesters (Invited)

A. Yusuf<sup>\*1</sup>; S. Ballikaya<sup>1</sup>; A. Yigit<sup>1</sup>; M. Yilmaz<sup>1</sup>

1. Istanbul Universitesi-Cerrahpasa, Engineering Sciences, Turkey

Wearable devices are compact electronic sensors that can be integrated with the body for health monitoring and wireless communication purposes. These devices are gaining attention due to their effectiveness in health monitoring, which can potentially save lives. Conventional wearable devices are powered by batteries, which have a short lifespan and are not environmentally friendly. Recharging or replacing these batteries can be challenging and costly. Research has shown that batteries in wearable devices can be replaced with energy harvesters (EHs). Thermoelectric generators (TEGs) can convert thermal energy into electrical energy, while piezoelectric energy harvesters (PEHs) can convert vibrations or human motion into electrical energy. However, due to the intermittent nature of their output, a single EH may not be sufficient to power a wearable device. To enhance the autonomy of wearable devices, multiple EHs can be integrated to convert both body motion and heat into electricity, enabling continuous energy generation once the device is worn. The proposed wearable device stands out from commercial devices because it is powered by at least two energy harvesters, providing free and sustainable energy.

### <u>S8 19th Intl Symp on APMT for Structural &</u> <u>Multifunctional Materials & Systems</u>

# S8- Microwave processing, SPS, flash sintering, high pressure assisted sintering, I

Room: Flagler A

Session Chairs: Wei Ji, Wuhan University of Technology; Gideon Grader, Technion - Israel Institute of Technology

#### 1:30 PM

#### (ICACC-S8-001-2025) Synchrotron X-ray multiscale observation of heterogeneous microstructures and defects in ceramics during sintering (Invited)

G. Okuma\*1

1. Busshitsu Zairyo Kenkyu Kiko, Japan

Synchrotron X-ray multiscale tomography is a 3D imaging technique that integrates both microtomography and nanotomography, enabling high spatial resolution measurements across a broad field of view. In this study, we demonstrate the use of this method to visualize the 3D evolution of microstructures across multiple scales in ceramic processes such as powder processing, sintering, and microfracture. The heterogeneity, complexity, and hierarchical nature of powder compacts contribute to a variety of defects that impact the quality, reliability of the final products. Defect formation and elimination are influenced by applied stresses during spark plasma sintering, as well as by internal stresses arising from differential and constrained sintering. Additionally, subsurface crack systems generated by Vickers indentation reveal how heterogeneous microstructures govern toughening mechanisms.

#### 2:00 PM

## (ICACC-S8-002-2025) Spark plasma sintering, microstructure and mechanical properties of Y-Ti-O ceramics (Invited)

L. He\*1; E. Hershkovitz2; T. Yoo2; H. Kim2; X. Pu3; K. Bawane4;

- F. G. Di Lemma<sup>4</sup>; T. Nakayama<sup>5</sup>; H. Suematsu<sup>5</sup>
- 1. North Carolina State University, Nuclear Engineering, USA
- 2. University of Florida, Materials Science and Engineering, USA
- 3. National Renewable Energy Laboratory, USA
- 4. Idaho National Lab, Characterization, USA
- 5. Nagaoka University of Technology, Japan

Fluorite-based compounds, including pyrochlore and defect fluorite-type structures, hold significant potential in the nuclear industry for applications such as nuclear fuel, inert matrix fuel, and nuclear waste forms. For example, Y2Ti2O7 pyrochlore, within the Y-Ti-O system, is considered a promising candidate for immobilizing high-level radioactive waste. However, distinguishing between the various structures of Y-Ti-O has been challenging in the literature, complicating efforts to establish clear structure-property relationships in this material system. Notably, Y<sub>2</sub>TiO<sub>5</sub> can exist in several polymorphs, including cubic, orthorhombic, and hexagonal phases within the lattice. To address these complexities, Y-Ti-O ceramics with various compositions were synthesized using spark plasma sintering. A comprehensive structural analysis of Y<sub>2</sub>TiO<sub>5</sub> was conducted using four-dimensional scanning transmission electron microscopy (4D-STEM) coupled with unsupervised machine learning, alongside X-ray diffraction and electron backscatter diffraction (EBSD). Additionally, various mechanical tests were performed to clarify the relationships between structure, composition, and mechanical properties.

# S8- Microwave processing, SPS, flash sintering, high pressure assisted sintering, II

Room: Flagler A

Session Chairs: Lingfeng He, North Carolina State University; Narsingh Singh, University of Maryland Baltimore County

#### 2:30 PM

# (ICACC-S8-003-2025) High pressure sintering of ultra-high temperature ceramics (Invited)

W. Ji\*1

1. Wuhan University of Technology, China

High pressure sintering technology is one of the most important research scopes for advanced new ceramic materials. It can not only resolve the contradiction between high density and fine grain structure during ceramic sintering, but also lead to unique microstructure and fantastic properties. In traditional sintering theory, atomic diffusion is considered as the dominate densification mechanism in pressure sintering. But in our study, it has been found that the plastic deformation and creep etc. caused by high pressure could dramatically improve the densification. The related unique microstructure could contribute to the high properties such as hardness and strength. Based on the new phenomenon, we investigated the densification behavior, microstructure evolution and properties of typical ceramics under different pressure scales. Combined with the modeling results, the dominate densification mechanism of high pressure sintering technology, and the relationship between dominate sintering mechanism and properties were studied.

#### 3:20 PM

#### (ICACC-S8-004-2025) Highly Textured Thermoelectric Materials by SPS Treatment of Electrospun Nanoribbons (Invited)

- G. Grader\*<sup>1</sup>; I. Maor<sup>1</sup>; A. Karlin<sup>1</sup>; K. Kruppa<sup>2</sup>; M. Mann-Lahav<sup>1</sup>; G. E. Shter<sup>1</sup>; A. Feldhoff<sup>3</sup>
- 1. Technion Israel Institute of Technology, Chemical Engineering, Israel
- 2. Leibniz Universitat Hannover, Germany
- 3. Leibniz University Hannover, Institute of Physical Chemistry and Electrochemistry, Germany

Misfit-layered calcium cobaltite [Ca2CoO3-6]0.62[CoO2] (CCO) is an outstanding p-type semiconducting thermoelectric with strong anisotropic properties. Texturing this material enhances its thermoelectric performance. The in-plane orientation of the grains improves the Seebeck coefficient and electrical conductivity, while the multi-scale parallel interfaces scatter phonons and reduce thermal conductivity. This talk will describe the synthesis of high-performance polycrystalline CCO ceramic by electrospinning of nanoribbons, followed by dual compaction process using spark plasma sintering (SPS) and edge-free spark plasma texturing. The combination of nanoribbon electrospinning and this multi-stage sintering technique was employed for the first time and resulted in exceptionally well-textured thermoelectric ceramics with excellent thermoelectric properties. At 1073 K, the ceramic exhibited an electrical conductivity of 268 S cm<sup>-1</sup>, a Seebeck coefficient of 247  $\mu$ V K<sup>-1</sup> and a heat conductivity of 3.3 W m<sup>-1</sup> K<sup>-1</sup>. In addition, the power factor and figure-of-merit reached enormously high values of 16.3  $\mu W$  cm  $^{\cdot 1}$  K  $^{\cdot 2}$  and 0.53, respectively. These results represent the highest thermoelectric performance reported to date not only for electrospun, polycrystalline calcium cobaltite fiber ceramics, but also for undoped polycrystalline calcium cobaltite ceramics.

#### 3:50 PM

# (ICACC-S8-005-2025) Spark plasma sintered $B_4C$ -SiC composites: Effect of sintering additives on mechanical and wear properties (Invited)

S. Jamale<sup>1</sup>; B. Kumar<sup>\*1</sup>

1. Indian Institute of Technology Roorkee, Metallurgical and Materials Engineering, India

The applicability of  $B_4C$  ceramics for structural and wear resistance components is restricted primarily due to processing challenges and limited understanding of mechanical and wear behavior. The present study consolidated  $B_4C$ , 10 wt% SiC and (0 & 6 wt%)  $Al_2O_3$ - $Y_2O_3$ powder mixtures by spark plasma sintering at 1600 – 1800 °C in argon atmosphere. A relative density of ~99% is obtained for the composites after sintering at 1600 °C due to liquid phase formation. Crack deflection, bridging and spitting increased fracture toughness. TEM analysis corroborated the absence of amorphous grain boundary phases. The material loss in sliding wear contacts against SiC is high for the composites sintered with  $Y_2O_3$  additives. The results highlight the influence of liquid phase precipitate composition on fracture and wear of  $B_4C$ -SiC composites.

#### 4:20 PM

# (ICACC-S8-006-2025) Enhancement of plastic deformability in ceramics by introducing refined fibrous eutectic microstructure

- Y. Aoki\*<sup>1</sup>; H. Masuda<sup>1</sup>; E. Tochigi<sup>2</sup>; H. Yohha<sup>1</sup>
- 1. Tokyo Daigaku Daigakuin Kolakukei Kenkyuka Kogakubu, Department of Materials Scient Aaud Engineering, Japan
- 2. Tokyo Daigaku Daigakuin Kogakukei Kenkyuka Kogakubu, Institute of Industrial Science, Japan

The inherent brittleness of high-strength ceramic materials has limited their application as structural materials. It has been recently reported that intrinsically brittle intermetallic or ceramic phase in fine lamellar eutectic composites with metal phase can exhibit microscopic plastic deformation at room temperature. Fine eutectic microstructure may improve plastic deformability of brittle material. Here, we demonstrated that Al<sub>2</sub>O<sub>3</sub>-GAP eutectic with the interphase distance of about 170 nm can show microscopic plastic deformation at room temperature. Al<sub>2</sub>O<sub>3</sub>-GAP eutectic sample with submicron-scale fibrous microstructure was produced by flash sintering technique, and then micropillars of Al<sub>2</sub>O<sub>3</sub> or GAP single crystal and the eutectic with a diameter of 1-2 µm and aspect ratio of 2.5 were obtained by FIB. Micropillar compression tests were performed at 25°C at a strain rate of  $1 \times 10^{-3}$  s<sup>-1</sup> using a nanoindenter. The Al<sub>2</sub>O<sub>3</sub>-GAP eutectic micropillars showed plastic deformation of up to 5%, while the Al<sub>2</sub>O<sub>3</sub> or GAP single-crystal micropillars exhibited brittle fracture. The TEM observation of the deformed eutectic pillar revealed the activity of basal slip in Al<sub>2</sub>O<sub>3</sub>, which is usually inactive at room temperature. The result implies that plastic deformation owing to the unusual dislocation activity can be triggered in the high-strength ceramics by refining eutectic microstructure.

#### 4:40 PM

## (ICACC-S8-008-2025) Finite Element Modelling of zirconium nitride flash sintering

R. Sabroj\*1; A. Durygin2; Z. Cheng1

- 1. Colorado State University, School of Materials Science and Engineering, USA
- 2. Florida International University, Mechanical and Materials Engineering, USA

Flash Sintering (FS) is a comparatively new technique for rapid densification of materials at significantly lower ambient temperatures. In FS, controlled voltage is applied directly across the sample and joule heating leads to sample temperature increase. Therefore, for materials whose electrical conductivity increases with temperature, under controlled voltage, the increased conductivity due to joule heating induces further increase in power dissipation.

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This snowball effect eventually leads to a surge in current or flash at a certain point and the sample sinters within a short period of time (minutes or seconds). However, for highly conductive and high-temperature ceramics like zirconium nitride (ZrN), their bulk electrical conductivity drops with temperature like metals, yet FS has successfully been demonstrated. In this work, a Finite Element Model (FEM) is developed using COMSOL Multiphysics 6.0 to understand the effects of various parameters such as DC voltage and mode of application (constant or linearly ramping), electrode material choice (graphite or molybdenum), pressure, thermal insulation, sample size, and sample conductivity with its dependence on temperature on FS behavior of ZrN. The results will be presented and the implications to the understanding of FS mechanism of ZrN like materials, will be discussed.

# <u>S9 Porous Ceramics Novel Developments and Applications</u>

# **S9-** Porous Ceramics- Novel Developments and Applications

Room: Ballroom 1-2

Session Chairs: Tobias Fey, Friedrich-Alexander University Erlangen-Nürnberg; Benoit Nait-Ali, Universite de Limoges

#### 1:30 PM

#### (ICACC-S9-001-2025) Study of Preparation and Performance of Porous/Dense Silicon Nitride Composite Structure for Hip Joint (Invited)

J. Yang\*<sup>1</sup>; F. Li<sup>1</sup>

1. Xi'an Jiaotong University, China

 $Si_3N_4$  material exhibits excellent biocompatibility, and stable chemical and physical properties, promising significant application in hip arthroplasty and orthopedic fields. The surface of artificial acetabular cup adopts a porous structure design, which facilitates inward bone growth and stable integration of the prosthesis. The interior is of dense structure coordinate with the liner and femoral head. In this study porous/dense composite  $Si_3N_4$  ceramic materials is prepared through the combination of in-situ solidification molding and template method. Based on the in-situ polymerization of organic monomers to achieve net size shaping, the preparation processes of dense  $Si_3N_4$  and porous  $Si_3N_4$  were investigated separately. The effects of sintering aid content and solid content on dense  $Si_3N_4$ , the effects of solid content and template holding time on porous  $Si_3N_4$ were explored. Ultimately, successful preparation of porous/dense composite  $Si_3N_4$  ceramic materials was achieved.

#### 2:00 PM

#### (ICACC-S9-002-2025) Design and Development of Biomassbased Foams for Multifunctional Applications

J. Zhang<sup>1</sup>; S. Gupta<sup>\*1</sup>

1. University of North Dakota, Mechanical Engineering, USA

Biomass is a vital but underutilized resource for manufacturing functional materials. In this presentation, we will novel manufacturing methods for fabricating porous materials from biomass. Intially, as a design paradigm - the proximate analysis of different biomass samples will be performed. Therafter, by using a customized pyrloysis process different types of tailored compositions will be fabricated with engineered porosity. Finallly, the mechanical and microstructural behavior of the biofoams will be documented for different functional applications.

#### 2:20 PM

(ICACC-S9-003-2025) In-situ formation of the microporosity of polymer-derived ceramics to stimulate superior OER activity of confined non-noble metal nanoparticles

S. Bernard\*<sup>1</sup>

1. CNRS, IRCER, France

The recent development of anion exchange membrane materials has led to the emergence of the anion exchange membrane electrolysers allowing the use of non-noble transition metals in the composition of catalysts for hydrogen (HER) and oxygen (OER) evolution reactions in alkaline media. However, their nanoscale synthesis is highly challenging to limit the overpotential, particularly at the anode (OER). The PDC (Polymer Derived Ceramics) route is a non-conventional way of designing ceramics by using preceramic polymers as precursors. The coordination (or direct reaction) of these precursors with metal complexes via the functional groups and/or ligands of the polymer makes it possible to trap transition metal nanoparticles in a micro-/mesoporous PDC matrix upon pyrolysis at low temperature. By considering the fact that preceramic polymers display an intrinsic ability to in-situ form and maintain a micropores range at low temperature pyrolysis, these metal nanoparticles become accessible while overcoming their stability issue during the catalysis process. Besides, the activity and selectivity can be simultaneously enhanced by taking advantage of the synergy between the metal nanoparticles and the encapsulating materials. This will be the content of this presentation that will introduce our very recent works on this topic.

# **S9-** Porous Ceramics- Novel Developments and Applications

Room: Ballroom 1-2

Session Chairs: Swantje Funk, Friedrich-Alexander-Universität Erlangen-Nürnberg; Michelle Weichelt, Friedrich-Alexander-Universität Erlangen-Nürnberg

#### 3:20 PM

## (ICACC-S9-004-2025) 2D-material engineered porous architectures for functional applications (Invited)

V. Brune<sup>1</sup>; T. Fischer<sup>\*1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Institute of Inorganic Chemistry, Germany

Due to their variable pore sizes and structural characteristics, porous materials have been utilized in diverse catalytic and sensing applications. Porous ceramic structures have been functionalized with layered 2D materials, which possess a high active catalytic surface area, to enhance performance. The outstanding properties of van der Waals (vdW) 2D transition metal chalcogenide-based materials, which show tunable and well-defined crystallographic structures and elemental compositions, offer a broad portfolio of exciting characteristics for catalytic applications, particularly in next-generation energy harvesting. The lack of control over the large-scale and homogeneous formation of 2D layered materials such as  $MX_2$  (M = transition metal, X = S, Se) in commercial production processes has motivated us to develop a simple synthetic approach using unique molecular building blocks for the fabrication of layered 2D materials. Molecular control enables the formation of binary compounds (MS, MSe, MS<sub>2</sub>, MSe<sub>2</sub>) with outstanding properties and well-defined formation pathways, enhancing the functional properties of modern 2D materials. Herein, we present 2D material-engineered porous architectures with enhanced catalytic properties for functional applications.

#### 3:50 PM

#### (ICACC-S9-005-2025) Fabrication of calcium phosphate-based composite porous scaffolds with unidirectional oriented pores using freeze-drying method

Y. Zusho\*1; S. Kobayashi2; T. Yokozeki1

- 1. Tokyo Daigaku, Department of Aeronautics and Astronautics, Japan
- 2. Tokyo Metropolitan University, Mechanical Engineering, Japan

In the development of artificial bones, the demand for porous scaffolds that can be quickly integrated with living bones is increasing. The freeze-drying method is used to achieve high porosity and unidirectional pore orientation to enhance cell penetration and meet biological requirements. Calcium phosphate ceramics have attracted significant attention as scaffold materials owing to their high osteogenesis, but it is difficult to meet the mechanical requirements of a single material. In this study, we fabricated a novel high-performance scaffold with excellent biological and mechanical properties by compositing it with different types of ceramics, such as alumina and silicon carbide. The sintering process is particularly important for the fabrication of ceramic composites. We established a method for fabricating ceramic composites by optimizing the addition ratio of each ceramic and the sintering conditions.

#### 4:10 PM

#### (ICACC-S9-006-2025) Optimization of Granulation for Improved Ceramic-Microsphere Composites Using Bio-Based Binders for Diverse Applications

A. De<sup>1</sup>; M. Jonsson<sup>2</sup>; F. Akhtar<sup>\*1</sup>

1. Lulea University of Technology, Division of Materials Science, Sweden

2. Nouryon Pulp and Performance AB, Sweden

This study focused on optimizing the co-granulation of powdered  $\alpha$ -alumina and nano-silica with expanded hollow microspheres (EHMs) using bio-based binders in a high-shear wet granulator. The objective was to develop a sustainable composite material with enhanced properties for thermal insulation and other applications. Various binders, including sucrose, chitosan, and cellulose nanocrystals, were evaluated while maintaining consistent granulation parameters to achieve granules with improved mechanical strength and optimal pore size distribution. The granules were analyzed for shape, size distribution, flowability, compressive strength, and thermal conductivity. Sucrose was the most effective binder, producing granules with good uniformity, flowability, and mechanical strength. Postcalcinated alumina granules exhibited high porosity and impressive compressive strength (~350 kPa at 13% strain), while silica granules demonstrated exceptionally low thermal conductivity (~0.03 W/m.K). These properties indicate suitability for catalyst support and energyefficient insulation applications. The findings highlight the potential of these composite materials for advanced uses, suggesting that future research should focus on optimizing the ceramics-to-EHMs ratio and binder concentrations to enhance performance and scalability for industrial applications further.

#### 4:30 PM

#### (ICACC-S9-007-2025) Automating the Future: High-Throughput Production of Porous Alumina Ceramics

E. Wolf<sup>1</sup>; K. G. Webber<sup>1</sup>; T. Fey\*<sup>1</sup>

1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

The high-throughput (HT) method, characterized by automated sample preparation and analysis, is already well established in the pharmaceutical and chemical fields. However, its application in materials science, especially in ceramics research, remains limited. Key areas in ceramics research that would greatly benefit from the use of HT processing are the analysis of phase diagrams or the evaluation of the relationship between microstructure and properties in porous ceramics. We present the first step toward automated processing of porous ceramics using the sacrificial templating method, using an automatic powder dispensing robot to improve accuracy and reduce manual work. Porous alumina ceramics with different porosities, pore geometries and sizes were successfully fabricated using different organic pore builders. Precise dosing enabled fine tuning of porosities, resulting in highly tunable mechanical and thermal properties. The microstructure was analyzed using  $\mu$ -CT technique to characterize pore shape, connectivity and size. Real structure models for mechanical FEM simulations were derived from the  $\mu$ CT measurements. These models were in agreement with the mechanical compression tests. Our results highlight the significant potential of high-throughput methods in advancing porous ceramic research, offering opportunities for increased efficiency and precision in material characterization and development.

#### 4:50 PM

## (ICACC-S9-008-2025) Thermal conductivity of porous ceramics: role of microstructure and environmental conditions (Invited)

B. Nait-Ali\*1; A. Alzina1; J. Bourret1; D. S. Smith1

1. Universite de Limoges, IRCER, France

Thermal conductivity of porous ceramics is a key property in various applications and fabrication processes. This property is strongly influenced by microstructural factors such as grain and pore size, pore volume fraction and spatial arrangement. Moreover, the orientation of anisometric pores, which can be influenced during processing, can lead to anisotropic behaviour that could be exploited in heat management. In addition to microstructural factors, the thermal conductivity of porous ceramics is also influenced by environmental conditions. Temperature affects both the conductivity of the solid phase and that of the gas. Furthermore, at elevated temperatures, a radiative contribution may come into play, becoming particularly significant in ceramics with high porosity. Relative humidity can also influence thermal conductivity. When placed in humid atmospheres, porous ceramics take up water which increases the material's ability to conduct heat. All these microstructural and environmental factors were investigated through experimental measurements on oxide ceramics, such as alumina and zirconia, two materials widely used in the ceramic industry. Analytical relations were applied to predict the experimental behaviour and further understand the role of each individual parameter. This approach provides insight for optimising ceramic microstructures for specific heat management applications.

### S12 Design and Applications of Nanolaminated MAX and MAB Phases Solid Solutions and 2D Counterparts

#### S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and 2D Counterparts

Room: Ponce de Leon

Session Chair: Miladin Radovic, Texas A&M University

#### 1:30 PM

#### (ICACC-S12-001-2025) Beyond MXenes: Quantum Confined 1D Titania-based Nanomaterials, Their Diverse Morphologies and Exceptional (Invited)

M. Barsoum<sup>\*1</sup>

1. Drexel University, Materials Science and Engineering, USA

Recently, we converted 15 binary and ternary titanium carbides, nitrides, borides, phosphides, and silicides into lepidocrocite-based, one dimensional, 1D, sub-nanometer nanofilaments, NFs,  $\approx$  5x7 Å<sup>2</sup> in cross-section by reacting them with a tetramethylammonium hydroxide, TMAH, aqueous solution at  $\approx$  85 °C range for tens of

hours. If the 5x7 Å<sup>2</sup> NFs were placed end to end they would span 600 million kms. In some cases, the conversion is 100 % precluding the need for centrifuges, filters, etc. We currently make 100 g batches in a lab setting. Depending on with what, and the order, the reaction products are washed, the 1D NFs self-assemble into loose, spaghettishaped fibers,  $\approx 30$  nm in diameter, fully inorganic TiO<sub>2</sub> gels, pseudo 2D sheets or porous mesoscopic particles. In all cases, the fundamental building block is 1D lepidocrocite NFs, ≈ 3 nm long, that self-assemble into the aforementioned morphologies. At this time, we believe our materials are the only thermodynamically stable 1D NFs in water, with important implications in photo- and chemical catalysis and water remediation. The production of hydrogen for times of the order of 6 months with production rates an order of magnitude higher than P25, will be discussed. The adsorption of cations like uranium, thorium and cationic dyes by the 1D NFs, that in some cases outperform high adsorption clays will also be discussed.

#### 2:00 PM

## (ICACC-S12-002-2025) Complex magnetism of bulk MAX phases (Invited)

C. Birkel<sup>\*1</sup>; N. Kubitza<sup>2</sup>; S. Kale<sup>1</sup>

1. Arizona State University, USA

2. Technical University Darmstadt, Eduard-Zintl-Institute, Germany

MAX phases - ternary transition metal-based carbides, nitrides and carbonitrides - are a large, and growing, family of layered solids. Their general composition is  $M_{n+}1AX_n$ , with n mostly being 1 (211 MAX phase), 2 (312 MAX phase) and 3 (413 MAX phase). There is a large variety of the elements, but the M element is typically an early-to-mid transition metal, A is a main group element (or late transition metal), and X is carbon and/or nitrogen. What are not a very common M elements are "magnetic" elements, such as manganese, iron and cobalt, because these elements form very thermodynamically stable antiperovskite structures that inhibit the formation of MAX phase structures, at least in bulk materials. In this talk, I will discuss our work on the synthesis of (potentially) magnetic MAX phases that are mainly based on chromium as the M element. We have developed different non-conventional preparation techniques, i.e based on microwave heating and sol-gel chemistry, to access new types of MAX phases. We characterize their structure and chemical composition in detail by a variety of diffraction, spectroscopy and microscopy techniques. The magnetic characterization reveals complex magnetic properties, for example in  $(V_{1-x}Cr_x)_2$ GaC, as well as tunable behavior as demonstrated for carbonitrides (such as Cr<sub>2</sub>GaC<sub>1-x</sub>N<sub>x</sub>) and Nb<sub>2</sub>SnC MAX phases that contain non-conventional A elements (e.g. V, Cr, and more).

#### 2:30 PM

# (ICACC-S12-003-2025) Processing of chemically complex MAX phases and their 2D derivatives (MXenes) (Invited)

N. Goossens\*1; K. Lambrinou2; J. Vleugels3

- 1. Empa, High Performance Ceramics, Switzerland
- 2. University of Huddersfield, School of Computing and Engineering, United Kingdom
- 3. Katholieke Universiteit Leuven Departement Materiaalkunde, Belgium

MXenes are electrically conductive nanometric 2D sheet-like transition metal carbides/nitrides, resulting from the chemical exfoliation of 3D nanolaminated  $M_{n+1}AX_n$  (MAX) phases. The precursor MAX phases are described by the  $M_{n+1}AX_n$  general stoichiometry, where M is an early transition metal, A is an A-group element, X is C and/ or N, and n = 1-4. Their broadly tunable structure and composition endows both MAX phases and their MXene derivatives with tailorable properties, which are gratefully exploited in application-oriented materials design. However, the quest for high-performance MXenebased devices is impaired by the challenging synthesis of adequate, etchable MAX phase precursors. The key towards highly pure MAX phase production encompasses careful lattice distortion balancing via meticulous unit cell engineering. This study elucidates the stabilizing effect of (chemically complex) solid solutioning on the M- and A-site for challenging MAX phase chemistries and addresses the adverse practical implications of inadequate processing conditions on the formation mechanism and final properties of the resulting MAX phase ceramics. Smart solid solution design holds immense potential for producing high-purity MAX phase ceramics under strongly restrictive compositional constraints, paving the road towards truly tailorable chemistry, purity, and properties in both MAX phases and their respective MXenes.

#### S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and 2D Counterparts

Room: Ponce de Leon

Session Chairs: Babak Anasori, Purdue University; Thierry Cabioch, University of Poitiers

#### 3:20 PM

(ICACC-S12-004-2025) Synthesis and characterization of ternary nanolaminated Carbide:  $Ti_2NbAlC_{1.82}$  and  $TiNbAlC_{0.91}$  (Invited)

S. Dubois\*1; T. Cabioch1; V. Gauthier1; P. Chartier1

1. PPRIME Institute, France

We report on the synthesis of  $[Ti_{1.x}Nb_x]_{n+1}AlC_n$  (MAX phases) by hot isostatic pressing starting with sub-stoechiometric titanium carbide, niobium and aluminum powders. In addition to a few TiC impurity, new 312 and 211 MAX phases, Ti<sub>2</sub>NbAlC<sub>1.82</sub> and TiNbAlC<sub>0.91</sub> are formed. The influence of the synthesis temperature is discussed as phases are only formed at high temperature whereas TiAl<sub>3</sub> impurities are present at quite low temperature. Its lattice parameters and Nb, Ti contents, deduced from Rietveld analysis of x-ray diffraction patterns and EDX analysis, are determined.

#### 3:50 PM

## (ICACC-S12-005-2025) Stability and Properties of MAX Phases with Compositionally Complex M-layers

M. Dujovic<sup>\*1</sup>; Z. Tan<sup>1</sup>; A. Srivastava<sup>2</sup>; M. Radovic<sup>1</sup>

- 1. Texas A&M University, Materials Science and Engineering (MSEN), USA
- 2. Texas A&M University, USA

This work focuses on MAX phase ternary carbides with chemical formula M2AlC where M is either Cr, Ti, Ta, V, Nb or a combination of them. Specifically, we focus on synthesizing M<sub>2</sub>AlC phases with two to five elements on M-site in equiatomic ratios starting from single M-element M<sub>2</sub>AlC. This approach for synthesizing MAX phases with compositionally complex M-layers is selected to avoid the formation of intermediate phases in the final microstructure due to possible incomplete reaction of elemental powders. While equiatomic M-element ratios are considered to (theoretically) maximize configurational entropy and, hence their stability. Our results show that out of 26 compositionally complex M2AlC examined in this study, only a few are found to be phase pure, while only one of them with four elements in the M-layers is entropy stabilized. Furthermore, the mechanical testing of these compositionally complex M<sub>2</sub>AlC suggests that the solid solution strengthening effect is not always dominant.

### 4:10 PM

## (ICACC-S12-006-2025) Synthesis of Ti-Si-C MAX-based materials via advanced reactive PVD techniques

A. Gitschthaler<sup>2</sup>; P. Doerflinger<sup>2</sup>; R. Hahn<sup>2</sup>; T. Wojcik<sup>2</sup>; J. Ramm<sup>3</sup>; C. Jerg<sup>3</sup>; S. Kolozsvári<sup>4</sup>; P. Polcik<sup>4</sup>; E. Ntemou<sup>5</sup>; D. Primetzhofer<sup>5</sup>; H. Riedl<sup>\*1</sup>

- 1. Technische Universitat Wien, Institute of Materials Science and Technology, Austria
- 2. Technische Universitat Wien, Christian Doppler Laboratory for Surface Engineering of high-performance Components, Austria
- 3. Oerlikon Surface Solutions AG, Switzerland
- 4. Plansee Composite Materials GmbH, Germany
- 5. Uppsala Universitet, Department of Physics and Astronomy, Sweden

MAX phases are nanolaminated compounds that traditionally follow the  $M_{n+1}AX_n$  (n = 1, 2 or 3) stoichiometry notation, comprising an early transition-metal (M), an A-group element (A) and carbon and/or nitrogen (X). Due to their layered structure and unusual interatomic bonding, they exhibit a unique combination of metallic and ceramic properties, combining high electrical and thermal conductivity with excellent oxidation and corrosion resistance. The synthesis, including different methods, still needs to be improved and heavily researched, as there is a discrepancy between theoretically predicted MAX phases and experimentally confirmed ones. Especially for the synthesis via PVD techniques, the extreme kinetic conditions far off thermodynamic equilibrium can be concurrently beneficial but also limiting in the phase formation. In more detail, the elevated temperatures required during PVD remain a significant problem, hindering a broad practical application of MAX phases as protective and functional coatings for next-generation technologies. Regarding this issue, cathodic arc evaporation and HiPIMS have great potential due to their high ionization degree. Thus, a variety of Ti-Si-C films have been grown in reactive plasma atmospheres by these advanced techniques and subsequently analyzed using a set of high-resolution techniques, including ERDA, RBS, HR-TEM, t-EBSD, SAED, and X-ray nano diffraction.

### 4:30 PM

### (ICACC-S12-007-2025) Super-MAX: On the Journey Towards Triple-site Solid-solutions of MAX Phases

I. Huck\*1; C. Birkel2

- 1. Technische Universitat Darmstadt, Chemistry, Germany
- 2. Arizona State University, USA

In the last years, the family of MAX phases has been growing rapidly to over 300 different compounds, whereof roughly half the compounds are solid-solutions. Amongst them, solid-solution phases with mixing on the X-site are considerably underrepresented and only few phases exhibit elemental mixing on more than one lattice site at a time. Here, we introduce a new solid-solution MAX phase by incorporating additional elements on all three lattice sites: a Super-MAX phase with the general formula  $(M_{1-x}M'_x)_2(A_{1-y}A'_y)(X_{1-z}X'_z)$ . While carbides can be readily synthesized from the respective elements, the synthesis of nitrides and carbonitrides often requires the use of precursors due to the gaseous nature and high stability of elemental nitrogen. Therefore, in a first step, binary nitride precursors were synthesized by non-conventional microwave-assisted heating. The subsequent formation of the triple-site MAX phase solid-solution is conducted by either using microwave heating or conventional furnace heating. We show  $(V_{1-x}Cr_x)_2(Ga_{1-y}Ge_y)(C_{1-z}N_z)$  as a first example of a Super-MAX phase. Refined lattice parameters show the expected distortion of the crystal structure by introducing elements of different atom sizes. Element-specific measurements further proof the formation of the new Super-MAX phase. Its initial magnetic properties hold promise on the journey towards long-range magnetic ordered bulk MAX phases.

### 4:50 PM

# (ICACC-S12-008-2025) Impact of MAX-Phases on fibre materials for electro-chemical cells

F. Jung\*1; M. Mazurkiewicz-Pawlicka2; L. Aretz3

- 1. RWTH Aachen University, Institut für Textiltechnik, Germany
- 2. Politechnika Warszawska, Faculty of Chemical and Process Engineering, Poland
- 3. GHI RWTH Aachen University, Germany

MAX phase ceramics, a class of materials that combine both metallic and ceramic properties, offer significant potential for applications in electrochemical cells. Their unique characteristics, such as self-healing and resistance to corrosive environments, make them particularly promising as fiber coatings in carbon fiber-reinforced composites. Within an interdisciplinary research project, RWTH an WUT investigate the integration of MAX phase ceramics with carbon fibers in critical fuel cell components, including gas diffusion layers (GDLs), electrodes, and membranes. Specifically, the research aims to enhance the fatigue strength of these components through the use of MAX phases. Preliminary results suggest significant improvements in durability and functionality, highlighting the potential of this material combination for future energy systems. The presentation will discuss the potential of the metal-ceramic MAX-Phase material for electrochemical cells.

## **<u>S14 Crystalline Materials for Electrical</u> <u>Optical and Medical Applications</u>**

### **S14- Optical Material I**

Room: Coquina A

Session Chairs: Luisa Bausa, Universidad Autonoma de Madrid; Kiyoshi Shimamura, National Institute for Materials Science

### 1:30 PM

## (ICACC-S14-001-2025) Lasing behavior of non-cubic fluorapatite (FAP) ceramics with nanocrystalline grains (Invited)

H. Furuse\*1; K. Takimoto2; S. Nakamura3; H. Sone2

- 1. National Institute for Materials Science (NIMS), Japan
- 2. Kitami Institute of Technology, Japan
- 3. Ibaraki University, Japan

We have studied the optical and laser properties of hexagonal Nd- or Yb-doped fluorapatite transparent ceramics with randomly oriented nanocrystalline grains. For Nd-doped materials, we investigated the laser oscillation at 1.0 and 1.3  $\mu$ m wavelengths for both FAP and S-FAP. For Yb:FAP, the temporal waveform of the laser power and the beam profile were measured. The maximum slope efficiency was over 10%, which is the highest slope efficiency for non-cubic ceramic materials. In the presentation, the details in both materials and output properties including microstructure, crystal structure, fluorescence properties and laser properties will be explained.

### 2:00 PM

## (ICACC-S14-002-2025) Self Q-Switched Transparent Ceramic Laser Rods

R. Osborne<sup>\*1</sup>; N. Cherepy<sup>2</sup>; A. Drobshoff<sup>1</sup>; S. A. Payne<sup>1</sup>

- 1. Lawrence Livermore National Laboratory, USA
- 2. Lawrence Livermore National Lab, Chemistry and Materials Science, USA

Combining transparent ceramics with additive manufacturing enables the fabrication of laser gain media with controlled doping profiles, such as planar and channel waveguides and laser rods with undoped endcaps and cladding. Self Q-switched Nd,Cr:YAG laser rods have been fabricated via additive manufacturing. Characterization of the rods, including their laser performance will be presented.

### 2:20 PM

### (ICACC-S14-003-2025) Development of Flexible Ceramics Films on Plastics Using Photo-Reaction Processes

T. Tsuchiya\*1

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

In recent years, the development of wearable devices has become a pressing issue in the development of an IoT society. Metal oxides have a wide variety of functions and have been used in sensors and electronic devices, but due to the high-temperature processes involved, it is difficult to form films on plastic substrates. To solve this problem, this research used photochemical reactions using excimer lasers to achieve low-temperature crystallisation of ITO transparent conductive films, as well as low resistance and work function control, and developed high-brightness OLEDs on plastic substrates. Furthermore, optical thin films such as VO<sub>2</sub>, ITO, and TiO<sub>2</sub> were created on polycarbonate, and the results of a weather resistance survey showed that the functionality and durability were improved by the photo-induced ceramic coating.

### 2:40 PM

## (ICACC-S14-004-2025) Prevention of Carbon Contamination in Yttria Sintered via SPS

J. Gild\*<sup>1</sup>; L. Backman<sup>2</sup>; A. R. Floyd<sup>1</sup>; B. Sadowski<sup>3</sup>; W. Kim<sup>1</sup>; S. Bayya<sup>1</sup>; J. Sanghera<sup>1</sup>

- 1. US Naval Research Laboratory, Optical Materials, USA
- 2. US Naval Research Laboratory, Spacecraft Engineering Division, USA
- 3. Jacobs Engineering, USA

There are numerous applications operating in very harsh environments that require rugged windows. Polycrystalline Y2O3 ceramic is a prime candidate for these applications due to the potentially high mechanical strength, wide transmission range of  $0.2 - 9 \,\mu m$ , high thermal conductivity of 14 W/mK, and isotropic structure. Y2O3 fabricated by Spark Plasma Sintering (SPS) has the potential to have fine grain sizes and rapid fabrication. Carbon contamination, however, is noted for oxide materials sintered via SPS due to the graphite tooling. In the present work, a variety of 25-50 µm thick metallic foils are utilized to prevent carbon contamination in the final specimen. The carbon contamination was examined as carboxylate absorption bands between 6 and 7 micron wavelength region. Ta foil was found to be superior to all other metals as a carbon blocker for improved transmission of the ceramic in both visible and infrared (IR). Inexpensive and thin foils of metals such as Ti and Zr proved suitable for IR transmission in materials where visible transmission is limited by structure or scattering from multiple phases such as 3YSZ or Y2O3-MgO composites.

### 3:20 PM

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## (ICACC-S14-005-2025) Nonlinear Optical Properties of 2D-Ferroelectric Heterostructures (Invited)

M. Ramirez\*<sup>1</sup>; D. Hernández-Pinilla<sup>1</sup>; G. Lopez-Polin<sup>1</sup>; J. Gomez-Herrero<sup>1</sup>; L. E. Bausa<sup>1</sup>

1. Universidad Autonoma de Madrid, Fisica de Materiales & IFIMAC, Spain

Second-harmonic generation (SHG) is a non-linear optical process that involves the conversion of two photons of same energy into a single photon of twice their energy. Efficient SHG occurs for crystals with broken inversion symmetry, such as transition metal dichalcogenide monolayers. Here we show the possibility of spatially tuning the non-linear optical response a monolayer  $MOS_2$  deposited on the polar surface of a periodically poled Lithium Niobate crystal. The modulation relies on the unique ability to modify the physical properties of ultrathin 2D materials through the underlying spontaneous polarization. Different factors affecting SHG such as the fundamental wavelength, pump power and polarization of the incident light will be discussed with particular emphasis on the role of light induced interfacial charge-transfer processes in 2D based ferroelectric heterostructures.

#### 3:50 PM

## (ICACC-S14-006-2025) Integration of Ferroelectrics and 2D Materials for Nanophotonics (Invited)

L. E. Bausa\*1; J. Fernandez Martinez<sup>2</sup>; D. Hernández-Pinilla<sup>2</sup>; D. Gallego<sup>2</sup>;

- P. Molina<sup>2</sup>; P. Ares<sup>2</sup>; J. Gomez-Herrero<sup>2</sup>; M. Ramirez<sup>1</sup>
- 1. Universidad Autonoma de Madrid, Fisica de Materiales & IFIMAC, Spain
- 2. Universidad Autonoma de Madrid, Física de la Materia Condensada & IFIMAC, Spain

The combination of 2D materials with ferroelectrics offers a powerful method for tailoring the optoelectronic properties of atomically thin Transition Metal Dichalcogenides (TMDs). In particular, our research delves into the dual influence of ferroelectricity and light on the optoelectronic behavior of monolayer (1L) MoS<sub>2</sub> placed on a periodically poled lithium niobate crystal. Through scanning micro-photoluminescence, we explore how excitation intensity, and ferroelectric domain walls affect the photoluminescence characteristics of 1L-MoS<sub>2</sub>. Our results identify a light-induced charging mechanism that varies with the orientation of ferroelectric domains and facilitates charge generation and transfer at the monolayersubstrate interface. Moreover, our findings shed light on the influence of intense, nanoscale-confined electric fields at the surfaces of LiNbO3 domain walls, demonstrating the ability to precisely control charge carriers in MoS<sub>2</sub>. This capability allows for the creation of deterministic p-n homojunctions with an unprecedented level of control. These insights open new possibilities for the development of advanced optoelectronic and photonic devices that integrate monolayer TMDs, exploiting the synergy between light-matter interactions and the surface selectivity afforded by ferroelectric domain architectures.

### 4:20 PM

### (ICACC-S14-007-2025) New Applications of Ceramic Phosphor Materials in LEDs and Lasers (Invited)

H. Menkara\*1

1. PhosphorTech, USA

Nearly all current white solid-state lighting (SSL) systems used for general illumination are based on the phosphor converted LED (pcLED) architecture, which offers a practical and mass producible structure for white light generation. Various ceramic phosphors are also being used to convert high energy ultraviolet/visible (UV/Vis) light to a wide range of wavelengths, including infrared. Laserbased SSL devices also exist and the application of laser-excited phosphor technology is now prevalent in medical applications, automobile headlights, image projection devices, even long-range flashlights. This study will present recent work on new phosphors used to convert narrow-band SSL emitters into both broadband and narrowband optical energy that cannot be achieved by LEDs alone. For example, UVA/UVB phosphors can be combined with UVC LEDs to produce full spectral coverage in the ultraviolet part of the spectrum. Similarly, near-infrared (NIR) and short-wave infrared (SWIR) phosphors can be combined with visible LEDs or lasers to produce a broadband emission throughout the infrared that can be used for a wide range of spectroscopy, medical, and hyperspectral imaging applications.

### 4:50 PM

### (ICACC-S14-008-2025) Low temperature synthesis of perovkite-QD materials using Novel Water-Assisted Solid-State Reaction method (Invited)

K. Toda\*1; W. Hikita1

1. Niigata University, Japan

In this study, we propose a novel soft chemical synthesis method, the water-assisted solid-state reaction (WASSR) method. This novel soft chemical synthesis method is very simple and can synthesize nanoparticle materials by simply storing or mixing raw materials with a small amount (typically 10wt%) of water in a reactor at low temperature below 500 K. Typical particle sizes (bellow 20 nm) of the samples prepared by the WASSR method were smaller than those (1 - 10 micrometer size) of the sample prepared by the conventional solid-state reaction method. For example, for the WASSR synthesis of the perovskite CsPbCl<sub>3</sub> quantum dot phosphor, a stoichiometric mixture of CsCl and PbCl<sub>2</sub> was mixed. Then, a small amount (10 wt%) of water was then added to the mixture and mixed with a mortar for 1 min to synthesize a single phase of CsPbCl<sub>3</sub>. The XRD pattern of the products are in good agreement with that of single phase CsPbCl<sub>3</sub>. The reaction mechanism of the WASSR method is different from a mechanochemical reaction, solution reaction, and hydrothermal reaction. he most likely mechanism is a novel water accelerated solid acid-base reaction on the surface. Our proposed low cost and low-temperature synthesis technique are promising for an industrial application in the processing of ceramic materials synthesis.

### **S18 Ultra-High Temperature Ceramics**

### **S18-** Compositionally Complex UHTCs I

Room: Coquina F

Session Chairs: Stefano Curtarolo, Duke University; Laura Silvestroni, Consiglio Nazionale delle Ricerche

### 1:30 PM

# (ICACC-S18-001-2025) From BIG-data to HOT-properties of high-entropy carbides and carbo-nitrides (Invited)

S. Curtarolo<sup>\*1</sup>

1. Duke University, Materials Science, Electrical Engineering and Physics, USA

Disordered multicomponent systems - occupying the mostly uncharted centers of phase diagrams - have been studied for the last two decades for their potential revolutionary properties. Very resilient compositions can be stabilized by maximizing entropy (configurational and/or vibrational) of (near) equimolar mixtures. The search for new systems is mostly performed with trial-anderror techniques, as effective computational discovery is challenged by the immense number of configurations: the synthesizability of high-entropy ceramics is typically assessed using ideal entropy along with the formation enthalpies from density functional theory, with simplified descriptors or machine learning methods. With respect to vibrations — even if they may have significant impact on phase stability — their contributions are drastically approximated to reduce the high computational cost, or often avoided with the hope of them being negligible, due to the technical difficulties posed in calculating them for disordered systems. In this presentation I will address many of the problems in the discovery of disordered systems, offer some data-based effective solutions, and discuss the avenues opened by the latter, especially for plasmonic-hyperbolic applications.

### 2:00 PM

### (ICACC-S18-002-2025) Strength of grain boundaries in (Ti-Zr-Nb-Hf-Ta)C + (Ti-Zr-Nb-Hf-Ta)B<sub>2</sub> high-entropy ceramics (Invited) **WITHDRAWN**

- A. Naughton Duszova<sup>\*1</sup>; M. Vojtko<sup>1</sup>; D. Medved<sup>1</sup>; O. Petruš<sup>1</sup>;
- M. Hrubovčáková<sup>1</sup>; P. Švec<sup>2</sup>; P. Hvizdoš<sup>1</sup>; J. Dusza<sup>1</sup>
- 1. Institute of Materials Research, Slovak Academy of Sciences, Slovakia
- Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia, Slovakia

Microcantilever bending, linear beam theory and micro/ nanofractography were used for the investigation of the strength of grain boundaries in recently developed (Ti<sub>0.49</sub>-Zr<sub>0.12</sub>-Nb<sub>0.13</sub>- $Hf_{0.11}-Ta_{0.15}C + (Ti_{0.82}-Zr_{0.04}-Nb_{0.08}-Hf_{0.03}-Ta_{0.03})B_2$  dual- phase high entropy ceramics. The reactive spark plasma sintered system has grain sizes of 2.2 mm and 3.4 mm of the carbide and boride phases, respectively. The majority of grain/phase boundaries show a continuous sharp ~ 1.5 nm wide segregation of Fe, Co and Ni impurities. Microcantilevers were focused ion beam milled from the carefully polished sample surface with random locations containing both carbide and boride grains and grain boundaries in the beam volume. All tested microcantilevers failed with the grain/phase boundaries as fracture origin with bending strength values from 3.8 to 7.3 GPa, depending on the location, size, orientation and character, of the boundaries. Fractographic analysis revealed that the fracture origins are mainly at the boride/carbide boundaries with average strength of 4.7 GPa, but boride/boride and carbide/carbide boundaries as fracture origins with higher strength values were detected, too.

### 2:30 PM

# (ICACC-S18-003-2025) Nb-Zr interdiffusion in a (Nb,Hf,Ta,Ti) $B_2$ -(Zr,Hf,Ta,Ti) $B_2$ high-entropy boride system

- A. Feltrin\*1; D. Lipke2; G. Hilmas2; W. Fahrenholtz1
- 1. Missouri University of Science and Technology, Materials Research Center, USA
- 2. Missouri University of Science & Technology, Materials Science & Engineering, USA

The incorporation of niobium (Nb) to high-entropy ceramics often results in a Nb-rich secondary phase, attributed to its slow diffusion rate, low solubility, or due to its different atomic size in comparison with other elements. Despite these observations, the kinetics of Nb diffusion within high-entropy ceramic systems remains unexplored. In this study, (Nb,Hf,Ta,Ti)B<sub>2</sub> and (Zr,Hf,Ta,Ti)B<sub>2</sub> high-entropy borides were synthesized by boro/carbothermal reduction of a mixture of transition metal oxides, carbon black, and boron carbide. Solid solution formation and densification of the reacted powders were done utilizing two-step spark plasma sintering at 2100 °C for 10 min. Boron carbide was added in 6 wt% excess for the (Zr,Hf,Ta,Ti)  $B_2$  and 2 wt% for the (Nb,Hf,Ta,Ti) $B_2$  resulting in materials with less than 2 vol.% oxide contamination. (Zr,Hf,Ta,Ti)B<sub>2</sub> exhibited a homogeneous solid solution, while the (Nb,Hf,Ta,Ti)B<sub>2</sub> showed Nb-enriched regions. (Nb,Hf,Ta,Ti)B<sub>2</sub>-(Zr,Hf,Ta,Ti)B<sub>2</sub> diffusion couples were heated to temperatures from 1900 °C to 2200 °C and the resulting composition profiles were analyzed to determine Nb-Zr interdiffusion coefficients and activation energies. The outcomes of this research are expected to provide a deeper understanding of the Nb kinetics in high-entropy borides.

### 2:50 PM

## (ICACC-S18-004-2025) Selective laser sintering and spark plasma sintering of compositionally complex carbide ceramics

B. Cui<sup>\*1</sup>; L. Trinh<sup>1</sup>; X. Chen<sup>1</sup>; L. Wadle<sup>1</sup>; Y. Lu<sup>1</sup>; Z. Hua<sup>2</sup>; K. Bawane<sup>2</sup>; L. Malakkal<sup>2</sup>; L. He<sup>3</sup>

- 1. University of Nebraska-Lincoln, USA
- 2. Idaho National Laboratory, USA
- 3. NC State University, USA

Two advanced manufacturing processes, spark plasma sintering (SPS) and selective laser sintering (SLS), have been developed for synthesis of (Zr,Nb,Ta,Ti,W)C compositionally complex ceramic (CCC) via reactive sintering of a powder mixture of constitute monocarbides. X-ray diffraction analysis confirmed that single-phase CCC can be formed by both SPS and SLS. While a homogenous microstructure with uniform metal element distributions was developed during SPS, three-layer microstructures with a thin TiC-rich layer and two TaC-rich layers along with a TiO<sub>2</sub>-rich surface layer containing W nanoparticles were formed during SLS. Cellular structures with W, Zr, and Ti element segregation and dislocations on cell boundaries were observed in the SLSed CCC sample, indicating the effect of non-equilibrium conditions on microstructure formation during laser melting followed by rapid cooling and solidification process. Compared to the SPSed CCC sample, the SLSed CCC showed enhanced hardness and reduced thermal conductivity, which may be related to unique cellular structures.

### 3:30 PM

### (ICACC-S18-005-2025) Aero-thermodynamic behavior of compositionally complex UHTCs in hypersonic/supersonic flows (Invited)

L. Silvestroni<sup>\*1</sup>; D. De Prisco<sup>2</sup>; R. Costanzo<sup>2</sup>; A. Cecere<sup>2</sup>; S. Mungiguerra<sup>2</sup>; R. Savino<sup>2</sup>

- 1. Consiglio Nazionale delle Ricerche, ISSMC, Italy
- 2. University of Naples Federico II, Department of Industrial Engineering, Italy

Aero-thermodynamic tests were carried out on two different ultra-high temperature ceramic (UHTC) composites based on ZrB<sub>2</sub>-SiC-TiB<sub>2</sub> and doped with NbC or VC. Hemispherical specimens with a diameter of 10 mm were exposed to subsequent hypersonic and supersonic flows of simulated air produced by an arc-jet plasma wind tunnel, at specific total enthalpies in the order of 20 MJ/kg. Different test configurations were selected, employing supersonic nozzles with different expansion area ratios (4 and 56.25, respectively), to achieve Mach numbers in the 3-6 range. Real-time surface temperatures were monitored by means of two-color pyrometer and an infrared thermocamera, and values between 1700 and 2700K achieved. One-dimensional chemical equilibrium models were used to characterize the flow field inside the test rig, to have a proper characterization of the thermo-fluid dynamic and chemical conditions in the different test configurations, including an estimation of the aero-thermodynamic loads on the specimens. Data were correlated to the microstructure evolution and oxidation mechanism.

### 4:00 PM

# (ICACC-S18-006-2025) Synthesis and Characterization of (CrMoTaVW)C\_{1+\delta} High-Entropy Carbide Ceramic

A. Sarikhani\*<sup>1</sup>; S. M. Smith<sup>2</sup>; S. Filipovic<sup>1</sup>; W. Fahrenholtz<sup>2</sup>; G. Hilmas<sup>2</sup>

- 1. Missouri University of Science and Technology, Materials Research Center, USA
- 2. Missouri University of Science & Technology, Materials Science and Engineering, USA

In recent years, high-entropy carbides (HECs) have attracted significant interest due to their exceptional physical properties. This study focuses on the synthesis and characterization of single-phase HEC ceramics with the composition (CrMoTaVW)C<sub>1+ $\delta$ </sub>. These ceramics were synthesized using commercially available metal-oxide and

carbon powders through a carbothermal reduction process. The resultant five-metal carbide powders were densified by spark plasma sintering (SPS) at varying temperatures to control grain size and microstructure. The microstructural and compositional analyses were performed using scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The face-centered cubic (FCC) crystal structure of these compositions was confirmed through X-ray diffraction (XRD), with lattice parameters determined using Rietveld refinement to compare ceramics grown under different conditions. Additionally, this work reports the electrical, thermal, and mechanical properties of these HECs synthesized under various conditions.

### 4:20 PM

## (ICACC-S18-007-2025) Arc melting of the Ti-Zr-Hf-Ta family of complex UHTC borides and carbides

A. Celik\*1; R. Haber1

1. Rutgers University, Materials Science and Engineering, USA

UHTC transition metal borides and carbides have attracted attention due to their remarkable material properties, including high melting temperature, high hardness, good strength, and chemical stability. Commercially available powders are generally limited to single-phase such as TiB<sub>2</sub>, ZrB<sub>2</sub>, HfB<sub>2</sub>, TiC, ZrC, HfC, etc. Most of the research done to date also has been on equimolar high-entropy compositions. Arc melting was utilized to fabricate both equimolar and non-equimolar solid solutions of Ti-Zr-Hf-Ta family of complex UHTC borides and carbides. Arc-melted ingots were milled down to fine powders using various comminution methods. Powder morphology, particle size distribution, particle shape and residual oxygen contents were examined through different characterization techniques.

### 4:40 PM

# (ICACC-S18-008-2025) Low Temperature Synthesis of High-Entropy Carbonitrides

S. M. Smith\*<sup>1</sup>; W. Fahrenholtz<sup>1</sup>; G. Hilmas<sup>1</sup>; S. Curtarolo<sup>2</sup>

- 1. Missouri University of Science & Technology, Materials Science and Engineering, USA
- 2. Duke University, Materials Science, Electrical Engineering and Physics, USA

Carbonitride ceramics have typically been synthesized by mixing commercial powders; yet high densification temperatures are needed to reach full solid solution. We produced three highentropy carbonitride compositions by first synthesizing a fourmetal carbide by carbothermal reduction. The resulting carbide powder was then mixed with the commercial nitride of the missing metal. (Hf, Nb, Ta, Ti, Zr)C<sub>0.8</sub>N<sub>0.2</sub>, (Hf, Mo, Ta, W, Zr)C<sub>0.8</sub>N<sub>0.2</sub>, and (Hf, Mo, Ta, Ti, V) $C_{0.8}N_{0.2}$  ceramics were finally obtained with spark plasma sintering. The densification temperatures ranged from 1850°C to 2000°C at soaking times ranging from 10-15 minutes. Scanning electron microscopy was used to examine the resulting microstructures and energy dispersive spectroscopy was used to determine the ratios of metals in the resulting ceramics. X-ray diffraction was used to determine the phases present in the reacted powders and the densified ceramics. The presentation will discuss feasibility of this synthesis route and how densification parameters affected the resulting microstructures.

### 5:00 PM

# $(ICACC\text{-}S18\text{-}009\text{-}2025) \ Phase \ evolution \ of \ SiC\text{-}based \ ceramics \\ derived \ from \ medium\text{-}entropy \ MXenes\text{-}modified \ polycarbosilane \\$

W. Li\*1; K. Lu1

1. University of Alabama at Birminghngham, USA

Polycarbosilane (PCS) precursors with an embedded mediumentropy MXenes network are produced via the polymer-derived ceramic (PDC) route. The ceramic yield of the medium-entropy MXenes-modified PCS is higher than that of pure precursor, and the shrinkage from polymer to ceramics reduces due to the incorporation of the medium-entropy MXenes which acts as a filler. Therefore, bulk medium-entropy MXenes-derived (Ti<sub>1/3</sub>Zr<sub>1/3</sub>Ta<sub>1/3</sub>)C/SiC ceramic monoliths are prepared by casting of preceramic polymers and pyrolysis. Moreover, the crystallization temperature of PCS precursors to SiC and degradation temperature of medium-entropy MXenes to (Ti<sub>1/3</sub>Zr<sub>1/3</sub>Ta<sub>1/3</sub>)C increase compared with pure precursor and single-phase MXenes due to mutual inhibition. Additionally, the obtained monolithic  $(Ti_{1/3}Zr_{1/3}Ta_{1/3})C/SiC$  ceramics show improved hardness and fracture toughness, which are much higher than SiC ceramics without the integration of MXene. The toughening mechanisms of pull-out, delamination, crack bridging, and crack deflection are characterized and clarified. This work demonstrates that medium-entropy MXenes are good reinforcements for enhancing the mechanical properties of structural ceramics, and also paves the way for the investigation of high-temperature properties of MXene-containing ceramics.

### **<u>S19 Molecular-level Processing and Chemical</u>** <u>Engineering of Functional Materials</u>

### **S19- Processing and shaping of molecular precursors I** Room: Ballroom 3

Session Chair: Peter Kroll, University of Texas, Arlington

### 1:30 PM

# (ICACC-S19-001-2025) Additive manufacturing of ceramics via sol-gel (Invited)

A. Zanini<sup>1</sup>; G. Franchin<sup>1</sup>; P. Colombo<sup>\*1</sup>

1. University of Padova, Industrial Engineering, Italy

Additive manufacturing technologies for ceramics typically rely on the use of powder-based feedstocks. This sometimes limits the possibility of successfully and accurately shaping complex components, as for instance when a significant difference in refractive index between the ceramic powders and the surrounding photocurable liquid exist in vat photopolymerization technologies, or when the size of the powders limits the minimum size of the nozzle used in extrusion-based technologies. The use of fully liquid feedstocks allows to overcome some of these limitations, while at the same time allowing to manufacture both oxide and non-oxide ceramic components. The sol-gel approach allows to obtain inorganic components by the thermal treatment of gels produced from alkoxides, even though several issues related to processing need to be overcome when shaping these materials by additive manufacturing technologies. In this lecture, examples will be provided of the fabrication of multicomponent glasses as well as carbide ceramics, for different applications.

### 2:00 PM

### (ICACC-S19-002-2025) Design of Novel 3D-Printed SiOC Ceramics as Promising Heterogeneous Catalysts

C. Youssef\*'; M. Obeid'; A. Bayout'; M. Nakhl²; D. VOIRY'; C. Salameh'; M. Zakhour²

1. Universite Montpellier Faculte des Sciences de Montpellier, France

2. Universite Libanaise, Lebanon

This research introduces a novel approach to the additive manufacturing of metal-modified SiOC ceramics using vat-based photopolymerization, specifically aimed at applications in heterogeneous catalysis. By incorporating nickel or copper nitrate into a photoactive polysiloxane resin, we developed a material that is fully compatible with vat-based photopolymerization, allowing precise control over both the geometry and porosity of the printed structures. After pyrolysis at 600°C, the metal-modified preceramic polymer transforms into amorphous silicon oxycarbide (SiOC) matrices with uniformly dispersed metal nanoparticles. These 3D-printed structures demonstrate considerable potential for catalytic applications due to their optimized architecture, large surface area, and well-distributed active sites. This study underscores the synergy between advanced 3D printing technologies and ceramic materials science, paving the way for innovative catalyst designs. The findings offer valuable insights into the development of sustainable catalytic materials, in particular showing strong potential as heterogeneous catalysts for hydrogenation and hydrogenolysis reactions.

### 2:20 PM

# (ICACC-\$19-003-2025) Scratch resistant lamellar zinc corrosion protection coating system using polymer derived ceramics (PDC)

J. Wendel\*1; S. Schafföner1; G. Motz1

1. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

Lamellar zinc coatings are widely used for corrosion protection in automotive and energy industries due to their very high performance while having a low thickness. To face the tendency towards higher operating temperatures, a lamellar zinc coating with increased temperature stability up to 400 °C using polysilazanes as matrix material was developed recently. However, the coating still suffers from high vulnerability to scratching. A possibility to increase the mechanical properties of the lamellar zinc coating would be the application of a scratch resistant top coat. The overall enhanced temperature stability of a polysilazane based zinc coating enables the application of a ceramic top coat via the PDC route. Therefore, the purpose of this study was to develop a ceramic top coat enhancing the scratch resistance of lamellar zinc coatings. The microstructure of the coating system was investigated by SEM while a scratch test (ISO 1518-1) and an abrasion test based on the linear Taber Abraser test (ASTM D 6279) were used to evaluate the wear resistance of the novel coating system. The combined coating system showed a threefold increase in scratch resistance and a reduced weight loss by a factor of about 21 compared to the lamellar zinc coating. Hence, the ceramic top coat was able to effectively protect the lamellar zinc coating from wear.

### 2:40 PM

# (ICACC-S19-004-2025) Processing and characterization of 3D-printed SiOC(N) ceramic via polymer derived ceramics route for biomedical and high temperature application

- R. Chaudhary\*1; F. Agostinacchio1; A. Motta1; G. D. Soraru1
- 1. Universita degli Studi di Trento, Department of Industrial Engineering, Italy

Additive Manufacturing (AM) of ceramics has recently gained significant attention due to its ability to produce intricate shapes with high dimensional accuracy. By integrating Fused Filament Fabrication (FFF), one of the inexpensive AM technologies, with the polymer-derived ceramics (PDC) process, we developed a novel method for producing SiOC(N) components with controlled porosity. The printed polymeric structure is infiltrated with a preceramic polymer (PCP) and further pyrolyzed in a controlled atmosphere, resulting in the final PDC structure. We studied the flexibility of the process for different wall thicknesses of the FFF-printed polymeric structure and observed successful infiltration of PCP for wall thicknesses  $< 600 \mu$ m, which allows fully dense ceramic struts. Thus, the process offers significant flexibility for fabricating complex ceramic components with desirable mechanical and functional properties, making them suitable for a myriad of applications in electronics, space, biomedical, and automotive industries. Preliminary in-vitro results reveal good metabolic activity and cell adhesion of human bone marrow-mesenchymal stem cells (hBM-MSC) after 7 days of activity. The versatility of this approach was further demonstrated by including composite materials (SiC/PU, Si/PU, and C fiber/PU), highlighting its broad applicability.

### **S19-** Processing and shaping of molecular precursors II Room: Ballroom 3

Session Chairs: Jenny Jouin, Institut de Recherche sur les Ceramiques; Paolo Colombo, University of Padova

### 3:20 PM

### (ICACC-S19-005-2025) 3D-Printed Catalytic Monoliths via Polymer-Derived Ceramics and Stereolithography for Enhanced Heterogeneous Catalysis (Invited)

C. Salameh\*1

1. Institut Européen des Membranes, France

We present the development of 3D-printed catalytic monoliths utilizing a combination of the polymer-derived ceramics (PDC) route and stereolithography. This innovative approach enables the fabrication of highly structured ceramic supports for heterogeneous catalysis, overcoming limitations in traditional catalyst support materials. The PDC route offers the flexibility to design ceramics with tailored properties, such as thermal stability, mechanical strength, and resistance to harsh chemical environments. By integrating this with stereolithography, we achieve precise control over monolith geometry and porosity, enhancing mass transfer and active site accessibility in catalytic processes. The resulting monoliths are robust and highly customizable, providing superior support for a variety of catalytic reactions, particularly in high-temperature and corrosive environments. Our work demonstrates the potential of combining additive manufacturing with advanced ceramic processing to create next-generation catalytic supports. These supports have been tested for their efficiency in catalytic applications, showing improved performance and durability compared to conventional systems. This approach represents a significant advancement in the development of tailored catalysts for optimizing heterogeneous catalysis.

### 3:50 PM

### (ICACC-S19-006-2025) Insights into Preceramic Polymer-Based Additive Manufacturing Inks via Rheological and Scattering Studies of Preceramic Polymer Grafted Nanoparticles

G. Germanton\*1; K. L. Martin2; A. Hossain1; N. D. Posey2; J. Ponder2;

C. Ramirez<sup>1</sup>; P. Gnanasekar<sup>1</sup>; L. Wiegart<sup>4</sup>; P. Polisetty<sup>1</sup>; D. Hallinan<sup>1</sup>;

- M. B. Dickerson<sup>3</sup>; S. Ramakrishnan<sup>1</sup>
- 1. Florida State University, FAMU-FSU COLLEGE OF ENGINEERING, USA
- 2. Air Force Research Lab, USA
- 3. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
- 4. Brookhaven National Laboratory, USA

Preceramic polymer grafted nanoparticles (PCPGNPs) offer unique advantages over other preceramic materials, including increased ceramic yield, controlled particle arrangement, and reduced volume shrinkage and mass loss. This study investigates the effects of low-temperature thermal treatments on the material transformations of PCPGNPs with a silica nanoparticle core and poly(1,1-dimethylpropylsilnae) corona suspended in SMP-877. The addition of PCPGNPs to SMP-877 increased the elastic modulus and viscosity, with percolation occurring between 50-60 wt% PCPGNP. Above this concentration, the particles formed a space-spanning network. Rheological and X-ray photon correlation spectroscopy (XPCS) measurements during thermal treatments demonstrated the effect of crosslinking on the resulting moduli and dynamics. When the neat PCPGNP grafts overlapped, the moduli increased, and a jammed state persisted even when cooled to room temperature, likely contributing to increased char yield. Understanding the thermal treatment of these hybrid materials is crucial for advancing their applications in turbine engines, advanced friction, and heatshielding components.

### 4:10 PM

### (ICACC-S19-007-2025) Chemical and Kinetic Analysis of a Hybrid Siloxane Gel and its Thermal Decomposition Products by Combining Thermogravimetry and Mass Spectrometry

R. Campostrini<sup>1</sup>; G. Guella<sup>2</sup>; P. Kroll\*<sup>4</sup>; M. Grigiante<sup>3</sup>

- 1. Universita degli Studi di Trento, Department of Industrial Engineering, Italy
- 2. Universita degli Studi di Trento, Department of Physics, Italy
- 3. Universita degli Studi di Trento, Department of Civil Environmental and Mechanical Engineering, Italy
- 4. The University of Texas at Arlington, Department of Chemistry and Biochemistry, USA

We present a quantitative TGMS (Thermogravimetric-Mass Spectrometer) analysis of the thermal decomposition of a hybrid polysilsesquioxane gel, (CH<sub>3</sub>)SiO<sub>1.5</sub>. The precursor with remaining functional groups -OH, -OEt, and -CH<sub>3</sub>, was synthesized through sol-gel processing of methyltriethoxisilane (MTES). TGMS was performed in the temperature range of 20–1000 °C. The m/z ion current (IC) curves of individual fragmentation products allow to follow chemical reactions. Integrating ion current (IC) curves provides quantitative information about the change of chemical composition. Processing the MS bands of 18 relevant IC curves yields the initial chemical composition of the gel,  $(CH_3)SiO_{1,20}(OH)_{0,29}(OEt)_{0,15}$ . Chemical composition change during pyrolysis and the mass loss measured with the thermobalance are consistent and supported by elemental analysis of powder residues collected after pyrolysis. A kinetic analysis of the decomposition uses TGMS data from different heating rates. Individual ion current (IC) curves are analyzed, and activation energies of individual release reactions are extracted. MS data yields detailed insight into the reaction kinetics of the release of individual siloxane oligomers at higher temperatures. Overall, we highlight the TGMS technique and show its versatility in polymer and ceramics processing.

### 4:30 PM

# (ICACC-S19-008-2025) Hydration layer formation by electric double layer of fine bubbles in CMP process

S. Suda\*1; S. Mochizuki1; A. Tsunoda1; M. Hase2; S. Soeya2

- 1. Shizuoka University, Engineering, Japan
- 2. National Institute for Materials Science, Japan

Chemical mechanical polishing (CMP) is an indispensable engineering or technology for planarization glasses or semiconductor substrates. Charge transfer reactions would occur by applying shear stress between a workpiece and an abrasive. The reactions would lead to the forming of softened hydration layers on the surface of glasses, which is referred to as the chemical polishing of the glass CMP process. Ceria and colloidal silica are generally used as glass CMP abrasives. Instead of these solid abrasives, we focus on fine bubbles as a novel abrasive material. Fine bubbles are generally charged negatively in water, and they have highly concentrated hydroxide ions in the vicinity of the gas-liquid interface of the bubbles. The charge transfer reaction for the hydration layer was evaluated by measuring the electric potential change under the CMP process. The amount of hydration layer after the CMP process was also investigated using SAXS and contact angles. The electric potential change for the fine-bubble solution was more significant than that for the bubble-free solution. SAXS and contact angle measurement revealed that the polishing with fine bubbles enhanced the hydration layer. Hydroxide ions in the vicinity of the fine bubbles enhanced the reactions, and the delicate bubbles would work as abrasives similar to colloidal silica.

### 4:50 PM

### (ICACC-S19-009-2025) Polymer-derived porous ceramics and polymeric membranes prepared via Pickering emulsions (Invited) P. Miele\*<sup>1</sup>

1. Ecole Nationale Superieure de Chimie de Montpellier, France

The fabrication of porous ceramic materials is of great importance for various applications in energy, catalysis, filtration and refractory applications. Achieving rational design of polymer- derived ceramics (PDC) with hierarchical porosity has been made possible with the use of porogen agents, direct foaming or (nano)casting. However, these approaches often suffer from complexity and limited control over the desired porous architectures. Here, we describe an innovative method for preparing porous polymer-derived ceramic (PDC) monoliths by combining the preceramic polymer route and the Pickering emulsion method. The emulsions were prepared using a SiOC precursor and stabilized with modified graphene oxide (GO) nanosheets. The effects of formulation and the chemical parameters on the final properties of Pickering emulsions will be discussed. As a proof of concept, the monoliths have been used as electrode materials for electrochemical energy storage in Li-ion batteries (LIBs). Following a similar strategy, we will present a new process for the preparation of porous hydrosoluble polymeric filtration membranes, of great interest in the context of green technologies development. In that case, the formation of the porosity of the membranes results from Pickering emulsion templating involving hexagonal boron nitride (h-BN) nanosheets as stabilizer.

#### 5:20 PM

### (ICACC-S19-010-2025) Straightforward design of 3D polymerderived ceramic architectures by extrusion-based 3D printing technology

S. Bernard\*1

1. CNRS, IRCER, France

There is a trend toward more performant or competitive materials with the objective to improve the efficiency of actual systems and to repel technological boundaries. Silicon Carbide (SiC) attracts strong interests due to its properties targeted for future materials and technologies especially in aerospace. Inherent difficulties to the traditional techniques for manufacturing such dense materials with a complex geometry can be overcome by the development of new manufacturing approaches and the deployment of synthetic paths where chemistry of materials and ceramic science are combined rationally. The Polymer-Derived Ceramics (PDC) route offers great opportunities in material sciences when combined with 3D printing. Here, the aim of this talk is to introduce a straightforward design approach consisting in tailoring the extrusion ability of polycarbosilanes to fit with a granule-based fused deposition modeling process and form after a two-step heat-treatment process at a relatively low temperature 3D stoechiometric SiC and derived composites parts.

### Tuesday, January 28, 2025

### 14th Global Young Investigator Forum

# GYIF- Life Cycle Assessment (LCA) of Ceramic and Composite Products

Room: Coquina G

Session Chairs: Yinsheng Guo, University of Nebraska-Lincoln; Bai Cui, University of Nebraska–Lincoln

#### 8:30 AM

### (ICACC-GYIF-008-2025) Mechanistic Understanding of Materials Corrosion Degradation in Nuclear Reactor Environments (Invited)

J. Xi\*1; N. Dailey1; W. Leng1; Y. Xu1

1. University of Illinois Urbana-Champaign, Nuclear, Plasma & Radiological Engineering, USA

The fast-growing energy demand and the need to limit greenhouse gas emissions have led to the acknowledgment of the importance of increasing nuclear energy efficiency, which requires nuclear materials can withstand more and more extreme environments. For example, the advances in nuclear reactors create exceptionally harsh working conditions for materials operating at higher temperatures and more chemically aggressive environments. Those extreme environments can degrade material's performance, thus requiring fundamental improvement in materials. However, the improvement of materials for nuclear applications is a daunting challenge, especially in the absence of a comprehensive understanding of the behavior of materials in extreme environments. Using examples from our research, I present strategies to overcome these challenges. Specifically, we integrate modeling with advanced experimental techniques to understand the relationship between microstructure/microchemistry, corrosion, and radiation responses in nuclear materials. In addition, I discuss strategies to design nuclear materials with enhanced corrosion resistant property, and how radiation couple with corrosion in materials. Altogether, these examples highlight the great potential of seamlessly integrating modeling and experiments into understanding and improvement of materials behavior in nuclear applications.

### 9:00 AM

#### (ICACC-GYIF-009-2025) Life-cycle assessment of 2D transition metal carbides (MXenes), and their use as functional additives in ceramics and electrocatalytic applications (Invited)

S. Nemani\*2; M. Firouzjaei3; A. Thakur1; M. Elliot3; B. Anasori2

- 1. Indiana University--Purdue University, Mechanical Engineering, USA
- 2. Purdue University, Mechanical Engineering, USA
- 3. University of Alabama, Civil Engineering, USA

MXenes are two-dimensional ceramic materials gaining major attention for various applications such as electrocatalysis, additives, and electromagnetic interference (EMI) shielding. Yet, comprehensive life-cycle assessments (LCAs) are still lacking. We performed a "cradle to gate" LCA to evaluate the cumulative energy demand and environmental impacts of lab-scale titanium carbide (Ti3C2Tx) MXene synthesis, comparing it with aluminum and copper foils used for EMI shielding. Results show electricity consumption has the highest environmental impact, with 1 kg of Ti3C2Tx MXene synthesis releasing 428.10 kg of carbon dioxide much higher than aluminum and copper foils. Furthermore, to utilize MXenes as functional materials, we investigate their compositional complexity towards enhancing hydrogen evolution reaction (HER) activity and investigate surfactant-free self-assembly of Ti3C2Tx MXene with ceramic matrices. By understanding life-cycle impacts, tuning HER activity through composition tailoring, and developing efficient incorporation strategies for ceramics, we address critical challenges in advanced ceramics and contribute to sustainable development goals.

### 9:30 AM

### (ICACC-GYIF-010-2025) Non-destructive Evaluation of Metallized Silicon Nitride Substrate under Thermal Cyclic Test by Digital Image Correlation (Invited)

M. Ngo\*1; H. Miyazaki1; T. Ohji1; M. Fukushima1

1. National Institute of Advanced Industrial Science and Technology (AIST), Multi-material Research Institute, Japan

In this work, non-destructive evaluation testing using Digital Image Correlation (DIC) technique was conduted to study the strain and dynamic bending behavior of a metallized Si<sub>3</sub>N<sub>4</sub> substrate under various consecutive thermal cycles with the temperature ranging from -40°C to 250°C, from the beginning of the test up to 2501 cycles. The substrate remained defect-free from 1 to 1500 cycles, as confirmed by Scanning Acoustic Microscopy (SAM) and 3D measurements using DIC. Deformation became evident when delamination started to propagate on the substrate after 2001 cycles and became significant after 2501 cycles. The deformation was in-situly measured throughout several consecutive cycles to observe dynamic behavior change of the substrate with temperature, especially at -40°C, room temperature (RT), and 250°C. Based on the DIC measurement results, we first confirmed the cyclic hardening of Cu and the thermal strain evolution with the number of thermal cycles on the defect-free substrate. Secondly, the dynamic bending behavior of the substrate along a whole thermal cycle after delamination was investigated, and the delemination was also evaluated. The study of the metallized Si<sub>3</sub>N<sub>4</sub> substrate using the DIC method throughout the entire reliability test revealed the behavior of each constituent material on the substrate during thermal cycling.

### **GYIF-Sustainable Materials Development**

Room: Coquina G

Session Chairs: Daniel Oropeza, University of California at Santa Barbara; Fiona Spirrett, Osaka University

### 10:20 AM

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### (ICACC-GYIF-011-2025) Development of Sustainable Composites and Manufacturing Technology for Future Air Mobility (Invited)

S. Chu<sup>\*1</sup>; C. Wohl<sup>1</sup>; C. Park<sup>1</sup>; V. L. Wiesner<sup>1</sup>; G. King<sup>1</sup>; M. R. Webster<sup>1</sup>; D. Burns<sup>1</sup>; S. Johnson<sup>1</sup>; E. Frankforter<sup>1</sup>; S. Miller<sup>2</sup>; M. Ranaiefar<sup>2</sup>; S. Vivod<sup>2</sup>; S. Malakooti<sup>2</sup>; D. Rinehart<sup>2</sup>; L. Abbott<sup>3</sup>; A. Santos<sup>3</sup>

- 1. NASA Langley Research Center, USA
- 2. NASA Glenn Research Center, USA
- 3. NASA Ames Research Center, USA

During the early stages of the evolution of the aircraft industry, the fabrication of aircraft structures primarily relied on a combination of natural composites, wire, and fabric materials. Aluminum alloys continued to dominate as the primary material of choice in the aerospace sector until recent times Currently, fiber-reinforced composites have gained wides and utilization across the aerospace industry. As the U.S. greenment and the aviation industry strive to achieve net-zero evolution emissions by 2050, the Sustainable Manufacturing of Alter II (SUMAC) project, supported by the Convergent Aerona are Solutions (CAS) program, aims to develop sustainably drived thermoplastic composites and manufacturing technologe for future aviation. A multidisciplinary team of experts drives this initiative through a collective effort. The team's key focus areas are sustainably derived thermoplastic resins, natural fiber reinforcement, composite manufacturing, structural health monitoring, computational materials modeling, and systems analysis. This presentation will give an overview of the SUMAC project, focusing on advancing the sustainability and resilience of future aviation. Topics include environmental impacts, challenges and technological feasibility, approaches and expected outcomes, partnerships with stakeholders, and future technology transition considerations.

### 10:50 AM

### (ICACC-GYIF-012-2025) Sustainable Ceramic Matrix Composites development: A Life Cycle and Multi-Criteria Analysis Approach (Invited)

A. Schneller\*1; D. Koch1; T. Langmann1; S. Bittmann1

1. University of Augsburg, Institute for Materials Resource Management, Germany

The increasing focus on sustainability is becoming more and more important in materials development. This is clearly evident, e.g., in attempts to reduce the CO2 footprint through the use of composite materials such as ceramic matrix composites (CMC). While research has so far focused on optimizing CMC properties, there is a growing need to consider the environmental impact of energy- and resource-intensive manufacturing processes. Life cycle assessments (LCA) for CMCs are still rare. This talk will look at the environmental optimization potential of the CMC manufacturing process, in particular liquid silicon infiltration, by analyzing the correlation between process parameters and material properties. By combining classical LCA with a multi-criteria analysis, the impact of changes in process parameters on environmental indicators and material performance is evaluated. A full understanding of the individual process steps is crucial for reducing resource and energy consumption. Thermophysical studies identify critical reaction zones during pyrolysis. In combination with in-situ experiments in an environmental scanning electron microscope, pyrolysis temperatures can be specifically lowered and holding times reduced. In-situ experiments are one aspect of the development of digital models of CMC processing, which can be used to achieve energy savings through digital optimization.

### 11:20 AM

## (ICACC-GYIF-013-2025) Carbon fiber recycling: methods and products

S. De La Pierre<sup>\*1</sup>; M. Ferraris<sup>1</sup>

1. Politecnico di Torino, DISAT, Italy

Fiber-reinforced composites are used as advanced materials in different sectors and their application has been continuously expanding. The increasing use of carbon fiber composites has raised attention about their disposal methods. Tons of composite waste coming from production scrap or end-of-life products have been accumulated every year and they must be recycled with a cost-effective approach and without causing pollution problems. Furthermore, the production of carbon fibers leads to environmental pollution, since carbon fiber manufacturing is an energy-intensive process. This project aims to analyze the different methods that have been developed to extract, and recycle, carbon fibers from Carbon Fiber Reinforced Polymers composites (CFRPs). More specifically, the recycling of carbon fibers using Mechanical, Thermal, and Chemical processing is reviewed. The first is based on crushing and milling the waste, while the other two on decomposing the waste employing thermal (pyrolysis and fluidized bed) and chemical (solvolysis) processes. The energy requirements, the final product outputs, and the recycled carbon fiber properties and composition are discussed for each technique. In conclusion, the most promising method is selected, discussing what can be recovered in energy terms and evaluating the method's sustainability.

### 11:40 AM

## (ICACC-GYIF-014-2025) C/C-SiC fabrication based on an alternative thermoplastic carbon precursor

M. Moos<sup>\*1</sup>; N. Langhof<sup>1</sup>; S. Schafföner<sup>1</sup>

1. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

Carbon fiber-reinforced silicon carbide (C/C-SiC) can be fabricated via the liquid silicon infiltration process. The three-step process is based on a carbon fiber-reinforced polymer (CFRP), which is processed into a carbon fiber-reinforced carbon (C/C) and then into a carbon fiber-reinforced silicon carbide. The properties of

the C/C-SiC can be tailored by the choice of the matrix polymer. Suitable matrix polymers need a low viscosity and a char yield after pyrolysis of > 50 %. The state-of-the-art polymeric carbon precursor is phenolic resin. However, thermoplastic materials such as polyetheretherketone (PEEK) also have been proven to be fitting candidates. PEEK is a high-performance polymer from the group of polyaryletherketones (PAEK). Another example of this group is polyetherketoneketone (PEKK). In this work, PEKK has been used as thermoplastic matrix material for the C/C-SiC fabrication. Its high char yield of > 65 % not only makes it a promising carbon precursor for C/C-SiC, but also for C/C materials. Yet, the high melt viscosity of PEKK leads to a microstructure with some matrix pores and not fully infiltrated fiber bundles in the CFRP. As a result, those fibers within a bundle react to silicon carbide in the C/C-SiC. Nonetheless, three-point bending tests of C/C-SiC samples show a promising mean flexural strength of 223 MPa, strain to failure of 0.61 % and Young's modulus of 39 MPa.

### FS6 Innovative material processing for diverse resource circulation loops

# FS 6- Recovery of critical/valuable materials from exhausted complex products

Room: Ballroom 5

Session Chair: Hidehiro Kamiya, Tokyo University of Agriculture and Technology

### 8:30 AM (ICACC-FS6010-2025) PV Panel Recycling and Resource Recycling Society (Invited)

D. Moriya<sup>1</sup>; M. Iwasaki\*<sup>1</sup>

1. Shinryo Corporation, Japan

In 2012, the Japanese government implemented a policy of purchasing renewable energy at a fixed price (Feed-in Tariff). The incentives this policy provided to the market were so powerful that the amount of PV panels installed in Japan grew rapidly. Shinryo Corporation has developed PV panel resource recovery technology in anticipation of the future era of mass PV panel disposal. EVA resin is a material necessary to protect PV panels from the elements and ensure their safe operation, but it also makes it difficult to recover resources from PV panels. Shinryo has developed a technology to remove EVA resin through heat treatment, enabling continuous processing of PV panels. The development of mechanical sorting system has made it possible to recycle recovered glassof the processed PV panels, which is difficult to use as a raw material for products. The recovered silicon cells are sold as silver-containing products, and Shinryo Corporation is currently studying the technology to separate silver and silicon.

### 9:00 AM

# (ICACC-FS6011-2025) Photovoltaic Panel recycle technology with low temperature decomposition (Invited)

T. Yamashita\*1

1. Kabushiki Kaisha Tokuyama Tokuyama Seizosho, Eco-Business Developement, Japan

The recycling method for pyrolyzing the photovoltaic module is a recycling method that can completely remove EVA, which is a sealing material, and can neatly separate the cell and glass. However, the backsheet material is mostly PET, and simple pyrolysis produces complex bonded carbide ("soot"). Soot deteriorates materials and requires energy to remove. We succeeded in suppressing the generation of soot by heating resin components such as PET and EVA, melting and dropping them into a ceramic filter supported by a catalyst, and performing an oxidation reaction around 500 degrees Celsius. We developed PV module heat treatment furnace and found the heating condition. We have completed a fully automated process, from removing the aluminum frame to sorting the parts after thermal decomposition. As a result, we got high purity components (glass, cells, electric wires) from disposed PV panel. All components have value as raw materials. We supplied glass for a demonstration test run by AGC Inc. to produce float glass from recycled materials. This test by AGC was conducted using the float glass production furnace at their Kashima Plant on March 18, 2024. Using cover glass supplied by Tokuyama as raw material, AGC successfully recycled this glass into float glass for the first time in Japan. For the next step, we study to recycle polly sillicon from cells.

### FS 6- Advanced powder processing both for carbon

### net zero and circular economy

Room: Ballroom 5

Session Chair: Hidehiro Kamiya, Tokyo University of Agriculture and Technology

### 9:30 AM

### (ICACC-FS6012-2025) Photocurable Suspension Design Toward 3D Structuring and Disassembling Process of Ceramic Green Bodies (Invited)

M. Iijima\*1; Y. Hiroshige1; J. Tatami1

1. Yokohama National University, Japan

Additive manufacturing using photocurable suspension is one of powerful process to enable optimized 3D structing of ceramic components. However, conventional processes involve long debinding to avoid structural collapse which is not favorable for carbon neutrality. Further, resource circulation, such as reuse of trial printed bodies, has not been well considered in these 3D structuring processes. Recently, we have proposed a new photocurable suspension which reagent particles are directly crosslinked by limited amounts of monomers. The designed suspensions were appliable to stereolithographic 3D printing process and processable thorough rapid debinding owing to small amounts of organics. Inspiring from the unique microstructure of the photocured bodies obtained from the newly designed suspension, which have nano-scaled polymer networks among the particles, herein, we demonstrate that the photocured bodies can be easily disassembled into primary particle size by a mild chemical reaction in aqueous solution. We believe that the proposed ceramic processing should play an important role in contributing with carbon neutrality (rapid firing) and resource circulation strategies.

# FS 6- Innovative material processing for diverse resource circulation loops II

### Room: Ballroom 5

Session Chair: Motoyuki Iijima, Yokohama National University

### 10:20 AM

### (ICACC-FS6014-2025) Nanoparticles dispersion and aggregation behavior control for easily degradable adhesion under electrical pulse stimulation (Invited)

H. Kamiya\*1; Y. Okada3; M. Kubo2; K. Matsuo1; M. Inutsuka1; T. Koita1;

- A. Narita<sup>1</sup>; C. Tokoro<sup>1</sup>
- 1. Waseda University, Japan
- 2. Tohoku University, Japan
- 3. Tokyo University of Agriculture and Technology, Japan

Our research group has been investigating the relationship between the molecular structure of organic ligands and the dispersion behavior of nanoparticles in organic solvents and polymers using experimental and computer simulation approaches. In our previous studies, we experimentally determined the molecular structure of the ligands to disperse nanoparticles of various materials in various organic solvents and polymers. We also analyzed the relationship between the interface structure and dispersion behavior using molecular dynamics and discrete element method simulations. We apply our previous method of controlling the dispersion and aggregation behavior of nanoparticles to the separation process of composite bonding materials. By dispersing conductive nanoparticles such as silver and carbon black in strong adhesive raw material organic molecules for automobiles and other large equipment, we attempted to establish a method for easily decomposing adhesives by high-voltage electric pulse stimulation. The high-voltage separation process and mechanism by dispersing nanoparticles in adhesive bonding polymers were analyzed using high-speed video cameras and other methods.

### 10:50 AM

## (ICACC-FS6015-2025) Controlled debonding of epoxy adhesives with conductive spots by pulsed discharge

K. Matsuo\*1; T. Koita<sup>1</sup>; M. Inutsuka<sup>1</sup>; K. Ota<sup>2</sup>; T. Honda<sup>2</sup>; R. Ogawa<sup>2</sup>; C. Tokoro<sup>3</sup>

- 1. Waseda Daigaku Riko Gakujutsuin, Japan
- 2. Kabushiki Kaisha Adeka Ogu Chuo Kaihatsu Kenkyujo, Japan
- 3. Waseda University, Japan

Composite materials, which are consisting of various metallic and non-metallic materials, are widely used in a variety of industrial products, including vehicles and aircraft. For assembling dissimilar materials, polymer adhesives such as epoxy resins are often used due to their advantages such as high strength, short working time, preventing Galvanic corrosion, and stress concentration. From the perspective of recycling, the assembled materials must be separated and collected individually after the end of product life. Thus, facile debonding method for the polymeric adhesives is required. A pulsed discharge is a promising method to debond the polymeric adhesives. In our previous study, polymeric adhesives joining two metal plates can be debonded by an explosive discharge by instantaneous applying of high-voltage electric pulses on each metal plate. We also demonstrated that a successful debonding requires a discharge inside the adhesive. To control the discharge position, it was effective to improve the conductivity of the polymer adhesive by the addition of carbon black (CB) to the adhesive. Nevertheless, even with the improved adhesive, debonding was not always successful due to the fluctuation of the discharge position. In this study, we aimed to control the discharge position more precisely using spotlike patterning of the adhesives with and without CB in the bonding surface.

## <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

### S1- Ceramics for Concentrated Solar–Thermal Power and Industrial Process Heat I

Room: Coquina E

Session Chairs: Dileep Singh, Argonne National Lab; Farhad Mohammadi, Ceramic Tubular Products, LLC

### 8:30 AM

### (ICACC-S1-011-2025) Opportunities for Ceramics Material Research and Development (R&D) for Concentrating Solar-Thermal Technologies (Invited)

K. C. Raghavan\*1

1. Department of Energy, USA

Concentrating solar-thermal (CST) plants capture the sun's energy from the collector field and convert it to thermal energy which can be stored and dispatched on-demand. Stored thermal energy can be utilized for power generation as well as for industrial processes. The Department of Energy (DOE) has set a target cost of electricity of \$0.05/kWh by 2030 with more than 12 hours of thermal energy storage (TES). To reach this target, DOE is adopting the technical strategy that focuses on supercritical sCO<sub>2</sub> Brayton cycle, operating at temperatures higher than 700°C and pressures of about 300 bar. For industrial processes, the temperature requirement is anywhere between 600°C and 1400°C for sectors including chemical production, refineries, steel and cement. For both power and industrial processes, the critical components - receivers, reactors, heat exchangers, etc. operate at high temperatures and harsh environments leading to material failure. To address the material failure challenges, Solar Energy Technologies Office (SETO) continues to invest in high temperature materials R&D. Ceramics constitute a large class of materials that can survive such harsh conditions. This talk will discuss the overall programmatic requirements of CST where ceramic materials R&D will play a significant role. The talk will also touch upon the opportunities and various funding mechanisms.

### 9:00 AM

### (ICACC-S1-012-2025) Design, Fabrication and On-Sun Performance Evaluation of Additively Manufactured SiC Receiver Components for CSP/CST Applications (Invited)

R. Sarrafi-Nour\*<sup>2</sup>; J. Shiang<sup>2</sup>; A. Kebbede<sup>2</sup>; D. Dunn<sup>1</sup>; H. McGuigan<sup>2</sup>; W. Costakis<sup>2</sup>

- 1. GE Aerospace, USA
- 2. GE Aerospace Research, USA

Increasing operating temperatures of solar receivers is paramount to the efficiency of concentrated solar thermal (CST) and solar power (CSP) systems. SiC has been the material of choice for application in high-temperature solar receivers. Funded by US Department of Energy, GE Aerospace Research in collaboration with Heliogen Holdings Inc and Sandia National Lab, is developing ultra-High Operating Temperature SiC-matrix Solar Thermal Air Receiver (HOTSSTAR) enabled by additive manufacturing. The program aims at demonstration of a techno-economically viable SiC air receiver technology to achieve exit air temperature of 1100°C. This presentation will discuss the design, initial prototype fabrication and on-sun testing of HOTSSTAR components. Feature test articles are fabricated using binder-jet printed SiC followed by melt-infiltrated reaction bonding process. To enhance the reliability of SiC test articles in thermal gradient and thermal shock environment of the application, sections of the component design maybe designed or reinforced with GE's MI SiC CMC. We report the test results under solar raidation exceeding 2000 suns, compare the thermal efficiency performance of the test articles with design model predictions, and discuss the next steps towards fabrication and testing of a full size HOTSSTAR module.

### 9:30 AM

### (ICACC-S1-013-2025) Topology Optimization, Additive Manufacturing and Experimental Testing of Particle Heat Exchangers

X. Qian<sup>\*1</sup>; M. Niemiec<sup>1</sup>; L. Bakke<sup>1</sup>; X. Yu<sup>1</sup>; K. Troyer<sup>1</sup>; J. Wu<sup>1</sup>; M. Wagner<sup>1</sup>; D. Negrut<sup>1</sup>; G. Nellis<sup>1</sup>; M. Anderson<sup>1</sup>

1. University of Wisconsin-Madison, Mechanical Engineering, USA

This talk provides an overview of our ongoing work directed towards improving the performance of particle heat exchangers (pHX) for concentrating solar power (CSP) applications. The approach is to integrate topology optimization (TO) and additive manufacturing (AM) to develop a modular pHX with dramatically improved heat transfer performance, manufacturability, cost effectiveness, and thermo-mechanical reliability. The combination of TO and AM allows the use of advanced heat transfer geometries and highertemperature Silicon Carbide (SiC) materials in the pHX in order to increase heat transfer performance and lifetime. The proposed pHX technology involves three integrated design-build-test components, including particle flow-based discrete-element modeling and continuum model-based TO for pHX design, binder jet additive manufacturing-based fabrication of pHX, and experimental validation of these models using imaging of particle flow and high-temperature testing of pHX. Initial results have shown that particle flow-based TO will lead to an advanced heat transfer geometry with much higher efficiency and durability than the baseline parallel-plate based HX. This project features synergistic collaboration among UW-Madison, GE Research, and Sandia National Laboratory.

### 9:50 AM

## (ICACC-S1-014-2025) Microstructure and Mechanical properties of diffusion bonded Ti<sub>3</sub>SiC<sub>2</sub> MAX Phase composites

- S. Bajpai\*1; D. Singh2
- 1. Argonne National Laboratory, Applied Materials Division, USA
- 2. Argonne National Lab, USA

Ti<sub>2</sub>SiC<sub>2</sub> MAX phase materials exhibiting high thermal conductivity and superior mechanical strength at high temperatures (>800°C) are promising for the next generation concentrating solar power (CSP) systems. However, for the real-life applications, scaling up of the small and simple shapes become mandatory. Reactive sintering of Ti+Si+2TiC powder via Spark plasma sintering at 1400 °C, 40 MPa, for 15 min, resulted in the formation of dense composites (~99%) having MAX phase  $Ti_3SiC_2(~91\%)$  and TiC(~9%). These pre-sintered Ti<sub>3</sub>SiC<sub>2</sub>-TiC composites were then diffusion bonded to themselves with and without Ti foil interlayer at 1100 °C and 1200 °C respectively, using spark plasma sintering. Microstructural analysis of the joined cross-sections confirmed the formation of Ti rich joint interlayer (~10 mm thick), resulting in decreased hardness from ~12 GPa for  $Ti_3SiC_2$  to ~9 GPa for joint interlayer. In contrast, for direct diffusion bonded Ti<sub>3</sub>SiC<sub>2</sub> composites, diffusion of elements forms a seamless microstructure resulting in uniform hardness of ~12 GPa across the interface, making these joints suitable for scaled up applications.

### 10:50 AM

#### (ICACC-S1-016-2025) Characterizations of Scalable, Infiltration-Free ceramic matrix composite

J. Wei\*1; A. Thukral1; K. Bhattacharyya1; G. Iftime1; R. Pandey1

1. SRI, Future Concept, USA

The time-consuming, and labor-intensive ceramic infiltration step is responsible for more than half of the manufacturing cost of ceramic matrix composite (CMC). This is especially true for CMC made with carbon fiber and carbon matrix. To make CMC cost-competitive in price-sensitive markets, like concentrated solar power, it is essential to innovate a CMC manufacturing process that skips the ceramic infiltration step. In this presentation, we will describe our work on how to optimize the thermomechanical properties of CMC for concentrated solar plants through investigation of the process-structure-properties relationship.

### 11:10 AM

# (ICACC-S1-017-2025) Impact of Scalable, Infiltration-Free ceramic matrix composite (SIFCMC) on concentrated solar receiver

J. Wei\*1; J. Martinek2; A. Couet3; S. Jagadeesh3; G. Iftime1

- 1. SRI, Future Concept, USA
- 2. National Renewable Energy Laboratory, USA
- 3. University of Wisconsin-Madison, USA

Ceramic Matrix Composite with high thermomechanical properties has the potential to improve the concentrated solar receiver by increasing its solar-to-thermal efficiency, reducing its cost, and extending its lifetime. However, the conventional CMC is too expensive for use in cost-sensitive applications. In this presentation, the characterization results of the reinforced carbon/carbon manufactured by the SIFCMC method are used in the concentrated solar receiver/reactor model to evaluate the receiver's performance. Furthermore, a model comparison between using SIFCMC and nickel alloy will be presented to demonstrate how the exceptional thermomechanical properties of SIFCMC transfer into the receiver's cost, performance, and lifetime.

### 11:30 AM

## (ICACC-S1-018-2025) Rapid printing of 3-D ceramic materials using microwave volumetric additive manufacturing

S. Mukherjee<sup>1</sup>; E. Rosenberg<sup>1</sup>; J. Vandenbrande<sup>1</sup>; E. Baluyot<sup>1</sup>; J. Schwartz<sup>1</sup>; M. Shusteff<sup>1</sup>; J. Tringe<sup>1</sup>; J. Kelly<sup>\*1</sup>

1. Lawrence Livermore National Laboratory, USA

Additive manufacturing has come a long way in the past 20 years to create complex 3D architecture that are hard to produce using traditional manufacturing methods. Many advances in the last 10 years have focused on expediting the time to create the 3D objects to rival methods aimed at industrial or large-scale production. One printing method of interest is volumetric additive manufacturing (VAM) using optical light, which can print a single object in one projection. However, VAM is unable to process resins that are opaque or have high loadings of powder. Our team has devised a strategy to overcome these limitations through microwave curing of ceramic binder mixtures to produce 3D ceramic objects. The microwave radiation thermally cures the epoxide-based binder in place to create 3D ceramic green body, and sintering the object forms the ceramic part. Current efforts in the materials side of the project revolve around identifying how the initiator concentration and the loading of the silicon nitride powder in the binder influences the exothermic reaction to enable the localization of the cured spot within the ceramic binder mixture, and identifying how the binder is removed during the post-processing sintering to form a solid ceramic object.

### 11:50 AM

### (ICACC-S1-019-2025) Reliability of Concentrating Solar Power Ceramic Components: Implication of Weibull 2- versus 3-Parameter Models

B. Barua\*1; P. S. Chaugule1; M. C. Messner1; D. Singh1

1. Argonne National Laboratory, Applied Materials Division, USA

The outlet temperature targets for Gen 3 Concentrating Solar Power (CSP) systems pose a significant challenge to the structural reliability of high-temperature metallic materials. Advanced ceramics present a promising alternative due to their high temperature strength and low thermal expansion. However, challenges like limited ductility, fabrication issues, and variability in failure strength must be addressed. CSP developers need to evaluate the viability of high-temperature ceramic components in system designs, considering factors such as probabilistic plant operating life. The Weibull 2-parameter distribution, conventionally used to characterize the variability in ceramic strengths, provides a nonzero probability of failure across the full range of applied stress, which can sometimes lead to conservative design assumptions, particularly for larger components. The 3-parameter Weibull model, with an additional parameter for threshold stress, allows for zero probability of failure when applied stress is at or below this threshold. This study evaluates the implications of using Weibull 2- versus 3-parameter models for reliability estimation of CSP receivers made from commercial SiC. Additionally, it presents a comparative design analysis of ceramic versus metallic receiver designs to assess the viability of advanced ceramics for high-temperature CSP applications.

## S2 Advanced Ceramic Coatings for Structural/Environmental & Functional Applications

### **S2- Environmental Barrier Coatings III**

Room: Coquina C Session Chairs: Jie Zhang, Institute of Metal Research, Chinese Academy of Sciences;

### 8:30 AM

### (ICACC-S2-010-2025) Multilayer design for Rare Earth silicatebased Environmental Barrier Coatings

S. Sampath<sup>1</sup>; E. Garcia<sup>1</sup>; J. Saputo<sup>\*1</sup>

1. Stony Brook University, Center for Thermal Spray Research, USA

Rare earth silicate-based coatings are envisioned as the best option for the volatilization barrier in multilayered TBC/EBC (Thermal/Environmental Barrier Coatings) systems to protect ceramic matrix composites (CMC) components in forthcoming power generation and aircraft/spacecraft turbine engines from the combustion atmo-sphere generated in operation. When these materials are deposited by atmospheric plasma spray (APS) in the form of coatings present high amorphous character and a shift from the original chemical composition that depends on the spraying conditions. This char-acteristic gives the advantage of producing coatings with different monosilicate/disilicate content just modifying the plasma parameters which allows the tuning of the thermomechanical properties of the deposited coatings. Three different silicate systems will be compar-atively presented in this work: Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> and YYbSi<sub>2</sub>O<sub>7</sub> studying their amorphous character, compositional changes, phase and microstructure evolution with thermal treatments. The suit-ability as volatilization layer of multilayer coatings produced with these systems will be comparatively discussed.

### 8:50 AM

### (ICACC-S2-011-2025) Oxidation performance under water vapor of PVD Y/Yb environmental barrier coatings

C. Y. Guijosa Garcia\*1; P. Mechnich1; U. Schulz1; R. Naraparaju1

1. DLR - German Aerospace Center, Institute of Materials Research, Germany

Environmental barrier coatings (EBCs) are proven to protect SiC-based materials against water vapor in gas turbine environments. The straightforward EBCs are typically comprised of two layers, ytterbium disilicates (YbDS) and a Si bond coat, and are applied by atmospherically plasma spraying (APS) method. YbDS offers high-temperature phase stability, however, it still experiences a detrimental volatilization rate under high velocity steam environment. Yttrium disilicate (YDS) on the other hand exhibits better water vapor resistance but lacks the high temperature phase stability. Combining both properties, Y/Yb disilicates might be very effective as EBCs. This study aims to produce a multi-component EBC system using Electron beam physical vapor deposition (EB PVD) Si bond coat and magnetron sputtering (Y,Yb) silicates on a SiC substrate. Further, EBC system has been tested under water vapor environment at high temperatures. Initial results have shown good adhesion between all the layers after deposition and crystallization heat treatment. The evolution of the microstructure after water vapor oxidation tests will be discussed.

### 9:10 AM

### (ICACC-S2-012-2025) Damage and Failure Analysis of Environmental Barrier Coatings under Extreme Environments: Multi-physics Modeling (Invited)

K. Chen\*1

1. National Research Council Canada, Aerospace Research Centre, Canada

Under adverse high-temperature environments, the premature failure of environmental barrier coatings (EBCs) is a preliminary phenomenon that can significantly limit coating applications to hot-section engines. The delamination and failure of EBCs typically occur within the topcoat and coating interfaces due to high-temperature water vapour corrosion, thermal mismatch stress and thermal gradient. This presentation shows a study of delamination and failure of EBCs using COMSOL multi-physics modelling methodologies. Heat transfer was cyclically implemented into the EBCs model to simulate the in-service operations. The stress distribution was analyzed versus thermal cycles by combining the thermally grown oxide SiO<sub>2</sub> (TGO) growth kinetics. Phase-field damage modelling was conducted to study crack propagation within the topcoat and its penetration behaviour across the coating interfaces. The effect of water vapour on crack propagation and failure of EBCs was investigated by combining experimentally measured TGO growth models under different water vapour conditions. Coating interface degradation was evaluated using the cohesive zone model to study interfacial delamination and its interaction with cracks distributed across the coating layers.

### S2- CMAS-type recession and mitigation strategies I

Room: Coquina C

Session Chair: Kang Lee, NASA Glenn Research Center

### 10:20 AM

### (ICACC-S2-013-2025) In situ Synchrotron X-ray Diffraction Studies Assessing the Responses of EB-PVD Ceramic Coatings due to CMAS Infiltration under Thermal Gradients

Z. Stein\*<sup>2</sup>; J. E. Förster<sup>1</sup>; P. Kenesei<sup>3</sup>; J. Park<sup>3</sup>; J. Almer<sup>3</sup>; J. Wischek<sup>1</sup>; M. Bartsch<sup>1</sup>; U. Schulz<sup>1</sup>; R. Naraparaju<sup>1</sup>; S. Raghavan<sup>2</sup>

- 1. DLR German Aerospace Center, Materials Research, Germany
- Embry-Riddle Aeronautical University, Aerospace Engineering, USA
- 3. Argonne National Laboratory, Advanced Photon Source, USA

Aircraft turbine engines operate in extreme environments. The ingestion and subsequent melting of calcium-magnesium-alumino-silicate (CMAS) particulates pose a significant threat to the longevity and performance of high-temperature ceramic-coated components, such as turbine blades. Improvements in engine efficiencies necessitate a more comprehensive understanding of the crucial response phenomena and mechanisms driven by the thermal and mechanical loadings experienced by turbine blades. Capturing these responses accurately require improvements in simulating the operational environmental conditions within a laboratory setting and enhancement on existing testing methodologies. This work encompasses high-resolution in-situ CMAS infiltration measurements on a thermomechanically-loaded high temperature yttria-stabilized zirconia ceramic coating through synchrotron X-ray diffraction. CMAS infiltration was captured within the exposed coating. A thermomechanical strain response and chemically-induced phase destabilization was observed in the exposed coating upon thermal cooling. This testing environment and in-situ experimental measurement capabilities enable the development of more resilient material systems, enhancing their ability to withstand increasingly extreme conditions in turbine engines and in other high-temperature applications.

### 10:40 AM

### (ICACC-S2-014-2025) Study of the effect of hydrogen in ASPS spraying on the microstructure of TBC and its resistance to CMAS solicitation

M. Gaudin\*1; S. Goutier2; G. Rivaud2; A. Joulia1; E. Béchade2; A. Kéromnès2

1. Safran Tech, France

2. Institut de Recherche sur les Ceramiques, France

One of the major advantages of Plasma Spray Suspension is its versatility in producing very different microstructures. These different microstructures can be achieved by varying the process parameters. The parameters that directly influence the microstructure are those that affect the kinetic and thermal properties of the particles. In the case of ASPS spraying using the Axial III Plus torch, Tarasi et al. have shown that gas flow rates have the greatest influence. In particular, the flow of hydrogen, a diatomic gas, is known to have a significant effect on the in-flight treatment of ceramic particles. In the present study, the effect of hydrogen on the in-flight treatment of particles and therefore on the microstructures was investigated using the Axial III Plus torch. Three microstructures with different morphological aspects (porous to dense), different mechanical properties (microhardness, porosity) and different thermal properties (diffusivity) were obtained. The TBCs were characterized on a thermal gradient CMAS test rig in order to study the effect of microstructure on CMAS attack resistance under thermal gradients. This study showed that increasing H<sub>2</sub> results in a densification of the TBC, which prevents CMAS infiltration into the coating and affects the CMAS resistance in the thermal gradient test.

### 11:00 AM

# (ICACC-S2-015-2025) Thermal Properties and CMAS Corrosion Resistance of Novel Rare Earth Phosphates (Sc\_{0.25}Lu\_{0.25}Yb\_{0.25}Er\_{0.25})PO\_4 for Environmental Barrier Coatings

B. P. Majee<sup>\*1</sup>; K. Bryce<sup>2</sup>; L. Huang<sup>3</sup>; J. Lian<sup>2</sup>

- 1. Rensselaer Polytechnic Institute, Department Of Mechanical, Aerospace, And Nuclear Engineering and Department of Materials Science and Engineering, USA
- 2. Rensselaer Polytechnic Institute, USA
- 3. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

Developing advanced environmental barrier coating (EBC) materials that simultaneously provide an appropriate coefficient of thermal expansions (CTEs), low thermal conductivity, and excellent CMAS and water vapor corrosion resistance is challenging. Herein, a single-phase multicomponent rare earth phosphate  $(Sc_{0.25}Lu_{0.25}Yb_{0.25}Er_{0.25})PO_4$  was synthesized, and its potential application for an EBC for SiC-based ceramic-matrix composites (CMCs) was investigated. The phase, CTEs, thermal conductivity, and microstructure are characterized using X-ray diffraction (XRD), dilatometry, laser flash technique, and scanning electron microscopy (SEM), respectively. The experimentally measured average CTE value is 6.46×10<sup>-6</sup> °C<sup>-1</sup>, which is close to that of the SiC-based CMC substrate (~4.5-5.5×10<sup>-6</sup> °C<sup>-1</sup>). The multi-component phosphates show low thermal conductivity (~3.0 W  $m^{-1}$  °C<sup>-1</sup> at 1000 °C) compared to its principal single-component REPO<sub>4</sub> (RE=Sc, Lu, Yb, and Er). The CMAS corrosion test at 1300 °C for different durations (5, 45, and 96 hours) shows the formation of dense and continuous reaction layers mainly composed of Ca<sub>8</sub>MgRE(PO<sub>4</sub>)<sub>7</sub> at the interface of phosphates/CMAS, and reaction layer halts CMAS penetration. Prolonged duration (45 and 96 hours) CMAS corrosion results show the formation of a disilicate (RE<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>) phase along with Ca<sub>8</sub>MgRE(PO<sub>4</sub>)<sub>7</sub>.

### 11:20 AM

### (ICACC-S2-016-2025) Molten silicate interactions with a luminate-based thermal/environmental barrier coatings

S. Berens\*1; C. S. Holgate1; C. G. Levi1; F. W. Zok1

1. University of California, Santa Barbara, Materials, USA

Rare-earth aluminate coatings are of interest as topcoat materials in thermal/environmental barrier coating (T/EBC) systems for both refractory alloy and CMC systems, owing to their high temperature stability in the moisture-laden gas turbine environment. Garnet formation is a promising strategy to mitigate attack by molten silicates by promoting the consumption of deposit components and formation of a protective film. Single-phase garnet coatings like Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> (YAG) dissolve and reprecipitate with a modified composition but are susceptible to substantial grain boundary penetration. A potential path to improvement is adding a second reactive phase to promote new garnet growth on existing (native) garnet, forming a barrier layer to further interaction. This study investigates the silicate interactions of YAG-based coatings with additions of 25 to 75 vol% YAlO<sub>3</sub> (YAP) to assess the formation and protectiveness of reaction layers through experiments using deposits with varied Ca:Si ratios. YAP reacts with the melt to form new garnet (G2) templating on native garnet (G1), which slows coating recession and mitigates penetration through pristine grain boundaries. Recession with high Ca:Si melts proceeds more slowly than with low Ca:Si, presumably because of differences in the  $YO_{1.5}$  solubility in G2. Implications for composite coating design will also be discussed.

### 11:40 AM

### (ICACC-S2-017-2025) Reactions between CAS Slag Melts and Ceramic Materials from TBCs or EBCs in Order to Find Protective Coatings for Components in Gasifier of IGCC

S. Kim\*1; M. Nam1; Y. Oh1; S. Lee1

1. Korea Institute of Ceramic Engineering and Technology, Engineering Materials Center, Republic of Korea

Gasifiers, which make syngas, mixture of hydrogen and carbon monoxide, are indispensable components of IGCC (Integrated Gasification Combined Cycle) power plants, operating under extreme environments characterized by high temperatures, elevated pressures, and exposure to corrosive slag melts. Corrosion by slag melts from raw coal feedstock, which is composed of calcia, alumina, and silica, has been a challenging issue in these components. In this study, reaction between slag melts and ceramic materials from TBCs or EBCs are examined in order to find the protective coatings for gasifiers, burners, and related components of IGCC. Mitigation approaches are explored primarily from a materials perspective as well. Special emphasis is placed on the effective strategies and their detailed components for minimizing slag corrosion in gasifier and burner systems.

## S3 22th Intl Symp on Solid Oxide Cells Materials Science & Technology

### **S3-Electrolysis and applications II**

Room: Ballroom 4 Session Chair: Federico Smeacetto, Politecnico di Torino

### 8:30 AM

### (ICACC-S3-008-2025) Advancing Production of e-Fuels through Pressurized Co-Electrolysis in Solid Oxide Electrochemical Cells (Invited)

J. Kupecki\*1; A. Niemczyk1; M. Bakala1; M. Kosiorek1; S. Jagielski1

1. Institute of Power Engineering - National Research Institute, Center for Hydrogen Technologies (CTH2), Poland

Solid oxide electrolyzers (SOE) offer a great advantage over low-temperature electrolyzers, which make them great candidates for intregration with downstream processes for synthesis of e-fuels. Moreover, SOE can be operated in co-electrolysis mode which makes it possible to simultaneously reduce H2O and CO2 in an electrochemical process. Additionally, co-SOE can be pressurized in order to increase activation resistance and elevate partial pressures of reactants at the triple phase boundary. Despite the great potential, up to date SOE were pressurized in only a few laboratories worldwide, therefore literature data are limited. In the recent study, two batches of 5 cm x 5 cm Ni-8YSZ supported cells with LSC oxygen electrode were investigated. Experimental studies included operation at the ambient pressure and measurements under pressurized conditions. The experimental campaing was constrained by two parameters (whichever occurs first): voltage equal 1.4 V or reaching limiting concentration of reactants at the outlet which correspond to carbon desposition isotherm under given working conditions. Upon completion of the in operando analysis, area specific resistance (ASR) was calculated and analyzed. The work integrates experimental tools and numerical modeling in order to predict performance and composition of gases exiting co-SOE.

### 9:00 AM

50

### (ICACC-S3-009-2025) State of the art of solid oxide cells from long-term operation to advanced post-test characterization (Invited)

A. Leon\*<sup>1</sup>; J. Schefold<sup>1</sup>; A. Micero<sup>1</sup>; S. Soille<sup>1</sup>

1. European Institute for Energy Research, Germany

High temperature steam electrolysis is advancing towards its industrialization to provide electrolytic hydrogen. The associated research and development targets to extend the durability of solid oxide cells, stacks, modules and ultimately the MW range and beyond electrolyzers. For that purpose, advanced electrolyte supported cells have been developed by the company Sunfire and three operation options have been explored by EIFER with a single cell test at high current density (-1.2 A/cm<sup>2</sup>) for 6,000 hours, with a compensation of the degradation by extending the temperature window of a cell to 100°C and with the demonstration of dynamic operation with ON/OFF switching in the millisecond scale of a 2.5 kW power stack. These operation strategies will be presented for cell and stack based on 3YSZ electrolyte. The cell performance and durability were characterized by appling in-situ impedance spectroscopy and complementary techniques based on X-ray fluorescence spectroscopy and X-ray diffraction. It will be shown that the degradation is mainly ohmic with contribution of electrodes at low temperature. 2D nanoscale mappings highlight the secondary phases formation at the interfaces and the evolution of the electrolyte structural phase. A comparison of the 8YSZ and 6Sc1CeSZ electrolytes analysis will be presented, and a correlation will be drawn to the measured ohmic degradation.

### 9:30 AM

# (ICACC-S3-010-2025) Impact of silicon contamination on high temperature electrolysis in MK35x solid oxide cell stacks

- A. Seidl\*1; S. Rothe1; S. Megel1; K. Develos-Bagarinao2; M. Kusnezoff1
- 1. Fraunhofer IKTS, Germany
- 2. National Institute of Advanced Industrial Science and Technology (AIST), Reserach Institute for Energy Conservation, Japan

Electrolysis with solid oxide cell stacks have the potential for high efficiency gas production when steam is available. To establish the technology on the market, an increase in performance and a reduction in the degradation rate are necessary which is often associated with impurities in the water vapor. Therefore, investigations on contamination effects of silicon in electrolysis mode were carried out. The stacks were contaminated with silicon by adding SiC or SiO<sub>2</sub> with different methods. A fixed volume fraction over the operating time could hardly be maintained since the material decomposes in the water vapor when placing it in a cartridge of the steam pipe of the test bench. That's why the initially high Si-concentration decreased during the operation. Results were shown and details of estimation of degradation will be given. The electrodes of electrolyte-supported cells essentially determine the degradation rate. Ni/GDC (nickel/gadolinia doped ceria) is used as a composite electrode on the fuel side. The cells were examined using various analysis methods (XRF, SEM, EDX, SIMS) to determine the influence of silicon on the electrode material. The results show that the Si-concentration in the samples is relatively low. It concentrates mainly at the fuel outlet. Both EDX and SIMS confirm silicon deposits on the GDC grains but not on Nickel or Nickel oxide.

### **S3- SOFC Applications**

Room: Ballroom 4

Session Chair: Eric Wachsman, University of Maryland

### 10:10 AM

# (ICACC-S3-011-2025) Development of metal-supported SOFC for vehicle application (Invited)

Y. Miura\*1

1. Nissan Jidosha Kabushiki Kaisha, Nissan Research Center, Japan

SOFC systems for both vehicle and stationary applications are developed in Nissan to reduce the carbon footprint. Metalsupported SOFCs exhibit higher mechanical strength compared to ceramic-supported SOFCs and are resistant to dynamic operation such as severe temperature distribution and redox. Fabrication process for metal-supported SOFCs has mainly involved powder metallurgy of ferritic steel particles or lase-drilling of metal plates. Since powder metallurgy allows for a higher open porosity of the metal-support compared to metal plates, it is particularly suitable for power generation under higher current density which required in vehicle applications. In automotive SOFC systems, compactness is required due to the limited space in the vehicle. As a solution to achieve system compactness, we have developed internal reforming SOFCs that integrates power generation and steam reforming by catalyst infiltration. After introducing Ni/GDC nanoparticles, power densities of 1.16 Wcm<sup>-2</sup> with hydrogen and 0.85 Wcm<sup>-2</sup> with methane are obtained at 600°C, 0.7 V. Since metal supports fabricated by powder metallurgy tend to have large surface areas, it degrades drastically under highly humidified conditions. To investigate appropriate composition of steel and morphology of the oxide film which prevent steam oxidation, the steam oxidation behavior of porous stainless steels with different Cr contents and additives is investigated.

### 10:40 AM

# (ICACC-S3-012-2025) Durability and kinetic effects of $\rm CO_2$ -rich mixtures on state of the art SOFC cathodes for applications in novel hybrid cycles (Invited)

M. Pagliari<sup>1</sup>; M. Marasi<sup>1</sup>; A. Donazzi<sup>\*1</sup>

1. Politecnico di Milano, Department of Energy, Italy

In the SOS-CO<sub>2</sub> cycle, a new hybrid cycle for blue power production, the SOFC cathode is fed with a dry CO<sub>2</sub>-rich oxidizing mixture (21%  $O_2$  79%  $CO_2$ ), and the anode is fed with a  $CH_4$ -based reformate mixture. While steam-rich mixtures degrade conventional perovskite cathodes, the kinetic consequences and the long term effects of dry CO<sub>2</sub>-rich atmospheres are much less known. State of the art Ni-YSZ SOFCs (25 cm<sup>2</sup>, SolydEra) with LSCF-GDC  $(La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta})$  and LSM-YSZ  $(La_{0.8}Sr_{0.2}MnO_{3-\delta})$  cathodes were tested under the SOS-CO<sub>2</sub> cycle's conditions (700°C, 0.85 V) up to 1300 h to verify possible deterioration due to CO<sub>2</sub>, with I/V and EIS measurements. The kinetic effect of CO<sub>2</sub> was studied via EIS on symmetric button cells with  $O_2/CO_2$  mixtures, between 700 and 550°C, and power law rates were derived. LSCF, LSM and LSC  $(La_{0.6}Sr_{0.4}CoO_{3-\delta})$  powder samples were also analyzed with operando XRD and NAP-XPS (Alba synchrotron, Barcelona) to investigate the temporal evolution of the bulk and surface properties of each perovskite, upon exposure to the 21% O<sub>2</sub> 79% CO<sub>2</sub> mixture at 700°C up to 3 h and 20 bar. The results showed that CO<sub>2</sub> inhibits the oxygen reduction reaction rate of the LSCF-GDC cathode, due to Sr carbonate formation. No kinetic effect and no carbonate were found on LSM-YSZ. In both cases, the effect of CO<sub>2</sub> revealed reversible when air supply was restored.

### 11:10 AM

### (ICACC-S3-013-2025) Internal Reforming SOFC Using Carbon-neutral Fuels Synthesized by Co-electrolysis SOEC (Invited)

H. Sumi $^{*1}$ 

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Previously, a long-term flight of a drone (UAV; unmanned aerial vehicle) driven by a solid oxide fuel cell (SOFC) using liquefied petroleum gas (LPG) was successfully demonstrated. However, LPG is a fossil fuel. To achieve a carbon-neutral society, syngas (H2+CO mixture) can be produced from steam and CO2 by a solid oxide electrolysis cell (SOEC) using renewable energy sources such as solar and wind power. As a result of quantitative analysis of the gas composition in this study, The H2/CO ratios of the product gases were identical to the H2O/CO2 ratios of the input gases for a co-electrolysis microtubular SOEC. The syngas with an H2/CO ratio of 2 can produce synthetic gasoline, kerosene, and diesel (e-fuel) via Fischer-Tropsch (FT) synthesis. Methanol (MeOH) and dimethyl ether (DME) are industrially produced from syngas. MeOH can be converted into gasoline (MTG; methanol to gasoline), olefin (MTO; methanol to olefins) such as ethylene and propylene, and aromatics (MTA; methanol to aromatics) such as benzene, toluene, and xylene. MTO will contribute to carbon-neutral manufacturing processes for commodity plastics (e-chemical). For mobile applications such as drones, robots, and vehicles, internal reforming SOFCs using MeOH and DME were successfully operated for 100 h in this study.

## S4 Advanced Materials for Thermoelectric and Thermionic Energy Conversion

# S4- Advanced Materials for thermelectric and thermionic energy conversion I

Room: Coquina D

Session Chairs: Sepideh Akhbarifar, The Catholic University of America; Michitaka Ohtaki, Kyushu Daigaku

### 8:30 AM

### (ICACC-S4-001-2025) Engineering of thermoelectric properties in half-Heusler and metal phosphide materials (Invited)

J. Bos\*1

1. University of St Andrews, United Kingdom

Thermoelectric conversion can be used to generate power, scavenge ambient heat and is used in thermal management. We have focused on intermetallic half-Heusler materials, and more recently on metal phosphides. Both are based on abundant elements and could provide a route towards sustainable thermoelectric energy conversion. In the half-Heusler materials, we pioneered the use of interstitial Cu in the leading XNiSn n-type compositions. This enables synergistic reductions of lattice thermal conductivity and improvements in the electronic quality of the materials. Competitive figures of merit, zT = 1 at 793 K are found for compositions with high X = Ti content. We have used aliovalent alloying in Zn<sub>0.5</sub>Ti<sub>0.5</sub>NiSb to achieve unusually low lattice thermal conductivities, far below expected based on mass and strain disorder. We postulate that this is driven by bond disorder, which also reduces the electronic quality of the materials. This limits the maximum achievable performance, requiring a careful trade-off between thermal and electronic parameters. Metal phosphides are underexplored but offer great structural diversity, often achieving low thermal conductivities, despite low gravimetric densities. CaCuP in particular seems to hold promise for applications based on its good mobility and large power factor, achieving zT = 0.5 at 793 K.

### 9:00 AM

## (ICACC-S4-002-2025) Strain engineering for boosting the thermoelectric performance of modulus-scale silicon (Invited)

B. Xu<sup>+1</sup>; R. Nagahiro<sup>1</sup>; Y. ikoma<sup>2</sup>; M. Kohno<sup>2</sup>; M. Ohnishi<sup>1</sup>; S. Terashima<sup>3</sup>; E. Iwase<sup>3</sup>; J. Shiomi<sup>1</sup>

- 1. Tokyo Daigaku, School of engineering, Japan
- 2. Kyushu Daigaku, Japan
- 3. Waseda Daigaku, Japan

Silicon thermoelectric materials are among one of the most promising candidates for low-cost, clean energy harvesting. However, a significant challenge lies in sufficiently reducing silicon's high thermal conductivity without compromising its electrical conductivity, especially when fabricating it in the module-scale. To address this issue, we employed a strain-engineering approach in addition to the conventional "size effect" strategy. Our research began with a high-pressure torsion process, through which we introduced inhomogeneous strain into nanocrystalline silicon. In this system, we verified the effectiveness of inhomogeneous strain, demonstrating that both interfacial and overall strain contribute to the reduction of thermal conductivity. Building on this insight, we applied the findings to a sintering process aimed at enabling the mass production of module-scale silicon thermoelectric materials. We proposed a three-dimensional architecture composed of nanosized grains connected by narrow conduction paths and developed a low-pressure, rapid sintering procedure for its fabrication. This structure effectively suppresses phonon thermal conductivity without compromising electrical conductance. The silicon exhibited superior performance compared to previous studies, as further demonstrated in a flexible thermoelectric device, which powered a wireless sensor continuously for 24 hours.

### 9:30 AM

### (ICACC-S4-003-2025) Micro-thermoelectric devices (Invited)

K. Nielsch\*1; H. Reith1

1. Leibniz Institute for Solid State and Materials Research, Institute of Metallic Materials, Germany

Sustainable energy harvesting and efficient thermal management are required for the development of highly integrated electronic devices, the Internet of Things, and flexible and wearable technology. Microthermoelectric devices, which are capable of generating electricity from waste heat or using electricity to generate local cooling, are a promising solution. The devices have, in particular, a smaller leg cross-section and height than their commercial, macroscopic counterparts and can thus offer a faster response, higher resolution and greater power density. They can also be integrated with multifunctional microelectronic devices. Here we present the development of micro-thermoelectric devices based on electrochemical deposition. We examine progress in device design, integration, characterization and performance, and explore potential applications in cooling, power generation and sensing. We also analyse the key challenges that need to be addressed to create high-performance devices and realize the full commercial potential of the technology.

### S4- Structure/property relationships, thermodynamics, and solid-state defect chemistry of thermoelectric/thermionic materials

Room: Coquina D

Session Chairs: Kornelius Nielsch, Leibniz Institute for Solid State and Materials Research; Navita Jakhar, Institute of Science and Technology Austria

### 10:20 AM

# (ICACC-S4-004-2025) Structure-thermal property relationships and low thermal conductivity materials (Invited)

G. S. Nolas<sup>\*1</sup>

1. University of South Florida, Physics, USA

Obtaining high performance devices is a complex problem for which new materials research is paramount, and continuously building a basic understanding of structure-property relationships is essential in advancing technological applications of interest. Moreover, investigations into new compositions expand our library of materials and provide potential new avenues for discovery, allowing for pathways towards the design of materials, and processing techniques, with targeted properties for specific applications of interest. Furthermore, an understanding of the thermal properties of materials is vital for any application of interest, and essential for thermoelectrics. In this regard, low thermal conductivity is obtained for specific structural and bonding features such as weak bonds, disorder, coordination preferences, lone pair electrons and anharmonicity. Motivated by these considerations, and my ongoing interest in thermal properties of matter as well as the study of previously unexplored materials and compositions, I will present results on the structure-property relationships of the recent materials my group has been investigating in providing an understanding of the fundamental properties of a variety of structure types, with a particular focus on thermal properties.

### 10:50 AM

## (ICACC-S4-005-2025) The emerging role of type II Si clathrate, an alternative low-density Si allotrope (Invited)

Y. Liu\*1; J. P. Briggs1; M. Singh1; R. T. Collins1; C. A. Koh1

1. Colorado School of Mines, USA

Like carbon, Si forms various crystalline allotropes beyond traditional d-Si. One such form includes expanded Si phases of guest-host structures with guest atoms occupying large interstitial sites in the cages or channels. Some of these structures have been stabilized under atmospheric conditions, opening up novel applications in optoelectronics, computing, PV, and energy storage. This work highlights advances in low-density Si allotropes, especially type II Si clathrates, inclusion compounds with Si cages encapsulating guest atoms, typically Na. By reducing Na levels to  $\sim 10^{18}$ /cm<sup>3</sup>, these low-doped clathrates are explored for semiconductor applications with Na as shallow donors. Their band edge characteristics show a direct bandgap near 1.7 eV and an absorption coefficient much higher than d-Si. Room-temperature PL in the near-infrared region suggests potential LED applications. Thermal diffusion of Li into clathrate frameworks synthesized Li<sub>x</sub>Si<sub>136</sub>, introducing a novel method for guest incorporation into Si clathrate with potential battery applications. Pulsed EPR spectra of Na donors in type II Si clathrate revealed spin behaviors similar to donors in d-Si, suggesting potential spin-based applications. These findings underscore the promise of low-density Si allotropes, especially Si clathrates, as viable alternatives to d-Si in advanced applications. Supported by NSF Awards 1810463 and 2114569.

### 11:20 AM

# (ICACC-S4-006-2025) Phases, microstructures, and thermoelectric Properties of n-type $Mg_3Sb_2$ -based thermoelectric materials (Invited)

S. Chen\*1

1. University of Houston, Physics and TcSUH, USA

N-type Mg<sub>3</sub>Sb<sub>2</sub>-based compounds exhibit excellent thermoelectric figure of merit (zT) while offering advantages in cost-effectiveness and superior mechanical properties. The composition of these materials involves careful alloying, such as Mg<sub>3.2</sub>Sb<sub>2-x-y</sub>Bi<sub>x</sub>Te<sub>y</sub>. However, the complexity of the defect microstructure impedes the advancement of high performance. For instance, our high-resolution transmission electron microscopy analysis suggests that the Bi phase form at the grain boundaries may act as scattering centers due to the difference in work functions with Mg<sub>3</sub>Sb<sub>2</sub>. In our recent study, we verify the presence of resistive grain boundaries and resistive phases in Mn-substituted compositions. These resistive grain boundaries and phases not only deteriorate the material's performance but also induce a transition from n-type to p-type behavior. Furthermore, the optimized composition results in an average zT of 1.37 and a peak zT of 1.74 was achieved at 573 K, with a zT of 0.72 measured at room temperature. Our work investigates the pivotal role of dopant concentration in the Mg<sub>3</sub>Sb<sub>2</sub> matrix, focusing on minimizing defect microstructure and improving the electronic and thermal transport properties.

### 11:50 AM

## (ICACC-S4-007-2025) Chemistry is Key in Solution-Based Thermoelectric Material Synthesis!

C. S. Fiedler<sup>\*1</sup>; M. Ibáñez<sup>1</sup>

1. Institute of Science and Technology Austria, Austria

Thermoelectric materials, which convert heat to electricity and vice versa, have many potential applications. However, current fabrication methods with superior performance are prohibitively expensive, limiting large-scale use. Solution processing offers a more affordable alternative with significantly lower temperatures, shorter reaction times, and more relaxed chemical purity requirements. Despite these advantages, the process's complexity arises from often-overlooked chemical transformations occurring during particle synthesis, purification, and densification. Alarmingly, many breakthrough studies lack detailed reporting of these steps, hindering reproducibility across laboratories. Herein, we emphasize the importance of these steps, particularly focusing on the often-neglected particle purification. Our investigation centers on a water-based, surfactant-free solution synthesis, a cost-effective method for producing thermoelectric powders, with SnSe selected due to its relevance in thermoelectric applications. We demonstrate the impact of leaching steps, purification solvent, annealing, and atmosphere

on thermoelectric performance. Our study reveals that differences in composition, such as the Sn:Se ratio and impurity content, are influenced by pre-densification steps. Our primary goal is to stress the importance of understanding chemical processes and detailed reporting to ensure material reproducibility.

## <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

### **S6- Battery Materials Design and Characterization I** Room: Coquina B

Session Chairs: Naoaki Yabuuchi, Yokohama National University; Olivier Guillon, Forschungszentrum Juelich

### 8:30 AM

# (ICACC-S6-009-2025) Thermal Runaway Risk and Li-ion Battery State-of-Health Monitoring (Invited)

H. Wang\*<sup>1</sup>; L. Lin<sup>1</sup>

1. Oak Ridge National Laboratory, USA

Thermal runaway is a major safety concern for Li-ion batteries. In practice, the cells have different chemistries, capacities and can be at different state-of-charge. It is difficult to compare thermal runaway risks among different cells. Only limited number of cells can be tested in a single study making comparison of test results impossible because test conditions are different. We developed a standard indentation test with Sandia Labs to use cell voltage and temperature as a function of time after the initiation of internal short circuit to calculate a thermal runaway risk (TRR) score. The test data and TRR scores are available via an open-access website. A summary of the thermal runaway data and analysis tools will be discussed. During the cell preparation and abuse testing of Li-ion cells, voltage and temperature are recorded to monitor the state-of-health (SOH) of the cell. They can be used to monitor potential cell damages and predict over-temperature and thermal runaway events. We recently added acoustic emission (AE) sensors to collect signals during mechanical and thermal abuse testing. The AE signals are sensitive to the internal gas generation and mechanical failures of the electrode materials. The gas generation signals occur below 100°C and can potentially be used as early warning of cell overheating to prevent thermal runway.

### 9:00 AM

### (ICACC-S6-010-2025) Thermochemical Pathways and Safety Strategies for Next-Generation Lithium-Ion Batteries: A Comparative Study of Liquid and Solid-State Systems (Invited)

V. Rikka\*1; W. Tang1; J. Jeevarajan1

1. UL Resarch Institutes, Electrochemical Safety Research Institute (ESRI), USA

As the global shift toward electric vehicles (EVs) accelerates, the demand for safer and more efficient lithium-ion batteries is at an all-time high. Achieving breakthroughs in energy density, cycle life, and safety, particularly under fast charging conditions, requires a deeper understanding of these systems' thermal and chemical behaviors. This study presents a pioneering thermochemical analysis of NMC811/Graphite (half and full) cells with a conventional liquid electrolyte (1.2M LiPF6 (3:7 EC: EMC)) in comparison to LLZO (Lithium Lanthanum Zirconium Oxide) solid-state electrolyte. Using a combination of analytical techniques, including thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC), coupled with gas chromatography time-of-flight mass spectrometry (GC-TOFMS), we have investigated the decomposition mechanisms and thermal stability of both cell types. We provide a mapping of safety hazards, such as electrolyte decomposition and thermal runaway, under fast charging and deep discharges. This approach not only contrasts the safety profiles between the liquid

and solid-state systems but also delivers actionable safety mitigation strategies for both. Also, our findings address a structured approach to establishing comprehensive safety protocols and guidelines that can influence the future of battery innovation.

### 9:30 AM

# (ICACC-S6-011-2025) $\mathrm{K_xFeO_2}$ as electrode material for K-ion batteries

- A. Sagot<sup>1</sup>; M. Sougrati<sup>3</sup>; V. M. Kovrugin<sup>1</sup>; L. Stievano<sup>2</sup>; V. Pralong<sup>\*1</sup>
- 1. CNRS ENSICAEN, France
- 2. Université de Montpellier, Institut Charles Gernardt Montpellier, France
- 3. CNRS ICGM, France

To meet future energy demands, developing beyond-lithium energy storage technologies has become a major part of global research activities. Potassium-ion batteries (KIBs) are promising technology thanks to their chemical and economic advantages. The majority of the work on layered transition oxide was done on the K<sub>x</sub>MnO<sub>2</sub> family due to their safety and price advantage. Interestingly, KFeO<sub>2</sub> structure is not a layered structure as for LiFeO<sub>2</sub> or NaFeO<sub>2</sub>; this structure is defined as FeO<sub>4</sub> tetrahedral linked by their corners. In electrochemistry, a reversible capacity of 60 mAh/g (for 0.3K<sup>+</sup>) was delivered. In our presentation, we will detail the electrochemical behavior of KFeO<sub>2</sub> and discuss the structure/properties relationship of this family of materials, showing interest in exploring such a system.

## S6- Electrode Materials Design and Characterization II

Room: Coquina B

Session Chairs: Olivier Guillon, Forschungszentrum Juelich; Naoaki Yabuuchi, Yokohama National University

### 10:15 AM

### (ICACC-S6-012-2025) Molten Solvate Electrolytes: Unique Transport Properties and Interfacial Reactions (Invited)

R. Tatara\*1; K. Dokko1

1. Yokohama National University, Japan

Conventional liquid electrolytes in Li-ion batteries are composed of Li salts dissolved in organic solvents, enabling the conduction of Li<sup>+</sup> ions. However, when the salt concentration exceeds approximately 3 mol/L, the resulting molten solvate electrolytes—or concentrated electrolytes—display markedly different characteristics compared to traditional electrolytes (~1 mol/L). These characteristics include reduced volatility and flammability, an expanded electrochemical window, enhanced rate performance driven by hopping conduction, distinct electrode reactions, and reduced interfacial reactivity. These changes are largely attributed to a decrease in the activity of free solvent molecules that are uncoordinated with Li<sup>+</sup> ions. This study explores the physicochemical properties of these concentrated electrolytes and examines their electrochemical behavior in the context of next-generation batteries.

### 10:45 AM

### (ICACC-S6-013-2025) Operando Optical Imaging Platforms to Study Battery Reactions (Invited)

X. Shan<sup>\*1</sup>; G. Thomas<sup>1</sup>; X. Zhao<sup>1</sup>

1. University of Houston, Electrical and Computer Engineering, USA

Increasingly complex and heterogeneous chemical reactions on the battery require the characterization methods to provide a complete picture of molecular interactions across the interface in situ. For example, the biggest challenge in accelerating the Li metal batteries towards higher energy density is the lack of fundamental understanding of interfacial chemical reaction. Inhomogeneity in reaction activity/deposition rate, chemical compositions, and ionic and electrical conductivity on the battery electrode will cause the non-uniform Li-ion diffusion, and lead to inhomogeneous

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nucleation and dendrite formation. We have developed a multimodal optical imaging platform to image the battery electrode reaction dynamics across the interfaces throughout the entire reaction process. We have developed reflection interference microscope (RIM) which allows us to study and image the SEI formation dynamics, and Li nucleation process. Using this system, we have comparied the SEI and Li nucleation in LCE, HCE and LHCE electrolytes. We have also developed optical microscope together with an in-situ Raman platform to study the solid state battery reactions in situ. We image the Li diffusion process through the cathode and solid electrolyte layer, and try to understand the battery performance and safety under high temperature conditions.

### 11:15 AM

# (ICACC-S6-014-2025) Electrode architecture design by high throughput style microstructure simulations (Invited)

H.  $Yu^{*1}$ 

1. Michigan State University, Computational Mathematics Science and Engineering, USA

While a battery's operational performance is dictated by electrode microstructures, its importance is often overlooked. As such, optimal performance of electrodes is hardly achieved, especially at high-rate cycling. Due to the complexities of Multiphysics coupling and complicated geometries in microstructures, electrode design to enhance cell performances still heavily replies on trial-and-error lab efforts. High-speed, high-fidelity microstructure simulations can provide a new reality to conduct on-chip, digital experiments to investigate the underlying complex relationship between intrinsic materials properties, microstructures, and cell performance of batteries. In this talk, we will demonstrate a framework able to simulate electrochemical processes directly on experimentally reconstructed electrode microstructures. Thanks to the unique capability of rapidly implementing direct voxel-based simulations, we will present a high-throughput style of large-scale autonomous microstructure simulations, which allows the screening of optimal secondary structures, e.g., tunnels, for high-capacity thick electrodes at high charge rates. We believe this technique will be greatly useful for battery developers and researchers.

## <u>S7 19th Intl Symp on Functional</u> <u>Nanomaterials & Thin Films for Sustainable</u> <u>Energy Harvesting</u>

# S7- Nanomaterials for energy conversion, storage and catalysis- II

Room: Flagler C Session Chair: Muhammet Toprak, KTH Royal Institute of Technology

### 8:30 AM

# (ICACC-S7-009-2025) Syngas economy with green hydrogen for rapid decarbonization of fuels and chemicals (Invited)

S. Kim<sup>1</sup>; Y. Song<sup>2</sup>; A. Karluk<sup>1</sup>; J. Mahmood<sup>1</sup>; C. T. Yavuz<sup>\*1</sup>

- 1. King Abdullah University of Science and Technology, Saudi Arabia
- 2. Max-Planck-Institut fur Kohlenforschung, Germany

To devise a sustainable energy portfolio, we must consider a hybrid model of renewable-energy-powered low-carbon fossil fuel production as a transitional energy technology. At the heart of such transition is synthesis gas (syngas), a mixture of gaseous carbon monoxide and hydrogen. Syngas is currently the primary source of hydrogen for vehicles and has been the core building block in the chemicals industry for liquids, particularly alcohols, olefins, and low molecular weight fuels. We have developed a Ni-Mo-MgO nanocatalyst that facilitates syngas production from the dry reforming of methane without coking or sintering, even after 35 days of continuous operation. Switching syngas production from steam reforming to dry reforming could provide gigatons of  $CO_2$  avoidance without significantly altering our lifestyle, this emissions relief could provide the necessary time for a successful implementation of future energy technologies. An estimated 15-50% reduction in carbon emissions is possible without any change to the infrastructure. Further reductions would be introduced if syngas was produced from a range of sources, such as biomass, waste, plastics, or paper. For green hydrogen through alkaline electrolysis, we have developed a robust nanocatalyst coated electrode that runs 1,000 hours at 1 A/cm<sup>2</sup> current density under a combined overall cell voltage of 3 V.

### 9:00 AM

## (ICACC-S7-010-2025) High entropy nanoparticles as oxygen catalysts for metal-air batteries (Invited)

A. Cabot\*1

1. Catalonia Institute for Energy Research, Spain

High entropy materials (HEMs) are solid solutions of five or more elements with high thermodynamic and kinetic stability, that hold great promise in the field of electrocatalysis owing to their high configurational entropy, subtle distortions of the atomic arrangement and electronic density, and potentially strong synergistic effects to optimize the adsorption energies and electrical conductivity. HEMs also offer numerous degrees of freedom to fine-tune the material structural, electronic, and catalytic properties. Overall, the use of HEMs is a powerful strategy to optimize the surface adsorption properties, catalytic active centers, electronic structures, and consequently the redox catalytic activity within different electrochemical technologies. I will present our recent work on the colloidal synthesis of HEM nanoparticles, discuss their electrocatalytic properties and demonstrate their potential as oxygen catalysts at the cathode of metal-air batteries.

### 9:30 AM

# (ICACC-S7-011-2025) Active site switching on high entropy phosphides as bifunctional oxygen electrocatalysts for rechargeable/robust Zn-air battery

R. He\*1; L. Yang1; A. Cabot1

1. Institut de Recerca en Energia de Catalunya, Spain

High-entropy materials offer a quasi-continuous spectrum of active sites and have generated great expectations in fields such as electrocatalysis and energy storage. Herein, we have synthesized FeCoNiPdWP high entropy phosphide (HEP) nanoparticles and explored their application as bifunctional electrocatalysts for the oxygen evolution and reduction reactions (OER/ORR). The HEPs exhibit an exceptionally low OER overpotential of 227 mV at 10 mA cm<sup>-2</sup>, attributed to the reconstructed HEP surface into a FeCoNiPdW high entropy oxyhydroxide with high oxidation states of Fe, Co, and Ni serving as the active sites. Additionally, Pd and W play crucial roles in modulating the electronic structure to optimize the adsorption energy of oxygen intermediates. For the ORR, Pd emerges as the most active component. In the reconstructed catalyst, the strong d-d orbital coupling of especially Pd, Co, and W fine-tunes ORR electron transfer pathways, delivering an ORR half-wave potential of 0.81 V with a pure four-electron reduction mechanism. Furthermore, the assembled zinc-air batteries demonstrate a superior specific capacity of 886 mA h gZn<sup>-1</sup> and maintain excellent stability for 700 hours. Overall, this study elucidates the role of each element in HEMs and provides a foundation for designing next-generation bifunctional oxygen catalysts.

# S7- Nanomaterials for energy conversion, storage and catalysis- III

Room: Flagler C

Session Chair: Andreu Cabot, Catalonia Institute for Energy Research

### 10:20 AM

# (ICACC-S7-012-2025) Defect Engineering in Hydrogenated ${\rm TiO_2}$ Hollow Spheres Toward Efficient Photocatalysis (Invited)

E. Moretti\*1; L. Liccardo2; M. Bordin1

- 1. Ca' Foscari University of Venice, Department of Molecular Sciences and Nanosystems, Italy
- 2. Istituto di Struttura della Materia-CNR (ISM-CNR), SS 14, Km 163.5, 34149 Trieste, Italy, Italy

Nanostructured TiO<sub>2</sub> is considered one of the best materials for photocatalysis due to its high surface area, reactivity, excellent chemical stability and ease of synthesis. However, its large energy bandgap limits the use of the full solar spectrum. This work demonstrates how the combination of defect and morphology engineering, e.g. the creation of defect-engineered nanostructured TiO<sub>2</sub> photocatalysts, may be a very good strategy to extend the light absorption ability up to the near-infrared region. In detail, hydrogenated TiO<sub>2</sub> hollow spheres (THS), composed of hierarchically assembled nanoparticles, significantly broaden the solar spectrum utilization and enhance charge generation for photocatalytic reactions such as organic pollutants photo-oxidation. Specifically, when applied for photodegradation of Ciprofloxacin, a common antibiotics, these photocatalysts enable to achieve over 80% degradation after 6 hrs under simulated sunlight. Photoelectron spectroscopy valence band analysis reveals an increase in oxygen vacancies correlated with the hydrogenation rate, establishing a direct link between hydrogenation degree and photocatalytic activity. Additionally, electron paramagnetic resonance identifies bulk Ti<sup>3+</sup> centers exclusively in hydrogenated THS. These results pave the way for highly efficient photocatalytic titania in applications such as water remediation and solar fuel production.

### 10:50 AM

### (ICACC-S7-013-2025) Study of carbon monoxide oxidation and hysteresis behavior on mesoporous silica supported metal nanocatalyst (Invited) *WITHDRAWN*

R. M. Al Soubaihi\*1; K. M. Saoud1; J. Dutta2

1. VCUarts Qatar, LAS, Qatar

2. Kungliga Tekniska Hogskolan, Applied Physics, Sweden

We utilized the sol-gel and self-templating processes in synthesizing three types of porous silica nanomaterials, mainly aerogels (SiO<sub>2</sub> AG), xerogel (SiO<sub>2</sub> XG), and nanosheets (SiO<sub>2</sub> NS). SiO<sub>2</sub> AG, SiO<sub>2</sub> XG, and SiO<sub>2</sub> NS are explored as metal support materials (M/SiO<sub>2</sub>) for environmental applications such as CO oxidation. The M/SiO<sub>2</sub> morphology was experimantally studied before, during, and after the CO oxidation reaction under various pretreatment and reaction parameters to understand the chemical and physical changes occurring on the catalyst. The catalyst pretreatment conditions can affect CO conversion efficiency at light-off temperatures  $(T_{ig})$  because of their effect on surface area and particle size, which have a substantial impact on diffusion and mass transport of reactants (CO, O<sub>2</sub>) and products (CO<sub>2</sub>) and active sites accessibility. The lowest  $T_{ig} \sim$ 195 deg.C and 65 deg.C for Pd/a-SiO<sub>2</sub> aerogel and Ag/a-SiO<sub>2</sub> aerogel catalysts treated in the  $CO/O_2$  mixture, respectively. The hysteresis behavior was explored on Pd/SiO<sub>2</sub>, and a normal hysteresis was observed due to the increased stability of the active sites. In contrast, the Ag/a-SiO<sub>2</sub> showed an inverse counter-clockwise CO oxidation hysteresis. Cyclic and long-term stabilities of the catalysts were investigated, where Pd/a-SiO<sub>2</sub> showed good stability for four consecutive cycles and long-term stability for ~ 27 hrs.

#### 11:20 AM

# (ICACC-S7-014-2025) Nanofibrous ceramic membranes in plasma-catalytic reactors for greenhouse gas conversion

- R. A. Yager<sup>\*1</sup>; A. Stanishevsky<sup>1</sup>; R. M. Nick<sup>1</sup>; T. Berry<sup>1</sup>; S. Nealy<sup>2</sup>
- 1. University of Alabama at Birmingham, Physics, USA
- 2. The University of Alabama at Birmingham College of Arts and Sciences, Chemistry, USA

Greenhouse gas (GHG) emissions have become a critical issue in recent years. Current technologies converting GHGs have issues with high cost and scalability. This is an investigation of low-pressure, non-thermal plasma enhanced catalysis using ultraporous (>90%) nanofibrous ceramic catalyst to convert GHGs. Preliminary data shows the incorporation of nanofiber catalytic membranes (NFCM) in low-pressure plasma systems can result in advanced plasma-driven catalysis with increased selectivity and efficiency. Dielectric barrier discharge (DBD) based plasma reactors with NFCM have been designed due to their low operating temperatures and their relatively low cost and simplicity in design. The NFCMs were derived using an uncommon process of high-yield, free surface alternating field electrospinning (AFES), which has shown to increase production rates compared DC electrospinning. Integration of NFCMs made of TiO<sub>2</sub>, ZrO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> and B<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> ceramic nanofibers into the plasma catalytic system have shown to improve selectivity of reactions with CO<sub>2</sub> and CH<sub>4</sub> into high-valued products such as O2, H2, MeOH, and various oxygenates. Nanofiber characterization methods including XRD, SEM, gas transport and mechanical testing determined the crystalline structure as well as their performance as catalysts. Gas chromatography, FTIR, and OES were used to measure the produced species of the reactions.

### 11:40 AM

## (ICACC-S7-015-2025) Improved robustness of spinel oxide catalysts for biomass utilizations

S. Yamaguchi\*1; Y. Nagashima1; T. Suyama1; T. Ozaki1; M. Ootani2

- 1. Osaka Research Institute of Industrial Science and Technology,
- Applied Material Chemistry, Japan
- 2. Kansai Catalyst Co., Ltd., Japan

To control climate changes, more amount of biomass has been utilized as one of renewable energy sources these days. Biomass can be converted to gasified gas containing hydrogen, carbon monoxide, and methane via gasification, a thermo-chemical process. Gasified gas also contains tar composed of long chain hydrocarbons and aromatic compounds that brings about clogging filters or flow channels. We have elucidated that tar can be reformed efficiently by reduced oxides containing Ni-Al spinel oxide (NAO) and NAO added with partial stabilized zirconia (NAZO). The conventional catalysts rolling granulated over porous alumina balls possess high activity for tar conversion but poor robustness. Especially, substances of NAO and NAZO peeled off easily from the catalyst surface. For evaluation of robustness, we adopted a shaking method for catalyst instead of a conventional measurement of crush strength. Peeled off amount of the catalyst was measured after shaking catalyst for a fixed period. More robust catalyst was obtained by optimizing the particle size distribution of catalyst and temperature for calcination. This catalyst is planned to be demonstrated in a power generation system converting biomass to electricity using solid oxide fuel cells. These results contribute to more stable, efficient, and less expensive power generation systems.

### 12:00 PM

### (ICACC-S7-016-2025) ZnO Nanowall/Polymer Hybrid Nanogenerators: Efficient Energy Harvesting for Wearable Devices

- G. Yüksel\*1; B. Göl3; S. Kinden2; E. Suvaci1
- 1. Eskisehir Teknik Universitesi, Materials Science and Engineering, Turkey
- 2. Eskisehir Teknik Universitesi, Electrical and Electronics Engineering, Turkey
- 3. Kahramanmaras Sutcu Imam Universitesi, Electrical and Electronics Engineering, Turkey

The rise of wearable devices in the 21st century has intensified concerns about energy demand, as traditional batteries often present recycling challenges. This scenario has spurred the development of flexible, alternative energy harvesting systems. Piezoelectric and triboelectric nanogenerators have emerged as promising solutions. Complying with EU RoHS regulations, lead-free materials such as ZnO have become a preferred choice for fabricating PENG and TENG. The research objective of this study was designing a flexible hybrid nanogenerators for wearable systems, combining ZnO nanowall arrays with polymers. ZnO nanowall arrays were synthesized on a flexible substrate by the hydrothermal method. Then, sandwich-like structures with ZnO nanowalls and various polymers were constructed as hybrid nanogenerators. The energy harvesting performance of these nanogenerators was measured under constant mechanical force. The results show that the incorporation of polymers into the ZnO nanowall-based piezoelectric system introduced a triboelectric effect, leading to 10-fold increase in output voltage. This enhancement is influenced by the static charge capacity of the polymer used. The study highlights the potential of ZnO nanowall/ polymer hybrid systems to enhance energy harvesting in wearable devices, offering a more sustainable and efficient alternative to traditional battery-powered systems.

## <u>S8 19th Intl Symp on APMT for Structural &</u> <u>Multifunctional Materials & Systems</u>

# **S8-** Green manufacturing, global environmental issues and standards

### Room: Flagler A

Session Chairs: Thi Mai Dung Do, Nagaoka University of Technology; Hyun-Sik Kim, University of Seoul

### 8:30 AM

(ICACC-S8-009-2025) Fabrication of  $Li_{3.5}Ge_{0.5}V_{0.5}O_4$ -based composite solid electrolyte (Invited)

S. Tanaka\*1

1. Nagaoka University of Technology, Materials Science and Technology, Japan

To fabricate oxide batteries, the sintering temperature of the solid electrolyte must be lower than that of conventional electrolytes, since it is necessary to co-sinter the solid electrolyte with the electrodes. However, among the candidate electrolyte materials, Li<sub>3.5</sub>Ge<sub>0.5</sub>V<sub>0.5</sub>O<sub>4</sub> (LGVO) is known to have a relatively low sintering temperature, but its ionic conductivity is not high at 10<sup>-6</sup> Scm<sup>-1</sup>. The purpose of this study was to develop a new composite solid electrolyte that combines LGVO with a high ionic conductive material, aiming to achieve both low-temperature sintering and high ionic conductivity. Specifically, we investigated the combination of LGVO with Li<sub>67</sub>La<sub>3</sub>Zr<sub>1.7</sub>Ta<sub>0.3</sub>O<sub>12</sub> (LLZTa), a material that exhibits high ionic conductivity. First, LGVO ceramics was fabricated at a sintering temperature of 700°C, and the relative density reached 96.3%. The ionic conductivity was 7.91×10<sup>-6</sup> Scm<sup>-1</sup>. Next, a mixed powder of LGVO and LLZTa with a volume ratio of 7:3 was prepared, molded, and sintered. The sintered body was produced at a sintering temperature of 700°C, and had a relative density of 72%. Finally, Li<sub>3</sub>BO<sub>3</sub> was mixed as a sintering aid,

and forming and sintering were carried out under the same conditions. As a result, the relative density of the sintered body was 90%, and the ionic conductivity was  $5.2 \times 10^{-5}$  Scm<sup>-1</sup>, both of which were higher than those of LGVO alone.

### 9:00 AM

### (ICACC-S8-010-2025) Effect of Raw Materials in Development of Ceramic Alkaline Balls for Alkaline Drinking Water (Invited)

L. K. Sharma\*1; C. Agarwal2

- 1. Mahamana Ceramic Development Organization, India
- 2. AEC Overseas Consultants, United Arab Emirates

Investigations were carried out for the development of Ceramic Alkaline Balls for drinking water by using different types of clays, calcium tri poly phosphate, calcined ox bones, Soda feldspar and calcite with different ceramic stains additives for colouring. Major and minor raw materials were used in different ratios. TDS and pH of water were tested before and after adding ceramic balls. Water absorption, apparent porosity of the balls were optimised to almost less than 1% by firing at 1180, 1200 and 1225°C for 120minutes soaking period. Balls fired at 1225°C for 120minutes soaking period with major raw material as calcium tri poly phosphate gave the best results with no increase in TDS, pH in the range of 8.4 to 8.8 with increase in dipping period of 25gms ceramic balls per litre of water from 120 to 240 minutes.

### 9:30 AM

# (ICACC-S8-011-2025) Biomineralization inspired fabrication of dense ceramics at low temperature

Z. Zou\*1

1. Wuhan University of Technology, China

Ceramics have widespread applications in many fields. However, ceramics are normally fabricated by powder sintering under high temperatures, causing extremely high energy consumption. Thus, the new fabrication technology of ceramics under mild conditions has attracted tremendous interest from researchers in recent years. By contrast, living organisms can produce biominerals under mild conditions. Here, taking inspiration from the biomineralization process, we manufactured aragonite ceramic composed of densely packed nanocrystals by in situ crystallization and densification of amorphous calcium carbonate (ACC) under pressure (300 MPa - 1 GPa) at low temperature (80 °C). The hardness and elastic modulus could reach 3.2 GPa and 65.6 GPa, respectively, which were significantly higher than those reported in previous studies and comparable to nacre. Besides, the flexural strength could also reach 49.0 MPa. The densification and crystallization mechanisms were investigated, highlighting the critical roles of water during the fusion of nanoparticles and ACC crystallization. Thus, our study provides new strategy for fabrication of dense ceramics at low temperatures.

### **S8- Design-oriented manufacturing and processing** Room: Flagler A

Session Chairs: Satoshi Tanaka, Nagaoka University of Technology; Hisayuki Suematsu, Nagaoka University of Technology

### 10:10 AM

### (ICACC-S8-012-2025) Engineering Thermal Conductivity in Liquid-Phase Sintered SiC Ceramics: Key Design Factors (Invited)

H. Kim\*1; Y. Kim2

- 1. University of Seoul, Republic of Korea
- 2. University of Seoul, Dept. of Materials Science & Engineering, Republic of Korea

Silicon carbide (SiC) is renowned for its exceptional thermal conductivity. Recent advancements have achieved a thermal conductivity of 261.5 W/m-K in polycrystalline SiC ceramics liquid-phase sintered (LPS) with  $Y_2O_3$ -Sc<sub>2</sub>O<sub>3</sub> additives at 2050°C under a

nitrogen atmosphere. The thermal conductivity of SiC is influenced by numerous factors, from the choice of additives to the sintering atmosphere. This study evaluates key factors determining the thermal conductivity of LPS-SiC, including lattice oxygen/nitrogen content, porosity, grain size, grain boundary structure, phase transformation, and additive composition. While examining each factor's impact on thermal conductivity, we also explore the interrelationships among these variables. We identify the most critical factors affecting thermal conductivity and, based on these findings, propose a comprehensive guide for engineers to develop high thermal conductivity LPS-SiC materials.

### **S8-** Polymer-based processing

Room: Flagler A

Session Chairs: Satoshi Tanaka, Nagaoka University of Technology; Hisayuki Suematsu, Nagaoka University of Technology

### 10:40 AM

# (ICACC-S8-013-2025) Effectiveness of potassium-based geopolymers in immobilizing the cesium and strontium ions

T. Do\*1; Y. Sajedah1; T. Suzuki1; T. Nakayama2; H. Suematsu3

- 1. Nagaoka University of Technology, Nuclear System Safety Engineering, Japan
- 2. Nagaoka University of Technology, Japan
- 3. Nagaoka University of Technology, Extreme Energy-Density Research Institute, Japan

Radionuclides in low- and intermediate-level nuclear waste, particularly long-lived isotopes, pose a significant environmental threat. In order to prevent their release into the environment the immobilization methods are important. Geopolymers, synthesized from aluminosilicate materials and alkaline activators, offer promising properties for nuclear waste solidification, including durability, radiation resistance, and the potential for low-temperature processing. This research investigates the feasibility of using potassium-based geopolymers for the immobilization of Cs-137 and Sr-90 from nuclear waste. The results indicate successful ion exchange between Cs<sup>+</sup> and Sr<sup>2+</sup> ions within the geopolymer matrix. While Cs<sup>+</sup> exhibited a 4.6% release, Sr<sup>2+</sup> was almost completely captured. To assess longterm radionuclide storage in a radiation environment, this study includes a three-month leaching behavior evaluation. The radiation resistance of the geopolymers will be simulated by evaluating their mechanical properties after exposure to the ETIGO III, an inductively pulsed electron beam accelerator with an output voltage of 2 MeV, a current of 5 kA, and a pulse width of 30 ns.

### 11:00 AM

## (ICACC-S8-014-2025) Novel Flexible Passive Wireless RLC Strain Sensor

K. Rivera\*

1. University of Rhode Island, Chemical engineering, USA

A passive wireless RLC strain sensor has been developed which is comprised of a silver microparticle infused polymer strain gage. The strain sensor is made from a 36:64 wt% silver microparticle powder and PDMS mixture. The passive wireless RLC strain sensor electromagnetic output was measured by inductively coupling it to a reader coil connected to a vector network analyzer analyzer and had a nonlinear gage factor ranging from 5 to -42.154 in the strain range of 150 $\mu$ E to 350 $\mu$ E. The silver microparticle:PDMS strain gage has the advantage of both having a small electrical resistance and large gage factor which allows a high quality factor when connected in series with an LC circuit to form a passive wireless circuit.

# S8- Joining, integration, machining, repair, and refurbishment technologies

### Room: Flagler A

Session Chairs: Satoshi Tanaka, Nagaoka University of Technology; Hisayuki Suematsu, Nagaoka University of Technology

### 11:20 AM

# (ICACC-S8-016-2025) Field-assisted sintering for the consolidation of high-temperature ceramics (Invited)

V. M. Sglavo\*1

1. University of Trento, Italy

Numerous research activities are trying to identify processes with lower environmental impact and, above all, with limited energy consumption for the production of ceramics. Among these, the very recently proposed techniques called flash sintering (FS) and ultrafast high-temperature sintering (UHS) appear extremely promising. An area where the above-mentioned issue is even more problematic is that of high-temperature ceramics, which can be typically consolidated only at very high temperature under the action of significant pressures and in inert atmosphere. The conditions are discussed here to achieve high density and no oxidation by using FS and UHS techniques with the aim to identify possible evolution of the process to real applications and actual issues which need further investigations. The correlation between the processing condition and material structure and composition is also analysed in detail.

## <u>S9 Porous Ceramics Novel Developments and</u> <u>Applications</u>

# **S9-** Porous Ceramics- Novel Developments and Applications

Room: Ballroom 1-2

Session Chairs: Swantje Funk, Friedrich-Alexander-Universität Erlangen-Nürnberg; Michelle Weichelt, Friedrich-Alexander-Universität Erlangen-Nürnberg

### 8:30 AM

# (ICACC-S9-009-2025) Fabrication of SiC Nanowire Based Elastic Aerogel (Invited)

H. Wang<sup>\*1</sup>; D. Lu<sup>1</sup>; L. Su<sup>1</sup>; S. jia<sup>1</sup>

1. Xi'an Jiaotong University, China

Because of the inherent brittleness of ceramic materials and the weak combination between nano ceramic particles, ceramic aerogels have the disadvantages of high brittleness and low strength. In this paper, the precursor pyrolysis combined with chemical vapor deposition and other methods are used to carry out the large-scale preparation of SiC nanowire elastic ceramic aerogel with SiC nanowire as the basic building unit. Using porous carbon template assisted pyrolysis as short carbon fiber three-dimensional framework and polysiloxane sol as raw materials through suction filtration, high-temperature pyrolysis, and oxidative decarburization, aerogel composed of SiC nanowires with high aspect ratio is obtained. The results showed that the optimum pyrolysis temperature was 1550 °C, When the pyrolysis temperature is too low, the polysiloxane pyrolysis is not sufficient, and the content of impurities such as SiOC ceramics in the aerogel is high; When the pyrolysis temperature is too high, the nanowires become coarser and the mechanical properties of the aerogels decrease. With the increase of polysiloxane content, the density of aerogels increased (5-30 mg/cm<sup>3</sup>), and the average diameter of nanowires increased (82~155 nm). The average diameter of aerogel with density of 10 mg/cm<sup>3</sup> is about 108 nm, the compression resilience is 49%, and the strength is 13 kPa.

### 9:00 AM

### (ICACC-S9-010-2025) Precursor Formulations for Isolvolumetric Synthesis of Nitride-Based Ceramics using Selective Laser **Reaction Sintering**

J. B. Spicer\*1; D. Zhang2; A. B. Peters3; M. Moorer1; Y. Rhim2

- 1. Johns Hopkins University, Materials Science and Engineering, USA
- 2. Johns Hopkins Applied Physics Laboratory, USA

3. Johns Hopkins University, Ralph O'Connor Sustainable Energy Institute, USA

The selective laser reaction sintering (SLRS) of precursors (Si or SiO<sub>x</sub>) in 100 vol%  $\rm NH_3$  was performed for  $\rm Si_3N_4$  production. Typical nitridation of Si powders occurs efficiently between 1100-1500 °C, where a combination of both  $\alpha$ - and  $\beta$ -phases are almost always formed. SLRS processing yielded nearly complete conversion to  $Si_3N_4$  (97.7wt%) with both  $\alpha$ -Si<sub>3</sub>N<sub>4</sub> and  $\beta$ -Si<sub>3</sub>N<sub>4</sub> having been produced using 3 W of laser power. Increasing laser power enhances chemical conversion by increasing temperatures at the laser-interaction zone. Near net-shape precursor mixtures were formulated to improve the surface microstructure of SLRS samples by compensating for conversion-induced volume changes. Our work to date has shown that the yield of  $\alpha/\beta$ -Si<sub>3</sub>N<sub>4</sub> from SLRS (~3:1  $\alpha/\beta$ -Si<sub>3</sub>N<sub>4</sub> from Si or Si/SiO) was greater than that reported previously by others which likely results from vapor-phase reactions that are prevalent in our work. For SLRS synthesis of Si<sub>3</sub>N<sub>4</sub> using Si or SiO<sub>x</sub> precursors, there appears to be the following trade-off: high local temperatures increase nitride yield but also lead to unusual layer morphologies; low local temperatures prevent consolidation and result in incomplete non-oxide conversion. We discuss SLRS processing conditions to identify those that possibly result in favorable microstructures and permit additive manufacturing of silicon nitride.

### 9:20 AM

### (ICACC-S9-011-2025) Evaluating the Effect of Porosity and Sintering Aid Composition on the Ablation Response of Silicon Nitride

M. Thompson<sup>\*1</sup>; A. Kimery<sup>1</sup>; R. Trice<sup>1</sup>

1. Purdue University, Department of Materials Engineering, USA

Silicon nitride (Si<sub>3</sub>N<sub>4</sub>) is a material of interest for high temperature radar frequency windows. However, there is limited data on the response of Si<sub>3</sub>N<sub>4</sub> to ablation. This descriptive study will document the effect of porosity and sintering aid composition on surface temperature and physical properties of Si<sub>3</sub>N<sub>4</sub> during ablation. In this study, billets of silicon nitride were slip cast at 30 vol.% solids loading in water, then thermally debound and pressurelessly sintered at 1850 °C. The following sintering aid compositions were assessed: 6 wt.% Al<sub>2</sub>O<sub>3</sub> / 2 wt.% Y<sub>2</sub>O<sub>3</sub>, and 5-15 wt.% Yb<sub>2</sub>O<sub>3</sub>. A commercially available  $\rm Si_3N_4$  plate with  $\rm Y_2O_3\text{-}Al_2O_3$  sintering aids served as the dense standard for comparison. These conditions represented approximately 0-40% porosity and two different glassy phases along the grain boundaries of Si<sub>3</sub>N<sub>4</sub>. Square plates with nominal dimensions of 20x20x5 mm were cut and ground for ablation testing and physical characterization. Relative density, surface roughness, scanning electron micrographs, and x-ray diffraction patterns of the top surface were obtained before and after ablation. Ablation was performed at two time points, 60 and 300 seconds, using an oxyacetylene welding torch under neutral atmosphere and a heat flux of 400 W/cm<sup>2</sup>. Change in mass, change in thickness, and front- and back-face temperatures were collected for each ablation condition.

### 9:40 AM

### (ICACC-S9-012-2025) Enhancing thermal and mechanical performance of silicon nitride via pore-driven grain growth

Y. Nakashima\*1; Y. Zhou1; K. Hirao1; T. Ohji2; M. Fukushima1

- 1. National Institute of Advanced Industrial Science and Technology (AIST), Japan
- 2. Yokohama Kokuritsu Daigaku, Japan

The enhancement of thermal conductivity and fracture toughness in silicon nitride (Si<sub>3</sub>N<sub>4</sub>) ceramics is strongly influenced by the growth of large, elongated grains. This study investigates the strategic introduction of controlled porosity within the green compact to facilitate grain growth and optimize densification. Four types of pore formers, with diameters of 2, 20, 30, and 100 µm, were used to introduce porosities ranging from 3 to 18 vol%. It was found that the presence of pores, irrespective of their size or volume, significantly promoted grain growth by minimizing grain-to-grain collisions within the pores. The larger pores contributed to the formation of more pronounced elongated grains. However, excess pore volume and larger diameters hindered the densification process. Among the pore formers used, those with a 30 µm diameter provided an optimal balance, resulting in an increase in fracture toughness and thermal conductivity, reaching values of 10.2 MPa  $m^{1/2}$  and 118.2 W/(m K), respectively, at 5 vol% porosity. These results demonstrate that the deliberate incorporation of pores into the green compact can effectively enhance the thermal and mechanical properties of Si<sub>3</sub>N<sub>4</sub> ceramics, provided that the pore-induced grain growth is utilized and the porosity is eliminated during sintering.

### **S9-** Porous Ceramics- Novel Developments and Applications

Room: Ballroom 1-2

Session Chair: Larissa Wahl, FAU Erlangen-Nürnberg

### 10:20 AM

#### (ICACC-S9-013-2025) Formulation and functionalization of durable porous silicate ceramics for water filtration incorporation of agro waste and biosourced additives

I. Maury Njoya\*1; G. LeComte Nana1; V. Chaleix2; Y. El Hafiane1; B. Nait-Ali<sup>1</sup>; A. Lengo Mambu<sup>2</sup>; C. Peyratout<sup>1</sup>

- 1. Institut de Recherche sur les Ceramiques, France
- 2. Universite de Limoges, Faculté des Sciences et Techniques, France

The present work is focused on the development of sustainable, high performance membranes based on West Cameroonian clays and groudnut husks for water filtration. To acheive this, three raw clays were selected. These materials were chosen beacause of their abundance and their beneficial properties. Different samples were prepared and the proportion of groundnut husk (C) were 0, 20 and 25 mass %. All samples were shaped by uniaxial pressing and sintered at 1100 °C. Results showed that, weight loss values were less thah 30 for all samples. Open porosity was highest (44-59 %) with 25 % C, proving the influence of C content on the porosity. Capillary rise test was in line with this trend. Flexural strength was more significant (4-6 MPa) on samples with 0 % C. SEM images revealed pores, sheets and intergranular contacts, so densification was effective. Further investigations are to be done on functionalization route and permeability properties on these samples.

### 10:40 AM

### (ICACC-S9-014-2025) Designing Future Materials: Tailoring Porous Ceramics through Microstructure Engineering and **Advanced Property Optimization**

### T. Fey\*1

1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

Cellular materials offer a wide range of applications such as catalyst support structures, lightweight materials, energy adsorption or energy storage materials. Due to various processing methods and different materials, a wide range of material properties such as thermal conductivity, mechanical strength or damping can be tailored, measured and verified with respect to the expected properties. Especially in heterogeneous and homogeneous porous structures and their composites, only globally effective material properties can be determined and measured. A major point of interest is the strengthening of porous ceramics by various possible techniques. Knowledge of the dominant influence of the microstructure on the mechanical properties is the key to designing materials

with desired properties. The combination of experimentally estimated material properties with microstructural models from  $\mu CT$  measurements offers the possibility to design the structures for future applications of porous ceramics.

### 11:00 AM

# (ICACC-S9-015-2025) Deformation Control Optimizes Kelvin Cell Architecture

- S. Funk\*1; T. Fey1
- 1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

The mechanical performance of porous and cellular structures is closely correlated with their micro- and macrogeometric design. The impact of architectural variations on the remaining physical properties, in particular strength, stiffness, and load distribution, is of critical importance. An optimized architectural design can result in a significant enhancement of these properties. This study examined the effects of stretching or compressing Kelvin cells with a 45° angle along the z-axis, resulting in architectures with variations of controlled deformation angles between 15° and 60°. The Kelvin cell Al2O3 structures were designed, 3D-printed, and sintered at 1600°C. It was found that depending on the deformation angle, the anisotropic volumetric shrinkage from 45° could be compensated for in order to achieve a non-deformed structure. The results of the compression tests indicate that variations in the deformation angles significantly affected the mechanical properties. This investigation highlights the potential for optimizing cellular structures in order to achieve specific mechanical properties, which can be readily achieved through the precision of the SLA printing process.

### 11:20 AM

### (ICACC-S9-016-2025) Energy-Reduced Fabrication of Light-Frame Ceramic Honeycombs by Replication of Additive Manufactured Templates

D. Köllner<sup>1</sup>; S. Niedermeyer<sup>1</sup>; M. Vermes<sup>1</sup>; S. Funk<sup>1</sup>; K. Kakimoto<sup>2</sup>; T. Fey\*<sup>1</sup>

- 1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany
- 2. Nagoya Institute of Technology, Graduate School of Eng., Dept. Mater. Sci. & Eng., Japan

Ceramic components require very high energy consumption due to synthesis, shaping, and thermal treatment. However, this study suggests that combining the sol-gel process, replica technology, and stereolithography has the potential to produce highly complex geometries with energy savings in each process step. We fabricated light-frame honeycombs of  $Al_2O_3$ ,  $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$  (BCZT), and  $BaTiO_3$  (BT) using 3D-printed templates with varying structural angles between -30° and 30° and investigated their mechanical and piezoelectric properties. The Al<sub>2</sub>O<sub>3</sub> honeycombs showed a maximum strength of approximately 6 MPa, while the BCZT and BaTiO<sub>3</sub> honeycombs achieved a d<sub>33</sub> above 180 pC/N. Additionally, the BCZT powder was prepared via a sol-gel process, and the impact of the calcination temperature on phase purity was analyzed. The results suggest that there is a large energy-saving potential for the synthesis of BCZT powder. Overall, this study provides valuable insights into the fabrication of complex ceramic structures with improved energy efficency and enhancement of performance.

### 11:40 AM

### (ICACC-S9-017-2025) Eco-friendly zeolite clinoptilolite functionalization with antimicrobial metallic nanoparticles: green synthesis and application

F. Gattucci\*1; M. Lallukka1; N. Grifasi1; M. Piumetti1; M. Armandi1; M. Miola1

1. Politecnico di Torino, DISAT, Italy

In response to the global focus on reducing airborne pathogens and ensuring clean air, natural zeolites have gained attention due to their exceptional adsorption capacity for toxic compounds. Clinoptilolite, a natural zeolite widely used in wastewater treatment and air purification, stands out for its high surface area and cation exchange capacity. This study explores the green functionalization of clinoptilolite with silver (AgNPs) and copper (CuNPs) nanoparticles to enhance its antimicrobial properties. Tannic acid was employed as a green reducing agent to achieve the in situ reduction of AgNPs and CuNPs on clinoptilolite. This eco-friendly method avoids the use of toxic reducing agents, organic solvents, and high temperatures required in traditional synthesis. The obtained materials were characterized using FTIR, FESEM, EDS, XRD, XPS, TEM, and the absorption and catalytic properties were tested through BET analysis and CO and ethylene reduction. The functionalized clinoptilolite (Clino-AgNPs and Clino-CuNPs) exhibits significant antimicrobial activity, as evidenced by zone of inhibition tests and bioaerosol contamination test. This work represent a promising solution for adsorbing toxic compounds while preventing pathogen growth, making it a valuable component for air purification systems and environmental sustainability efforts.

## S12 Design and Applications of Nanolaminated MAX and MAB Phases Solid Solutions and 2D Counterparts

### S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and 2D Counterparts

### Room: Ponce de Leon

Session Chairs: Konstantina Lambrinou, University of Huddersfield; Thierry Cabioch, University of Poitiers

### 8:30 AM

### (ICACC-S12-009-2025) Entropy Stabilization and Order-Disorder Transitions in Multi-Transition Metal MAX phases and MXenes (Invited)

B. C. Wyatt<sup>1</sup>; B. Anasori<sup>\*1</sup>

1. Purdue University, Materials Engineering, USA

The family of two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, is one of the largest 2D material families, with over fifty synthesized compositions. MXenes are primarily synthesized through the top-down selective etching of their precursor MAX phases. Consequently, the design of new MXene compositions depends on the synthesis of novel MAX phases. In 2021, a new research area emerged within MAX/MXenes: high-entropy MAX and MXene phases, making MXenes one of the first 2D materials to enter the field of high-entropy research. In these phases, four or more transition metals are combined as solid solutions within the 2D atomic planes. In this talk, I will present a systematic study of over 30 multi-transition-metal MAX/MXene phases, incorporating different numbers and types of transition metals in the M layers. The goal is to understand the influence of entropy versus enthalpy on the formation of these phases. By combining various elements and analyzing the atomic layer-by-layer composition of the MAX phases, we determine how many transition metals are required to form fully disordered high-entropy MAX phases. Additionally, we demonstrate how to synthesize novel high-entropy MXenes from these phases and explore some of their properties.

### 9:00 AM

### (ICACC-S12-010-2025) Exploring the Potential of Clay Minerals and MXenes for Biomedical Applications: A First-Principles Study of 2D Hybrid Materials (Invited)

D. Cakir\*<sup>1</sup>

1. University of North Dakota, Physics and Astrophysics, USA

The search for innovative biomedical materials has driven growing interest in two-dimensional (2D) materials due to their exceptional properties and versatility. Among these, clay minerals and MXenes stand out as promising candidates, offering distinct structural and functional features suitable for bioapplications. In this study, we use first-principles calculations to investigate the chemistry, structural properties, and biomedical potential of clay minerals, MXenes, and their heterostructures. Our focus includes the interactions between various amino acids and clay minerals or MXenes with different surface terminations, aiming to create nanocomposite biomaterials with enhanced performance. By comparing the unique features of clay minerals and MXenes, we explore their roles in hybrid materials and the potential synergistic property enhancements from heterostructure formation. This research aims to uncover new opportunities for applying these advanced 2D materials in the biomedical field, particularly in areas such as tissue engineering, where their unique properties hold promise for significant advancements.

### 9:30 AM

### (ICACC-S12-011-2025) Direct Etching of MAX Phases to MXene Nanosheets Using Quaternary Ammonium Fluorides: Implications for Energy Storage and Degradation Stability (Invited)

V. Kotasthane<sup>1</sup>; Z. Tan<sup>1</sup>; K. Y. Lee<sup>1</sup>; J. Yun<sup>2</sup>; E. Pentzer<sup>1</sup>; J. Lutkenhaus<sup>2</sup>; M. Green<sup>2</sup>; M. Radovic<sup>\*1</sup>

- 1. Texas A&M University, Materials Science and Engineering, USA
- 2. Texas A&M University, Artie McFerrin Department of Chemical Engineering, USA

Traditional top-down etching of MAX phases using HF remains a prevalent approach in MXenes sythesis, but it poses serious scalability challenges due to associated health risks. Alternative methods often require high temperatures or additional intercalation steps. To overcome these limitations, we propose using a safer family of quaternary ammonium salts, such as tetramethylammonium fluoride (TMAF), with a suitable solvent for MXene synthesis. The large quaternary ammonium cation size facilitates simultaneous intercalation and exfoliation during etching, eliminating the need for separate intercalation steps and additional chemicals. Single or few-layer Ti3C2Tz and Ti2CTz MXenes were successfully synthesized by directly etching their corresponding MAX phases in aqueous solutions of TMAF and HCl. Notably, the resulting MXenes exhibited tunable functional group distributions, dependent on the etching duration and concentrations of TMAF and HCl. This method yielded over 30 wt% of single- or few-layer MXene nanosheets, highlighting its scalability. Furthermore, Ti3C2Tz MXenes produced using this method showed excellent degradation stability in aqueous dispersions compared to those synthesized using conventional methods, though Ti2CTz MXenes did not demonstrate the same stability improvements.

### 10:20 AM

60

# (ICACC-S12-012-2025) Using neutron and synchrotron X-ray diffraction to probe and quantify bulk-sample turbostratic disorder in MAX-Phases and other layered materials

A. A. Coleman\*1; R. Springell2; J. Kelleher

- 1. Rutherford Appleton Laboratory, ISIS, United Kingdom
- 2. University of Bristol, Phsyics, United Kingdom

Turbostratic layering commonly occurs in materials with weak interlayer bonding and is just one of several features that uniquely affect layered materials such as MAX-Phases. The presence of these features can greatly impact the micromechanical properties, particularly the material's response to mechanical stress. While turbostratic layering may be visualised by a thin sample lift-out in TEM, a spectral analysis method would provide a non-destructive, large-volume method of disorder quantification. In turn, this would improve statistical fitting of other microstructural features, such as particle size estimation in diffraction analysis. Neutron diffractograms of MAXTHAL ( $Ti_3AlC_2$ ), various nuclear graphites and Transition-Metal Dichalcogenide NbSe<sub>2</sub>, were fit using a standard Rietveld refinement method in GSAS-II and consistently outlying features were analysed using Fityk. Common features in peak broadening among diffractograms of these samples are identified by single-peak

fitting and Rietveld refinement. Once these features of broadening are quantified, it may provide a key to improving refinement-based fits of data from diffraction techniques, including neutron and x-ray diffraction and electron backscatter diffraction (EBSD).

## S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and

### 2D Counterparts

Room: Ponce de Leon Session Chair: Deniz Cakir, University of North Dakota

### 10:40 AM

# (ICACC-S12-013-2025) Engineering MXenes and their hybrids for Energy Applications (Invited)

### M. Naguib<sup>\*1</sup>

1. Tulane University, Physics and Engineering Physics, USA

MXenes, a large family of 2D transition metal carbides and nitrides, are represented by the general formula  $M_{n+1}X_nT_x$ , where M stands for an early transition metal, X represents carbon or nitrogen, n varies from 1 to 4, and T<sub>x</sub> indicates surface terminations. These materials offer a highly versatile platform for intercalation and the formation of unique hybrids, enabling a broad range of applications. Their ability to host ions and their exceptional tunability make them especially attractive for various uses. In this talk, we will explore the engineering of MXenes and their hybrids for energy storage and environmental applications. For example, by engineering MXene multilayers through pre-intercalation, an areal capacitance as high as 5.7 F/cm<sup>2</sup>-a record for MXene-based materials-has been achieved. Additionally, by incorporating nitrogen-doped graphene-like carbon between Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> layers to create a heterostructure, the capacity and stability of sodium-ion and lithium-ion batteries can be significantly enhanced, with specific capacity effectively doubling. Moreover, we will share our recent research on MXene hybrids used as sorbents for radioactive iodine, a byproduct potentially generated by nuclear energy systems.

### 11:10 AM

### (ICACC-S12-014-2025) Mechanisms of Deformation and Failure in Single-Crystal MAX Phase (Invited)

M. Radovic<sup>2</sup>; A. Srivastava\*1

- 1. Texas A&M University, USA
- 2. Texas A&M University, Materials Science & Engineering, USA

The single-crystal-level mechanical response of MAX phases is characterized using small-scale mechanical testing of specimens machined from individual grains via focused ion beam milling or utilizing as-grown single crystals. Our results demonstrate that the onset of plastic flow in MAX phases is highly orientation-dependent and follows non-classical crystallographic slip, influenced strongly by the stress acting normal to the basal planes. We also analyzed the effects of different MX layers and stacking sequences on this non-classical slip behavior. Furthermore, our findings show that MAX phases tend to cleave easily along the basal planes, especially when the driving force for crystallographic slip is insufficient. However, when deformation is constrained normal to the basal planes, MAX phase crystals deform by kinking. The complete results of these experiments, as well as computational analyses to better understand the experimental observations and their implications on the macroscopic response of the material, will be presented.

### 11:40 AM

### (ICACC-S12-015-2025) Laser Ablative Patterning of MoAlB Ceramics for Hydrophobic Surfaces (Invited)

B. Cui<sup>\*1</sup>; S. Ruiz<sup>1</sup>; R. Wall<sup>1</sup>; L. Wadle<sup>1</sup>; Y. Yoo<sup>1</sup>; Y. Lu<sup>1</sup>; C. Wohl<sup>2</sup>; V. L. Wiesner<sup>2</sup>

- 1. University of Nebraska-Lincoln, USA
- 2. NASA Langley Research Center, USA

Through a novel laser ablative patterning (LAP) process, the present work reported the increase in wetting contact angle of molybdenum aluminum boride (MoAlB) and reduction of dust adhesion. The LAP technique employed picosecond laser pulses to form a cross-hatch pattern with micropillars on ceramic surfaces. The wetting behavior was successfully transitioned from hydrophilic ( $\theta < 90^\circ$ ) to hydrophobic ( $\theta > 90^\circ$ ), which may be related to Wenzel or Cassie-Baxter mechanisms. Parameters such as laser fluence and number of laser scans were varied to study their effects on ceramic surface characteristics. Dust adhesion experiments were performed on these hydrophobic ceramic surfaces, which showed that the adhesion of lunar soil simulant dust particles was significantly reduced in the patterned MoAlB surface. The patterned MoAlB samples were further examined using the SLIDE testbed to evaluate the wear performance.

## **<u>S14 Crystalline Materials for Electrical</u>** <u>Optical and Medical Applications</u>

### **S14- Optical Material II**

Room: Coquina A

Session Chair: Matthias Müller, Radiation Monitoring Devices Inc

### 8:30 AM

### (ICACC-S14-012-2025) Synthesis and Luminescence Enhancement of Novel Deep-red Emitting Phosphor SrCa<sub>2</sub>Ga<sub>2</sub>O<sub>6</sub>:Mn<sup>4+</sup> (Invited)

W. Hikita\*1; Y. Nasuda2; H. Okura2; K. Toda1

1. Niigata University, Graduate School of Science and Technology, Japan

2. Fuso Chemical Co., Ltd., Japan

 $\rm Mn^{4+}$ -doped oxide phosphors display deep-red emission peakes between 650 and 730 nm under n-UV or blue light irradiations.  $\rm Mn^{4+}$ -activated phosphors are strongly attracted because they are useful in the field of plant cultivation. In particular, Tululitemineral structure-related phosphors, such as Ca<sub>14</sub>Zn<sub>6</sub>Al<sub>10</sub>O<sub>35</sub>:Mn<sup>4+</sup>, Ca<sub>14</sub>Zn<sub>6</sub>Ga<sub>10</sub>O<sub>35</sub>:Mn<sup>4+</sup>, and Ca<sub>7</sub>Mg<sub>2</sub>Ga<sub>6</sub>O<sub>18</sub>:Mn<sup>4+</sup>, are well studied because they can be efficiently excited by n-UV light. Recently, we found a novel deep-red emitting phosphor SrCa<sub>2</sub>Ga<sub>2</sub>O<sub>6</sub>:Mn<sup>4+</sup> from the solid solution system of Sr<sub>3</sub>Ga<sub>2</sub>O<sub>6</sub>-Ca<sub>3</sub>Ga<sub>2</sub>O<sub>6</sub>, and elucidated its crystal structure as a new member of Tululite-mineral structure family by the single crystal XRD analysis. Moreover, we successfully enhanced its luminescence properties by doping Ba<sup>2+</sup> ions. Ba<sup>2+</sup>-doped SrCa<sub>2</sub>Ga<sub>2</sub>O<sub>6</sub>:Mn<sup>4+</sup> showed strong deep-red emission under blue light as well as n-UV light.

### 9:00 AM

### (ICACC-S14-010-2025) New feldspar, BaMgSi<sub>3</sub>O<sub>8</sub>

K. Toda\*<sup>1</sup>; W. Hikita<sup>1</sup>

1. Niigata University, Japan

BaMgSi<sub>4</sub>O<sub>10</sub>:Eu<sup>2+</sup> shows strong blue luminescence under UV irradiation. While it has excellent luminescence properties, the luminescent phase had not been identified. In this study, single-crystal samples of BaMgSi4O10:Eu2+ phosphor were prepared. The chemical composition and crystal structure were identified by single-crystal XRD structural analysis. As a result, it was found that the correct luminescent phase of the BaMgSi<sub>4</sub>O<sub>10</sub>:Eu<sup>2+</sup> phosphor is a material with a composition of BaMgSi<sub>3</sub>O<sub>8</sub>:Eu<sup>2+</sup>. Composition BaMgSi<sub>3</sub>O<sub>8</sub> is the first compound with a feldspar structure composed only of Si.

### 9:20 AM

#### (ICACC-S14-011-2025) Control of the emission and excitation Energies in Pr<sup>3+</sup>-activated perovskite oxide–oxynitrides by bandgap engineering

Y. Sato<sup>1</sup>; S. Noda<sup>1</sup>; J. Odahara<sup>1</sup>; R. Yanamoto<sup>\*1</sup>; T. Hasegawa<sup>3</sup>; S. Yin<sup>3</sup>; J. Jia<sup>4</sup>; M. Kakihana<sup>2</sup>

- 1. Okayama Rika Daigaku, Department of Chemistry, Japan
- 2. Osaka Daigaku, SANKEN, Japan
- 3. IMRAM, Tohoku University, Japan
- 4. Waseda Daigaku, Global Center for Science and Engineering, Japan

In this study, we investigated the photoluminescence properties of  $Pr^{3+}$ -activated  $CaM_{x}Ta_{1-x}O_{2+x}N_{1-x}$  phosphors (M: Zr and Hf) across a compositional range from 0.0 to 1.0. This solid-solution system provides the potential to finely tune the maximum excitation wavelength by adjusting the O/N and Zr (or Hf)/Ta ratios, which directly influence the bandgap energy between the valence and conduction bands. Consequently, the sharp emission peak from  $Pr^{3+}$  in the solid-solution system can be excited by near-UV or blue light if the bandgap energy is tuned within the range of 2.8 to 3.2 eV. The solid-solution samples were synthesized using the polymerizable complex method, followed by heat treatment under an NH<sub>3</sub> gas flow at 900-1100°C. XRD patterns confirmed that all samples exhibited a single-phase perovskite structure. In the case of  $CaZr_{x}Ta_{1-x}O_{2+x}N_{1-x}$ phosphors, the absorption associated with bandgap excitation shifted to higher energy as the Zr<sup>4+</sup> concentration increased. Specifically, the bandgap energy was successfully tuned from 2.8 to 3.2 eV by controlling the Zr<sup>4+</sup>/Ta<sup>5+</sup> and O/N ratios as x increased from 0.70 to 0.90. Moreover, the solid-solution system exhibited intriguing photoluminescent behavior, with single emission peaks observed at 612 nm when the bandgap energies were tuned to approximately 3.0 eV in samples with x values around 0.75.

### **9:40** AM

# (ICACC-S14-009-2025) Dense, transparent Ce: $Y_3Al_5O_{12}$ films from flame made nanopowders for white light applications (Invited)

R. M. Laine\*1; E. Yi1

1. University of Michigan, Materials Science and Engineering, USA

Flame made metal oxide nanopowders enable processing of dense, transparent thin (< 50 µm) films of Ce3+ doped Y3Al5O12 for white light applications. The addition of very small amounts of SiO2 (0.14 wt. %) and the use of a final 95:5 N2:H2 atmosphere sintering step permits nearly complete removal of pores from films originally sintered in O2. Furthermore, the introduction of this final step allows reduction in processing temperatures needed to effect Ce4+ reduction to Ce3+ by several hundred degrees below typical temperatures of > 1600 °C. At 20–50  $\mu$ m, the reported films are also much thinner than previously reported for the same materials normally produced by solid state reactions of micron size powders. Spectrofluorometric measurements of the dense transparent films exhibit excitation spectra centered around 450nm and broad emission spectra in the 470-750 nm range with two peaks centered at 537 and 570 nm, confirming their applicability as a phosphor for white light emitting diodes.

### 10:30 AM

### (ICACC-S14-013-2025) Luminescence Property of Ceramic Phosphors Synthesized by the Melt Quenching Technique (Invited)

K. Toda\*1; W. Hikita1

1. Niigata University, Japan

For rapid screening and synthesis of new ceramic phosphors, we have applied novel synthesis technique "Melt Quenching Synthesis". In the melt synthesis, the mixture of oxides or their precursors is melted in a short period of time (5-60 seconds) by a strong light radiation in Xe arc imaging furnace. A spherical molten sample

where multiple cations were mixed homogeneously was directly solidified on a Cu hearth. The Melt Quenching reactor system has some advantages; i) the whole part of solid reactants can be kept at a steady temperature, and ii) heat can be transferred very fast to substances because each reactant is perfectly melted. The phosphors synthesized by the "Melt Quenching Synthesis" show superior luminescence property because of high homogeneity, high crystallinity and relatively few defects. This novel technique is powerful tool for rapid screening and improvements of phosphor materials.

### 11:00 AM

### (ICACC-S14-014-2025) Processing of Diamond with Defects for Single Photon Emission for Quantum and Sensing Applications

L. N. Ramasubramanian<sup>1</sup>; R. N. Singh\*<sup>1</sup>

1. Oklahoma State University, School of Materials Science and Engineering, USA

Diamond is a fascinating wide-bandgap semiconductor for many applications in quantum electronics, quantum sensing, and as a single photon emitter. These applications require diamond-containing nitrogen-vacancy (N-V) and siliton vacancy (Si-V) point defect centers that can be excited with variant to display unique optical emission characteristics, including angle photon emissions. The challenge for these applications requires processing high-quality diamond crystals containing V V or Si-V defect centers for the greatest sensitivity and applicability. Our research focuses on understanding the diamond nucleation mechanisms and incorporating N or Si dopants in situ to meet these challenges. Processing by Microwave Plasma Enhanced Chemical Vapor Deposition is explored to synthesize N- and Si-doped diamond single crystals containing these defects. The diamond crystals are characterized by Scanning Electron Microscopy (SEM), Raman, and Photoluminescence (PL) spectroscopies. These results and a brief overview of the promise of diamond for quantum applications will be presented.

### **S14- Scintillator I**

Room: Coquina A

Session Chair: Biwu Ma, Florida State University

### 11:20 AM

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### (ICACC-S14-015-2025) Scintillation properties of single crystalline lutetium oxide doped with rare earth grown by floating zone method (Invited)

T. Yanagida\*<sup>1</sup>; D. Nakauchi<sup>1</sup>; K. Okazaki<sup>2</sup>; K. Watanabe<sup>4</sup>; T. Kato<sup>1</sup>; N. Kawaguchi<sup>3</sup>

- 1. Nara Institute of Science and Technology, Japan
- 2. Nara Institute of Science and Technology, Materials Science, Japan
- 3. Nara Institute of Science and Technology, Graduate School of Materials Science, Japan
- 4. Kyushu Daigaku, Japan

Scintillators are one of the luminescent materials and are used in ionizing radiation detectors. When ionizing radiations are irradiated to scintillators, they are absorbed by scintillators via electromagnetic interactions or nuclear reactions, and absorbed energies are converted to low energy (few eV) photon emission. Scintillators have been utilized in many applications, including medical, security, environmental monitoring, resource exploration, and high energy physics. In this study, we focused on rare earth doped Lu<sub>2</sub>O<sub>3</sub> as a new scintillator since it has a high effective atomic number of 69 and a high density of 9.4 g/cm<sup>3</sup>. Rare earth elements (Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, and Yb) 1% doped Lu<sub>2</sub>O<sub>3</sub> single crystals were synthesized by the floating zone method. After cut and polish, photoluminescence properties and scintillation properties of them were systematically investigated.

### 11:50 AM

# (ICACC-S14-016-2025) Gd\_3Al\_5O\_{12} and GdAlO\_3 transparent thick film phosphors prepared using chemical vapor deposition for scintillation phosphors

A. Ito\*1

1. Yokohama National University, Graduate School of Environment and Information Sciences, Japan

 $Gd_3Al_5O_{12}$  (GAG) and  $GdAlO_3$  (GAP) crystals doped with  $Ce^{3+}$  ions are expected to be scintillation phosphors that will exhibit high scintillation light yields and short fluorescence lifetimes. However, GAG is thermally unstable, and GAP is prone to cracking when cooled down, making them difficult to grow crystals from the melt. In the present study, we synthesized  $Ce^{3+}$ -doped GAG and GAP transparent thick film phosphors using chemical vapor deposition and studied their optical and luminescence properties.

### **<u>S17 Advanced Ceramic Materials and</u> <u>Processing for Photonics and Energy</u>**

# S17- Advanced Ceramic Materials and Processing for Photonics and Energy I

Room: Coquina H

Session Chair: Tohru Suzuki, National Institute for Materials Science

### 8:30 AM

### (ICACC-S17-001-2025) Novel Materials Chemistry for Applications in Energy Storage and Conversion (Invited)

N. Pinna\*1

1. Humboldt-Universität zu Berlin, Department of Chemistry, Germany

The current trend in various energy applications, ranging from batteries to electrolizers, lays in the control of structural, physicochemical and morphological properties of materials and their interfaces. During this presentation, recent scalable strategies for nanostructured materials synthesis, targeting energy and environmental applications will be discussed. Especially, we will focus on one-pot strategies for the fabrication of hybrid and complex nanomaterials focusing on the importance of the organic-inorganic and inorganic-inorganic interfaces. Among the examples presented, we will discuss the synthesis of complex nanostructures and the stabilization of metastable phases for applications in energy, catalysis and environmental remediation. We will see that nowadays the available strategies allow a control in terms of composition, crystalline structure, morphology and nanostructuration that would have been unimaginable just few years ago. Finally, the open challenges the field is currently facing and possible further developments which are needed to meet the always growing demand for high performing materials will be also discussed.

### 9:00 AM

### (ICACC-S17-002-2025) Next-Gen Innovations: How Green Nanomaterials Are Shaping the Future of Clean Energy (Invited)

### R. Naccache\*1

1. Concordia University, Chemistry and Biochemistry, Canada

Nanomaterials have garnered significant interest with their compact size, versatile and tunable surface chemistry, simple and low-cost synthesis. While some of the reported works have focused on catalytic applications, their investigation as heterogeneous catalysts for the production of biofuels such as biodiesel remains unexplored. Biodiesel fuel production remains one of the most promising alternatives to non-renewable fossil fuels such as conventional oil and diesel. However, many challenges persist in its production particularly related to the tedious purification processes, high cost of production and unsustainable practices. Thus the need for the development of novel and sustainable heterogeneous catalysts is required. Here we show that these nanomaterials can trans/esterify the conversion of oils to biofuels with sustained catalytic efficiency for at least five reaction cycles. Our second and third-generation catalysts allow for a significant reduction of reaction temperature and operate at ambient pressure without a significant increase to the catalyst loading. Our work now tackles waste and inedible oils in order to reduce the overall cost of the process. This cost-efficient, sustainable and effective heterogeneous catalyst can have positive economic and environmental repercussions that can further drive academic and industrial research in this burgeoning area.

### 9:30 AM

### (ICACC-S17-003-2025) Synthesis of mixed and high etropy metal oxides with unique surface properties in supercritical conditions (Invited)

R. M. Richards\*1

1. Colorado School of Mines, Chemistry, USA

The ability to manipulate earth abundant metal oxides presents an important potential technology to develop sustainable materials with novel properties. These materials are of interest due to the coordination environments that can be achieved and to the high degree of control over properties that can result from tailoring the exposed facets and from mixing metal oxides. The Richards' research group has developed techniques based on supercritical solvents to produce a number of new nanoscale metal and metal oxide materials that have demonstrated unique surface activities through controlled faceting as well as novel intercalation strategies that impart robustness. The initial synthesis of MgO and NiO with (111) facets as the primary surface has been followed by recent work utilizing a multiscale characterization platform to discover the underlying phenomena associated with the electrolytic properties of NiO(111) for Li ion batteries and electrochromics. Joint experimental-theoretical work with collaborators unravelled the potential of (111) polar surfaces for carbon capture. Most recently, doped and mixed metal oxides (including high entropy systems) have been achieved through the use of supercritical conditions during synthesis and solvent removal. Here, recent highlights regarding these materials and their applications will be presented.

### 10:20 AM

# (ICACC-S17-004-2025) Selenization of Ni-hexacyanoferrate-based nanocubes: properties and catalytic performances (Invited)

F. Polo\*1; E. Lushaj1; T. A. Shifa1; E. Moretti1

1. Universita Ca' Foscari, Molecular Sciences and Nanosystems, Italy

In recent years, extensive efforts have been devoted to design and synthesize highly active, earth-abundant, and low-cost alternative catalysts for oxygen evolution reaction (OER). Prussian-blue analogue (PBA) materials have attracted research interests for a long time owing to their intriguing stimuli-responsive electron transfer properties. Facile synthetic routes and an improved knowledge of their properties helped spreading their use in different research field, including the energy storage. Moreover, the development of hierarchical nanostructures with controllable composition proved to be a new pathway to tune their physico-chemical properties. In this presentation, we describe a two-step protocol to synthesize composite nanocubes, constituted of nickel hexacyanoferrate (Ni-HCF) and trigonal selenium, in which the characteristics of PBAs and chalcogenide-based materials are merged. The electronic, structural, and optical properties have been fully characterized and their performances have been tested in the oxygen evolution reaction (OER) to comprehensively understand the structure-performance relationship. The new material features low charge transfer resistance and high current delivery providing enhanced kinetics toward OER.

### 10:50 AM

# (ICACC-S17-005-2025) Understanding and tailoring carbon dots (Invited)

A. Tagliaferro\*1; M. Bartoli2

- 1. Politecnico di Torino, Department of Applied Science and Technology, Italy
- 2. Istituto Italiano di Tecnologia, Italy

Since nanomaterials suddenly burst onto the scene of research, their impact has been steadily growing. New field of applications have been proposed on a yearly basis, if not faster. Although applications in fields like catalysis, energy, ... have been proposed, the greatest excitement was raised in the field of biological applications. Their potential use in biological environments has become a rather prominent topic, with applications including drug delivery, cancer therapy, localized heating and chemical probes. However, promoting a proof of concept to a real-world product devoted to human health is rather challenging. As biocompatibility needs to be guaranteed, given that tests to check it must compulsorily be run, carbon-based nanomaterials appeared among the most promising in this respect. This led many research groups worldwide to focus on carbon dots, carbon-based nanostructures having size down to a few nanometres. However, a deep understanding of the correlations among production routes, structures and properties is required to really open the gate towards applications. In this talk, we will highlight the interplay among production parameters and precursors, elemental composition and local structures, and properties. We will eventually show how, given a sought property, how to select the most appropriate structure to achieve it and the best precursors and production route to realize such a structure.

### 11:20 AM

### (ICACC-S17-006-2025) Toward Enhanced Energy Density through Interface Engineering in All-Solid-State Batteries (Invited)

T. Song\*<sup>3</sup>; J. Park<sup>2</sup>; J. Kim<sup>2</sup>; S. Lee<sup>2</sup>; J. Kim<sup>2</sup>; I. Hwang<sup>2</sup>; M. Kim<sup>2</sup>; S. Myeong<sup>2</sup>; H. Lee<sup>2</sup>; M. Ryu<sup>2</sup>; G. Lee<sup>2</sup>; S. Han<sup>2</sup>; J. Sun<sup>2</sup>; J. Jeong<sup>1</sup>; Y. Lee<sup>1</sup>; U. Paik<sup>2</sup>

- 1. Hanyang University, Department of Battery Engineering, Republic of Korea
- 2. Hanyang University, Department of Energy Engineering, Republic of Korea
- 3. Hanyang University, Department of Energy Engineering, Department of Battery Engineering, Republic of Korea

All-solid-state batteries (ASSBs) incorporating sulfide-based solid electrolytes with superior ionic conductivity represent promising candidates for next-generation energy storage solutions, owing to their potential for enhanced safety and high energy density facilitated by metallic anodes. Lithium metal, with its exceptional theoretical specific capacity (3860 mAh/g) and low electrochemical potential (-3.04 V versus the standard hydrogen electrode), is particularly attractive as an anode material. Nonetheless, its practical implementation is constrained by significant interfacial challenges, including contact degradation during cycling, which accelerates lithium dendrite propagation, and chemical instability at the Li/sulfide electrolyte interface. This work examines these fundamental degradation mechanisms from both electrochemical and mechanical perspectives, proposing advanced strategies in interface engineering to reinforce the stability of the Li metal and sulfidebased solid electrolyte interface. By employing these engineered interfaces, the developed ASSBs exhibit a marked suppression of dendritic growth and mitigation of deleterious interfacial reactions, resulting in enhanced electrochemical stability and improved energy density.

### 11:50 AM

### (ICACC-S17-007-2025) Unveiling kinetic dynamics in buffer layer formation during chemical bath deposition for enhanced solar cell efficiency

I. Gushchina\*1; C. Rossi1; S. Slimani1; D. Peddis2; D. Colombara1

- 1. Universita degli Studi di Genova, Chemistry and Industrial Chemistry, Italy
- 2. Istituto di Struttura della Materia Consiglio Nazionale delle Ricerche, Materiali e Dispositivi, Italy

Metal oxides and heterostructures play pivotal role in advancing modern technologies e.g., photovoltaics (PV). In particular, for Cu(In,Ga)Se<sub>2</sub>-based solar cells metal oxides/chalcogenides (e.g. Zn(O,S),  $In_2S_3$ ,  $Zn_{(1-x)}Sn_xO$ ,  $Zn_{(1-y)}Mg_vO$ , etc.) serve as a buffer layer and act as safer alternatives to toxic CdS buffer currently in use. Chemical bath deposition (CBD) allows an effective surface defect passivation, preventing the charge recombination in photovoltaic device. Therefore, this method is widely used for solar cells buffer layer fabrication. This work is focused on  $Zn_{(1-x)}(Sn/Mg)_xO$ materials and understanding the kinetics of thin film formation during CBD. In several studies the aforementioned buffers show an inhomogeneous composition of the film negatively affecting the final device, step-by-step investigation of film formation would help to unravel the growth mechanism. To address this, we use dynamic light scattering (DLS) to measure the size of the growing particles as a function of temperature. In addition, elemental analysis is performed to examine the distribution of elements within the film, ensuring compositional uniformity. This study will offer a better understanding of the buffer layer fabrication process to significantly improve the PV efficiency in the future.

## **S18 Ultra-High Temperature Ceramics**

### **S18- Novel Processing Methods**

Room: Coquina F Session Chairs: Ian McCue, Northwestern University; Christopher Weinberger, Colorado State University

### 8:30 AM

# (ICACC-S18-010-2025) Design Stability of Nanostructured TaC Composites (Invited)

I. McCue\*1; C. Ott1

1. Northwestern University, Materials Science and Engineering, USA

Ultra-high temperature ceramics (UHTCs) have garnered significant interest for use in next-generation hypersonic structures due to their high melting points, excellent thermo-physical properties, and reasonably-low densities. UHTCs have been used as monolithic materials or coatings, but additional functionality (e.g., ablation resistance and transpiration cooling) can be introduced by fabricating porous form factors. Here, we demonstrate the synthesis and properties of porous UHTCs derived from nanoporous refractory metals via gas-phase carburization. This talk will detail the fabrication of nanoporous metal precursors, kinetics of low-temperature ceramic conversion, and stability of these materials at high temperatures. In addition, proof-of-concept composites and their enhanced properties will be presented.

### 9:00 AM

# (ICACC-S18-011-2025) Pressureless Sintering of Hafnium Diboride-Silicon Carbide Particulate Composites

### T. W. Moore<sup>\*1</sup>

1. US Army Combat Capabilities Development Command Army Research Laboratory Aberdeen Proving Ground, USA

Hafnium diboride - silicon carbide has typically been produced by pressure assisted means, such as spark plasma sintering or hot pressing. However, these methods greatly limit the geometrical complexity that can be obtained from a sintered part without resorting to extensive diamond grinding. To enable the production of near net shape components, pressureless sintering of HfB<sub>2</sub>-SiC particulate composites with 20 vol% SiC was studied by mixing these two materials with various sintering aids and sintering at temperatures between 2000°C and 2300°C. Reactive sintering aids using stoichiometric blends of Hf metal and amorphous B were able to produce composites with >99% theoretical density at 2100° with the added benefit of the reaction products being one of the primary constituents. Further investigation into this Hf-B blend was conducted to determine how varying the amount of sintering aid would affect the densification, microstructure, hardness, and oxidation resistance of the resulting material.

### 9:20 AM

### (ICACC-S18-012-2025) Gas Chemistry Influences on Titanium Carbide Fiber Growth by Laser Chemical Vapor Deposition

K. J. Mitchell\*1; G. Thompson2

- 1. University of Alabama, Interdisciplinary Materials Science PhD Program, USA
- 2. University of Alabama, Metallurgical & Materials Engineering, USA

Laser Chemical Vapor Deposition (LCVD) is a process in which fibers are deposited from a gaseous precursor into a solid phase under a traversing laser focal point. Here, we report the growth of titanium carbide (TiC) fibers and tubes dependent upon a hyperbaric hydrogen-rich, hydrogen-balanced, and hydrogen-lean environment referenced to changes in the titanium tetrachloride and ethylene gas mixture. X-ray diffraction confirmed the deposition of B1 TiC. Depending on the hydrogen concentration, the TiC encased a carbon-rich core or formed a hollow tube, with these formations explained by thermophoresis. Energy dispersive spectroscopy noted a radial compositional gradient of titanium and carbon with electron microscopy confirming a hatch-like pattern of nanoscale Ti-precipitates in TiC near the edges of the deposit, with such microstructures explained by changes in carbon solubility in TiCx with decreasing temperature. The associated mechanical properties of these fibers/tubes were measured and correlated to the LCVD processing conditions.

### 9:40 AM

### (ICACC-S18-013-2025) Synthesis of Ultra High Temperature Ceramics by Spark Plasma Sintering: non-reactive and reactive routes

- T. Menard\*1; F. Rebillat2; J. Braun3; L. Maillé4
- 1. Laboratoire des Composites Thermostructuraux, France
- 2. University Bordeaux, Laboratory of thermostuctural composites, France
- 3. CEA, France
- 4. University of Bordeaux Laboratory for Thermostructural Composites (LCTS), UMR 5801, France

During atmospheric re-entry, the leading edges of vehicles experience temperatures exceeding 2000 °C, requiring the use of refractory materials with passivating behavior instead of common materials like C/C or C/resin composites. Ultra-High Temperature Ceramics (UHTC) are promising candidates, either as coatings or matrix materials for C/C. Key UHTC constituents include carbides (ZrC, HfC) and borides (ZrB2, HfB2), which form a porous oxide layer during oxidation. To enhance protection, SiC can be added to generate a glassy phase that fills the porosity and reduces oxygen diffusion. Spark plasma sintering (SPS) effectively produces dense UHTCs while minimizing synthesis temperature (1900°C) and time (minutes). This study aims to synthesize UHTCs via SPS, using reactive sintering to lower processing temperatures. The chosen system is (Zr,C,Si,B), with ZrB2+SiC (20 vol.%) as a reference material. A thermodynamic approach guides the selection of initial elements and compounds, with ZrB2 being the most stable at sintering temperature, followed by ZrC and SiC. Microstructures from both reactive and non-reactive routes are compared using SEM, EDS, and XRD. The materials' oxidation resistance is tested under an oxidizing environment with an oxyacetylene torch, establishing a relationship between composition, sintering route, and oxidation resistance.

### 10:20 AM

### (ICACC-S18-014-2025) The Role of Surface Energies and Dopants in Controlling Transition Metal Carbide Powder Shape

Y. Huang<sup>1</sup>; C. R. Weinberger<sup>\*1</sup>

1. Colorado State University, Department of Mechanical Engineering, USA

Tailoring powder shape through controlled crystal growth is a potential method to control precursor powders for UHTC ceramics. This method further has the potential to created tailored powders, which can improve sintering as well as change properties of these materials. However, there are large gaps in our understanding of what controls the as-grown crystal shapes. In this talk, we examine how carbide crystals can be controlled through their surface energies via carbon vacancies and transition metal doping. Specifically, we use DFT modeling to examine how carbide stoichiometry changes the surface energies and subsequent shapes of cubic carbide crystals. Then, we demonstrate how doping with different transition metals can also change these equilibrium shapes. These results are then compared to experimental observations of transition metal carbide powders to provide a better understanding of what controls carbide particles shapes and how processing conditions can affect it.

### 10:40 AM

### (ICACC-S18-015-2025) Synthesis of Binary Solid Solution Powders via Boro/Carbothermal Reduction and Arc Melting

Z. Ayguzer Yasar\*<sup>1</sup>; R. Haber<sup>1</sup>

1. Rutgers The State University of New Jersey, Material Science and Engineering, USA

Ultrahigh-temperature ceramics (UHTCs), such as titanium diboride (TiB2), zirconium diboride (ZrB2), and tantalum diboride (TaB2), have exceptional thermal and mechanical properties required for hypersonic, nuclear power, and tooling applications. However, UHTC composites are difficult to produce due to the need for high-purity powder and the importance of particle size distribution. Furthermore, multicomponent boride powders are not commercially available. In this study, titanium diboride, zirconium diboride, and tantalum diboride as single and binary borides were successfully synthesized by boro/carbothermal reduction and arc melting method. It was observed that high-purity and submicron single and multi-component boride powders can be produced by this method.

### 11:00 AM

### (ICACC-S18-016-2025) Synthetic Method of Oxidized Zr-based polymer Precursor for PIP Method using the Sol-Gel Method

J. So\*1; K. Lee1; S. Kim1; M. Park1; S. Lee1

1. Korea Institute of Materials Science, Republic of Korea

Ultra-high-temperature ceramics (UHTC) are promising materials in the aerospace and defense industries. Their unique properties, including high heat resistance and ablation resistance, have made UHTC indispensable materials in the aerospace industry. Among UHTC, Zr-based ceramics (ZrO<sub>2</sub>, ZrC) are widely used due to their high melting points exceeding 2800°C. One of the densification methods for Zr-based ceramics is the polymer infiltration & pyrolysis (PIP) method. In the PIP method, a liquid polymer precursor with low viscosity is necessary for efficient infiltration into matrix. Typically, Zr-based ceramic precursors have been synthesized through sol-gel reactions with zirconium alkoxides and carbon sources. These carbon sources often contain hydroxyl functional groups, which facilitate the sol-gel reaction but can complicate control over the molecular weight of the product, resulting in significantly increased viscosity. Therefore, new synthetic strategies are required to increase ceramic yield while reducing precursor viscosity. In this present versatile, enabling the production of both ZrC and ZrO2 depending on the carbon source's presence, we will introduce a novel oxidized precursor for the fabrication of ZrC and ZrO2. The carbon source used in our study acts as a solvent, effectively decreasing the viscosity of the precursor and promoting a stable infiltration process.

### **<u>S19 Molecular-level Processing and Chemical</u>** <u>Engineering of Functional Materials</u>

# S19- Precursor-derived high-entropy ceramics and UHTCs

Room: Ballroom 3 Session Chair: Gunnar Westin, Uppsala University

### 8:30 AM

# (ICACC-S19-011-2025) A New Route to High Entropy Nitride Compounds (Invited)

R. M. Laine\*1; J. Heron2

1. University of Michigan, Materials Science and Engineering, USA

2. University of Michigan, USA

The Laine group has, over the last decades, formulated ceramic precursor design principles in two reviews, that can serve as criteria for the work proposed here. A primary focus must be on the synthesis of processable precursors typically defined as meltable, soluble or malleable which implies introduction of extraneous ligands that prevent early crosslinking while imparting processability. Unfortunately, said ligands must be lost on thermal conversion to the target HEN reducing final ceramic yields. Phase purity. With HENs, it may be that some impurities such as C or Si will improve delta S and favor stability. The small number of HENs described primarily in the Russian literature to date offer FCC structures. To our knowledge there are no publications on the use of precursors to process HENs; although there is one modest patent on the subject. A further observation is that most of the reported materials are sintered at temperatures of 1800-2200 °C. In principle, precursors may reduce processing temperatures given essentially atomic mixing at the outset reducing diffusion distances but not necessarily temperatures needed to access the correct phase purity. In our precursor approach to HENs, we have reported the need to heat to 1800°C to obtain good crystallization of AlN; however, in our next systems much lower temperatures provide targe materials as powders and thin films.

### 9:00 AM

### (ICACC-S19-012-2025) Molecular Precursor Strategies for High-Entropy Oxides (Invited)

- Z. Aytuna<sup>1</sup>; T. Fischer<sup>\*1</sup>; S. Mathur<sup>1</sup>
- 1. Universitat zu Koln Mathematisch-Naturwissenschaftliche Fakultat, Institute of Inorganic and Materials Chemistry, Germany

Entropy stabilized multi-cation oxides are of significant interest in heterogeneous catalysis due to higher number of active sites, when compared to simple binary oxides, which reduces for example the overpotential or alters the selectivity in catalytic transformations. To control the enthalpy of mixing and suppress potential phase segregation, the use of molecular metal alkoxides for chemical cross-linking of different metal centers shows promise in creating homogenous

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high entropy chemical preceramic networks. While traditional solidstate processing requires high temperature, molecular precursors with a preformed metal oxygen framework provide a straightforward reaction pathway for the desired metal oxide materials. Moreover, homogeneous mixing of molecular precursors in solution processing provides unrivalled homogeneity and low temperature processability of high entropy oxide materials. This talk will highlight the synthesis and processing of transition metal alkoxide precursors via solution processing into high-entropy oxide materials, and their application in electrocatalytic water splitting.

### 9:30 AM

## (ICACC-S19-013-2025) Ultrahigh Temperature Ceramics from Electrified Pyrolysis (Invited)

S. Ren<sup>\*1</sup>

1. University of Maryland, USA

Compositionally complex ceramics provide a significant advantage over traditional ceramics when it comes to operating in extreme environments, their high-temperature stability, highly distorted lattices and unique metallic, covalent, and ionic bonding. In this talk, we report the synthesis of compositionally complex ceramics with excellent high-temperature stability using a preceramic molecular approach based on the crosslinking of transition metal salts with the short-chain silicon monomers. Using molecular monomers instead of long-chain polymers (i.e., preceramic polymers) allows for precise control over the dispersion of transition metals at the atomic level and the formation of dense, pore-free ceramics, which was not possible using the preceramic polymer approach. We crosslinked transition metal elements from groups 4-6 with preceramic monomers, resulting in compositionally complex ceramics with a lower pyrolysis temperature. These ceramics can be additively manufactured onto various metals and conformal structures to enable thermal management of the metal base via suppressing oxidation at elevated temperatures. Besides thin film coatings, the feedstock can also be used to fabricate bulk ceramic pellets. Furthermore, the speed and scalability of the ceramic formation enables rapid screening of different compositions as oxidative barrier coatings on metals or other intricate structures.

# S19- Conversion, decomposition, and structural formation of molecular precursors

Room: Ballroom 3

Session Chair: Thomas Fischer, University of Cologne

### 10:20 AM

### (ICACC-S19-014-2025) Single Source Precursors for Spinel Ferrites in Chemical Vapor Deposition

S. Diel<sup>1</sup>; T. Fischer<sup>\*1</sup>; S. Mathur<sup>1</sup>

1. Universitat zu Koln Mathematisch-Naturwissenschaftliche Fakultat, Institute of Inorganic and Materials Chemistry, Germany

Spinel ferrites are a stable, yet versatile class of ternary metal oxide materials of the genera structure MFe<sub>2</sub>O<sub>4</sub> with different applications, ranging from magnetic materials to heterogeneous catalysts. While traditional solid-state synthesis relies on high temperature processing, molecular single-source precursors open new process parameter windows in chemical vapor deposition (CVD). Here, trinuclear bimetallic alkoxides have been identified as adaptable precursors with preformed metal-oxygen framework, desired stoichiometry (M:Fe ratio = 1:2) and correct oxidation states of the metal centres. Although, these properties facilitate the materials formation from molecular precursors, the synthesis, handling and identification of optimal process parameters to yield phase pure target materials remains a challenge. With the support on operando techniques, the film formation can be studies in detail and provide meaningful data for process optimization. Moreover, external magnetic fields can support the phase formation and microstructure evolution for enhanced functional properties. This talk will highlight the synthesis and application of different bimetallic spinel ferrites in chemical vapor deposition and the application of the resulting nanostructured spinel thin-films in electrochemical water splitting reactions.

### 10:40 AM

### (ICACC-S19-015-2025) Development of Highly Weather-Resistant Components Using Photo-induced Metal organic decomposition (MOD) and Resource Recycling

T. Tsuchiya\*1

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

The chemical solution method is expected to be applied to various industrial fields as an energy-saving process because it has good control of the metal composition and does not require a vacuum device. On the other hand, it is generally difficult to combine it with metal or resin substrates that do not have heat resistance because the decomposition of organometallic compounds and the crystal growth of metal oxide thin films require heating processes at 500 °C or higher. From this perspective, we have developed a coating and Photo irradiation method that uses the photochemical reaction of metal-organic compounds with ultraviolet lasers or, lamp. In this paper, we will report on the technology for coating ceramics with high weather resistance on plastic and metal substrates and on resource recycling using Photo-induced MOD. This work was partially supported by Council for Science, Technology and Innovation: CSTI, Cross ministerial Strategic Innovation Promotion Program(SIP), Building a Smart Infrastructure Management System(Funding agency Public: Works Research Institute)

### 11:00 AM

# (ICACC-S19-016-2025) Growth control of nanocrystals: A deeper understanding of surface energetic contributions

R. Castro\*1

1. Lehigh University, Material Science & Engineering, USA

Nucleation and growth are critical processes controlling synthesis and application of functional oxide nanoparticles. For this later, high temperature applications can activate growth modes, compromising features only present due to the nanoscale dimension. In this talk we present an effective strategy to control the growth of nanocrystals by targeting reduction of the driving force: surface energies. By providing experimental data, we demonstrate that thermodynamics of nano-oxides can be designed to minimize growth potentials, being an important contributor for stabilization and nucleation control. By using Zirconia and Aluminates as model systems, we describe how thermochemistry plays a critical role in those engineering processes.

### 11:20 AM

## (ICACC-S19-017-2025) From precursor to nanoparticle formation, size control and structural study (Invited)

J. Jouin<sup>\*1</sup>; F. Remondiere<sup>1</sup>; J. Gambe<sup>1</sup>; A. Lemarchand<sup>1</sup>; O. Masson<sup>1</sup>; P. Thomas<sup>1</sup>

1. Institut de Recherche sur les Ceramiques, France

The liquid phase synthesis of materials is a powerful way to obtain samples which could otherwise not be prepared by conventional methods. This is particularly useful when dealing with nanomaterials, as starting from metal organic precursors favors a better control of the nucleation/growth phenomena. In this work, the synthesis of nanoparticles of metal oxide compositions was performed in the ZrO<sub>2</sub>, ZnO, SnO<sub>2</sub> and TiO<sub>2</sub> systems, using different controlled methods such as non-hydrolytic solvothermal synthesis. The objective was to obtain crystallized particles with uniform sizes of less than 5 nm to correlate the synthesis parameters with the size and local structure of the samples. Indeed, for such small sizes, the bulk-based structural models do not apply anymore and specific properties are identified. For all the selected chemical systems, the synthesis of very small crystallized particles was successful. In this case, the presence of residual water and thermal parameters is as important as the choice of the reagents. The samples were analyzed by conventional X-ray diffraction, pair distribution function and transmission electron microscopy in order to determine their average and local structure as well as their morphology. Locally, the atomic structure of the particles are clearly different from the bulk structures when the sizes are inferior to 5 nm.

## 14th Global Young Investigator Forum

### **GYIF-Sustainable Materials Development** / **Eco-Design Principles for Ceramics and Composites** Room: Coquina G

Session Chairs: Stefano De La Pierre, Politecnico di Torino; Srinivasa Nemani, Indiana University

### 1:30 PM

### (ICACC-GYIF-015-2025) Specialized Data-Driven Framework for Designing Compositionally Complex Ceramics for Energy Storage and Conversion (Invited)

B. Ouyang<sup>\*1</sup>

1. Florida State University, Chemistry and biochemistry, USA

The emerging of data driven materials research and generative artificial intelligence has revealed exciting opportunities for designing ceramic materials for energy storage and conversion. Particularly, training a foundation AI with enormous computational data may serve as useful starting point to explore complex ceramic design space. In this talk, we will present our recent progress on developing specialized database and machine learning models emphasizing on compositionally complex ceramic materials for energy storage and conversion applications. Leveraged on our house developed computational dataset that contains > 100,000 DFT computed compositionally complex ceramics across periodic table, our talk will cover understandings across two aspects: 1) What is the most adequate dataset and machine learning framework that can make best use of domain knowledge of ceramics for energy storage and conversion; 2) From which aspects large computational dataset can help to discover the synthesizability and stability of ceramics for energy application? Our talk will also cover our understanding of the advantages of specialized dataset and AI agent compared to more generic AI for broad scope of materials science.

### 2:00 PM

### (ICACC-GYIF-016-2025) Abrasive Effects of Lunar Regolith on Material Wear for Long-Term Lunar Application

Z. Stein\*1; C. Wohl2; V. L. Wiesner2; S. Raghavan1

- 1. Embry-Riddle Aeronautical University, Aerospace Engineering, USA
- 2. NASA Langley Research Center, Advanced Materials and Processing Branch, USA

Long-term operations on the Moon's surface require materials that can withstand the harsh lunar environment. Lunar dust and regolith pose significant threats to the long-term durability of materials used in lunar applications. Lunar dust, easily perturbed and dispersed, adheres and abrades materials due to its rough and irregular grain morphology. More closely representing this abrasion action through experimental laboratory testing is critical in assessing the durability of potential lunar candidate materials used in mechanical, sensor, and humanbased systems. In this study, the performance of materials using Taber abrasive wheels made from lunar regolith simulant was assessed and compared to results obtained using standard ceramic-based abrasion materials. The results highlight a difference in the abrasive wear rates between the lunar regolith simulant and the standard ceramic-based abrasive. Utilizing the mechanisms and testing capabilities of this two-body abrasive interaction leveraging regolith-based abrasives may more closely represent the interplay between materials and lunar dust, which is vital for assessing the long-term viability of materials for extended lunar missions. Improved lunar testing capabilities may also enhance evaluations of the long-term performance degradation of passive and active dust mitigation method.

### 2:20 PM

## (ICACC-GYIF-017-2025) Improving sustainability in gas turbine engines through mindful material selection (Invited)

C. S. Holgate\*1; S. Berens1; N. Basilyan1; C. G. Levi1

1. University of California, Santa Barbara, Materials, USA

The world's ongoing transition towards sustainability and minimizing the use of fossil fuels demands materials design breakthroughs. Two particularly challenging industries to improve are aerospace and natural gas power generation, both of which rely on gas turbine engines. Their efficiency can be greatly improved by burning fuel hotter, but this accelerates wear on the internal components. A critical engine component is ceramic thermal or environmental barrier coatings, typically consisting of a rare-earth (RE) oxide and either  $ZrO_2$ ,  $HfO_2$ , or  $SiO_2$ . These coatings are susceptible to attack by silicate debris, which melts in the hottest parts of the engine and drives severe thermomechanical stresses in the brittle coatings. The extent of damage depends on the chemical interaction between the coating and the silicate melt, which in turn depends on the rare-earth species chosen. In this work, the impact of the RE choice is investigated through exposing three RE<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> coatings to molten silicates. The findings will be discussed in the context of choosing a RE species that balances performance with sourcing sustainability (e.g., mining, availability in the crust).

# GYIF- Energy and Material-Efficient Manufacturing Processes

### Room: Coquina G

Session Chairs: Mark Du, Argonne National Laboratory; Yuki Nakashima, National Institute of Advanced Industrial Science and Technology (AIST)

### 3:20 PM

### (ICACC-GYIF-018-2025) Harsh Environment Material Manufacturing for Clean Energy Technologies at Idaho National Laboratory (Invited)

J. Rufner\*1; A. Preston1; A. Gorman1; X. Zhang1

1. Idaho National Laboratory, Materials and Manufacturing, USA

Idaho National Laboratory (INL), a multi-disciplinary national laboratory with the mission of changing the world's energy future, is the home to the Center of Excellence for Field Assisted Sintering Sciences, and dedicated to the advancement of clean energy technology. An important part of enabling clean energy deployment requires creating material solutions specific to each of their operating environments, which are quite harsh. INL has been at the forefront of researching and developing such materials capable of withstanding harsh environments and extreme conditions, including high temperatures, radiation, mechanical stress, and corrosive environments. Advanced manufacturing, specifically with advanced sintering technologies such as electric field assisted sintering (EFAS), is a powerful pathway that is poised to open access to many materials for harsh environments that were previously out of reach. INL is driving the scientific research, development, and deployment of field assisted sintering at both small and large length scales. Methodology, benefits, and projects using EFAS to enable technologies such as fusion and fission energy, embedded sensors for material health surveillance, materials for aerospace utilization, corrosion resistant alloy fabrication, molten salt and concentrated solar power/thermal systems, and critical material manufacturing will be presented.

### 3:50 PM

### (ICACC-GYIF-019-2025) Flexible Chemical and Fuel Production using Protonic Ceramic Electrochemical Cells (PCEC) for Energy and Materials-Efficient Manufacturing Processes (Invited)

D.  $Ding^{*1}$ 

1. Idaho National Lab, Hydrogen and electrochemistry, USA

Protonic ceramic electrochemical cells (PCECs) are solid-state electrochemical devices using the proton-conducting oxide as the electrolyte. Besides power generation as fuel cells, PCECs is an emerging technology that could be employed for flexible chemical manufacturing by using a range of feedstocks. Economically competitive PCEC systems have distinct advantages over their counterparts at lower or higher temperatures, but further technology development and widespread market acceptance will require continuous innovation of materials and structures in order to improve cell performance, enhance system lifetime and reduce cost. Herein, we report the advancement of PCEC with new electrode component, catalyst integration, unique electrode structures as well as deep investigation on the state-of-the-art electrolyte materials to enable high-performance and robust operation for chemical and fuel production when sustainable feedstocks (e.g. steam, carbon dioxide and nitrogen) are used. Special emphasis is placed on intermediate temperatures, which shows potentials of PCEC as process intensified manufacturing processes technologies compared with those industrial mature processes. At the end, we will also highlight INL's effort on advanced manufacturing processes to scale up the technologies.

### 4:20 PM

### (ICACC-GYIF-020-2025) Hexagonal boron nitride incorporated electrospun polyvinylidene separators with enhanced thermal conductivity and stability for safer Li-ion batteries (Invited)

B. Kottathodi\*1; W. Tang1; J. Jeevarajan1

1. UL Research Institutes- ESRI, USA

Because conventional lithium-ion batteries (LIBs) have limitations at high temperatures, their safety still remains a serious issue, which restrict the large-scale energy storage applications in different sectors including electric vehicles. The separator plays a critical role in ensuring the safe and efficient operation of LIBs and the present study focuses on the fabrication of hexagonal boron nitride (h-BN) incorporated polyvinylidene fluoride (PVDF) separator by the electrospinning technique. h-BN has excellent thermal conductivity and mechanical stability, and when incorporated into the highly porous electrospun PVDF matrix, promotes efficient heat dissipation in the separator during cell cycling. Additionally, this distinct fusion also improves the separator's wettability, ionic conductivity, and mechanical stability, which lead to better electrochemical performance. This presentation demonstrates h-BN-PVDF as a promising separator material with enhanced thermal stability that avoids thermal shrinkage, which ultimately prevents battery short circuit, allowing for safer LIBs.

### 4:50 PM

# (ICACC-GYIF-021-2025) Sustainable Lunar Construction Using Freeze Casting and Sintering of Regolith (Invited)

S. S. Hossain<sup>\*1</sup>; J. W. Bullard<sup>1</sup>

1. Texas A&M University, Department of Civil and Environmental Engineering, USA

Space agencies are undertaking missions that aim to establish a permanent human base on the Moon within next two decades. Transporting resources from Earth to support that effort is prohibitively expensive, so the success of these plans will on-demand manufacturing of infrastructure, tools, and replacement parts using indigenous materials and energy sources. We explore the use of lunar regolith as the primary raw material in the sustainable fabrication of construction materials by freeze casting and sintering. We show that high-fidelity synthetic regolith can be transformed into lightweight or dense load-bearing components with intricate shapes through freeze casting, using a small volume of non-recyclable additives. Freeze casting has great potential to utilize the cold vacuum environment of the lunar polar regions for the freezing and sublimation steps, which may reduce the energy consumption required for shape fabrication. The key parameters, including the regolith composition, particle size distribution, and sintering conditions, play crucial roles in developing the physical and mechanical properties of the final material. This study paves the way for future research into scalable manufacturing methods that could support a long-term human presence on the Moon, reduce reliance on Earth-supplied materials, and enhance the sustainability and feasibility of in-situ resource utilization.

### FS6 Innovative material processing for diverse resource circulation loops

# FS6- Innovative material processing for diverse resource circulation loops II

Room: Ballroom 5

Session Chairs: Enrico Bernardo, University of Padova; Katsuya Teshima, Shinshu University

### 1:30 PM

#### (ICACC-FS6016-2025) Optimizing Concrete Performance with Recycled Crushed Glass Aggregate (Invited)

- D. Alterman\*<sup>1</sup>; C. Tokoro<sup>2</sup>; C. Gerber<sup>1</sup>; A. Narita<sup>3</sup>; T. Koita<sup>2</sup>;
- D. Jozwiak-Niedzwiedzka4
- 1. University of the Sunshine Coast, Australia
- 2. Waseda University, Japan
- 3. Waseda University, Sustainable Energy & Environmental Society Open Innovation Research Organization (SEES), Japan
- 4. Polska Akademia Nauk, Poland

This paper explores the feasibility of using recycled crushed glass as an aggregate replacement in concrete pavers and its effects on strength properties. The findings indicate that while recycled glass impacts strength, the effect is not detrimental. Results support the use of glass aggregate in construction, consistent with previous research. Though some mixes showed a slight reduction in compressive strength, flexural strength improved with more glass content. The slower rate of strength gain, potentially leading to long-term improvements, is an important factor for design consideration. Environmental conditions affected strength gain, though most mixes achieved design strength within 28 days. The slower pozzolanic reaction rate of glass can be managed through careful design and extended curing. No significant changes in slump or bleed water were noted, with a slight increase in air content, indicating mix designs can accommodate these variables. Durability concerns, particularly Alkali Silica Reaction were addressed by using fly ash and selecting appropriate aggregate size. Image analysis showed smooth, non-cubic glass aggregates, which enhanced flexural strength without affecting workability. In conclusion, recycled crushed glass is a viable aggregate replacement in concrete pavers, offering environmental and economic benefits when appropriate design measures are taken.

### 2:00 PM

### (ICACC-FS6017-2025) Novel fabrication and disassembly processes for ceramic devices by chemical reactions near room temperature for material recycling (Invited)

Y. Yamaguchi\*<sup>1</sup>

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Most of ceramic devices are fabricated by co-sintering process at 1000 °C, recently, these processes are expected to change into cleaner process which can reduce the  $CO_2$  emission in the device fabrication. In addition, these ceramic devices were difficult to disassemble for

the material recycling. Then, these are often scraped. In this study, we introduce the process for obtaining the dense ceramic material using acid-base reaction and a novel decomposing process of ceramics under 200 °C using similar solution to densification, which can disassemble layered ceramic devices. For the fabrication of dense ceramics, amorphous hydrous metal oxide powders were pressed and molded to pellet shape which are used as precursors. These precursor pellets were immersed into alkaline earth hydroxide solution and kept blow 150 °C, then, the dense complex oxide ceramic can be obtained. For example,  $BaZrO_3$  can be prepared with over 90 % relative density. In addition, prepared dense ceramics can be decomposed to powder state using the chemical treatment in same alkaline earth hydroxide solution.

### 2:30 PM

### (ICACC-FS6018-2025) Sintering Kinetics and Optimization of Polymer Sintering for Improved Filter Performance (Invited)

M. Kaneko\*1

1. NITTETSU MINING CO., LTD., MACHINERY AND ENVIRONMENT, Japan

Sintered polymer filters, which are renowned for their durability and longevity in comparison to nonwoven alternatives, are increasingly regarded as a promising technology for the circular economy. Nevertheless, the theoretical comprehension of the sintering process for polymer materials like polyethylene remains constrained, particularly in regard to manufacturing. One reason for this limitation is that the final product's performance is influenced by variations in particle size distribution, particle shape, molecular weight among polymer suppliers. The objective of this study was to investigate the manner in which the particle size distribution and temperature dependence of melt viscosity of polymer particles are reflected in the sintering process. We introduced a kinetic model that quantifies the neck growth between polymer particles, thereby enabling us to examine the changes in tensile strength and air permeability of porous products as sintering progresses. Moreover, by modifying the polymer type and sintering conditions and examining the internal structure, we investigated the influence of powder characteristics on filter performance. Our findings indicate that a theoretical understanding of the polymer sintering process can facilitate the optimization of the manufacturing process, the reduction of variability in production, and the achievement of consistent product quality.

# FS6- Advanced powder processing both for carbon net zero and circular economy II

#### Room: Ballroom 5

Session Chairs: Dariusz Alterman, University of the Sunshine Coast; Yuki Yamaguchi, National Institute of Advanced Industrial Science and Technology (AIST)

### 3:20 PM

### (ICACC-FS6019-2025) Advanced Membrane Technology for Direct Air Capture: Utilizing Ionic Liquid Mixtures and Nanoceramics (Invited)

T. Makino\*<sup>1</sup>

1. National Institute of Advanced Industrial Science and Technology, Japan

To achieve the 1.5°C scenario of the Paris Agreement, reaching carbon neutrality by 2050 and achieving negative emissions afterward are essential. Alongside decarbonizing electricity and conserving energy, CCUS from emission sources is crucial. Post-2050, deploying negative emission technologies (NETs), such as direct air capture with carbon storage (DACCS), is necessary. Although DACCS is currently costly, future advancements could reduce these costs. Conventional DAC methods require significant thermal energy for CO<sub>2</sub> recovery. Our research explores membrane-based DAC (m-DAC), which can primarily operate on renewable energy without thermal energy. Given the low atmospheric CO<sub>2</sub>

concentration (0.04%), efficient membranes are required. Facilitated transport membranes (FTMs) show promise for low-concentration  $CO_2$  capture. Ionic liquids (ILs) are promising materials due to their high  $CO_2$  permeability and non-volatility. We have developed optimized IL mixtures for m-DAC, achieving a  $CO_2$  permeability of 25893 Barrer and  $CO_2/N_2$  selectivity of 10059. We produced a mass-production prototype IL membrane using Roll to Roll technology with a nanoceramic layer, achieving a  $CO_2$  permeance of 1104 GPU and  $CO_2/N_2$  selectivity of 3556. This exceeds conventional polymer membranes' performance. Our presentation will detail this advanced membrane's characteristics.

#### 3:50 PM

### (ICACC-FS6020-2025) Flux-grown crystal innovation for circulating water systems - Data-driven/AI & high-throughput processes (Invited)

K. Teshima\*<sup>1</sup>; T. Yamada<sup>1</sup>; F. Hayashi<sup>1</sup>; N. Isu<sup>1</sup>; A. Tanaka<sup>1</sup>; C. Terashima<sup>2</sup>; S. Oishi<sup>1</sup>

- 1. Shinshu University, Institute for Aqua Regeneration, Japan
- 2. Tokyo University of Science, Research Center for Space System Innovation, Japan

Recently, we have developed a number of high-performance crystals grown by the flux method, which we refer to as "Shindai Crystals (i.e., High performance crystals grown at Shinshu University)". We have also demonstrated their practical applications in various fields. The flux method represents one of the principal techniques for the growth of liquid-phase crystals. The method is environmentally friendly, simple, and inexpensive, and it can produce inorganic crystals at temperatures much lower than the melting point. In this regard, the flux method has been employed to fabricate a variety of highly crystalline particles and composites at relatively low temperatures. We have employed our flux method to fabricate crystalline particles of diverse designs, including next-generation batteries, visible light-driven photocatalysts for solar-thermal hydrogen production and ion exchangers for water purification. Lately, we have been particularly focused on solving the water issues in the world. Additionally, we are collaborating with a start-up company to develop a device that will enhance water circulation. Moreover, we are integrating data-driven and AI methodologies for efficient material exploration and proposing a high-throughput robotic system. Acknowledgements: this research was partially supported by CSTI-SIP, JST-GteX, Aichi Grant and JSPS-KAKENHI.

### FS6- Circular economy perspectives for inorganic waste/wastewater valorisation/stabilization I Room: Ballroom 5

Session Chairs: Yuki Yamaguchi, National Institute of Advanced Industrial Science and Technology (AIST); Dariusz Alterman, University of the Sunshine Coast

### 4:20 PM

# (ICACC-FS6021-2025) Enhanced waste glass upycling by engineered alkali activation

F. Carollo<sup>1</sup>; Z. Muhammad Jamshaid<sup>1</sup>; G. Tameni<sup>1</sup>; P. Sgarbossa<sup>1</sup>; E. Bernardo<sup>\*1</sup>

1. University of Padova, Industrial Engineering, Italy

Despite the general perception, glass is not fully recyclable. Significant amounts of glass cullet, especially as fine powders ('glass fines'), are still landfilled. Fines typically concentrate heterogeneities (e.g. metal, polymer and ceramic particles) which complicate both remelting (closed loop recycling) and valorization in new glass-based products (open loop recycling). The chemical attack of glass fines suspended in diluted alkaline solutions (NaOH, KOH<3 M) offers nwe opportunities. OH<sup>-</sup> ions promote the cleavage of Si-O-Si, Si-O-Al, Si-O-B bonds, in a first stage, resulting in the formation of Si-OH, Al-OH, B-OH groups at the surface of particles. Adjacent particles, upon

drying of suspensions, undergo welding by condensation of the same Si-OH, Al-OH, B-OH groups and formation of new strong bonds. The voids between packed particles concentrate both alkali ions and products of glass dissolution in a gel, which may be solubilized by immersion in acid solution or in boiling water. The resulting product is a porous cementituous glass-based matrix matching well, in terms of strength-to-density and thermal conductivity, with conventional lightweight concrete. We will discuss the application to a vast range of industrial glasses (container glass, glass for LCD displays, opal glass) as well as to glasses from the melting of incinerator bottom ashes and the energy savings, upon drying, provided by microwave heating.

### 4:40 PM

### (ICACC-FS6022-2025) Pumice stone, refractory brick and cork wood on the facade of buildings to mitigate noise pollution in urban street canyons

- J. Rendón Giraldo\*1; H. A. Colorado L.<sup>2</sup>
- 1. Universidad de Antioquia, CCComposites Laboratory, Colombia
- 2. Universidad de Antioquia, Colombia

The behavior of ambient noise in urban street canyons is conditioned by elements that are not only linked to the noise source, which is usually road traffic, but also to the different materials that make up the facade of buildings. The different materials related to the facades of buildings such as glass, stone and cement mixtures cause highly reverberant environments that increase the level of noise pollution in pedestrian areas. To evaluate these conditions, a 1:10 scale model was used, which was equipped with a linear array of tweeters that simulated the noise produced by a vehicular source circulating on a road and measurements of the sound level meter on the pedestrian sidewalk. In this work, different materials such as pumice stone, refractory brick and cork wood are related, which, located in 16.7% of the facades of buildings in urban street canyons, can mitigate up to 5.1 dBA in frequency bands between 125 and 500 Hz.

### 5:00 PM

# (ICACC-FS6023-2025) Tailoring of secondary metal oxide raw materials for sustainable ceramics in concentrated solar thermal technology

G. Alkan\*1; P. Mechnich2; D. Kenn3; P. Friedrich3

- 1. Deutsches Zentrum fur Luft- und Raumfahrt DLR, Germany
- 2. DLR German Aerospace Center, Institute of Materials Research, Germany
- 3. Rheinisch-Westfalische Technische Hochschule Aachen, Germany

Metallurgical slags are considered as promising sustainable and economical secondary oxidic raw materials to prepare spherical ceramic particles to be used in concentrated solar thermal technology (CST) as high-temperature stable heat absorptance and storage medium. In this study, non-ferrous fayalitic slags from copper and lead industry were assessed as secondary raw materials in a comparative manner. The influence of chemistry, crystal quality and phase composition on CST related functional properties such as heat capacity, solar absorptance and high temperature stability was studied. Moreover, copper fayalitic slag was exposed to the adapted smelting process with subsequent thermal treatment to tune crystal quality and phase content. The effect of cooling rate in smelting process and thermal treatment conditions on crystal quality and phase formation mechanisms has been investigated. The controllability of material properties by adaptive smelting and heat treatment, and their effect on CST related properties is discussed.

## <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

### S1- Ceramics for Concentrated Solar–Thermal Power and Industrial Process Heat II

Room: Coquina E

Session Chair: Kamala Raghavan, Department of Energy

### 1:30 PM

### (ICACC-S1-020-2025) Development of a SiC based Heat Exchanger for Concentrated Solar Application\* (Invited)

D. Singh<sup>\*1</sup>

1. Argonne National Lab, USA

High-temperature heat exchangers that can operate above 700°C and up to 20 MPa fluid pressures are needed for efficient heat transfer in the future concentrating solar power plants. At these temperatures and pressures, metal heat exchangers degrade in structural performance. In this regard, heat exchangers based on advanced materials is needed. In this presentation, design and development of a SiC-based heat exchanger will be discussed. Ceramic-to-metal approach to integrate the heat exchanger for performance testing will be presented. Finally, on-going efforts in the process scale-up of the ceramic heat exchanger will be highlighted. \*This work was supported by the U.S. Department of Energy's (DOE) Office of Energy Efficiency and Renewable Energy (EERE) under the Solar Energy Technologies Office (SETO) Award Number 38479 at Argonne National Laboratory operated under Contract no. DE-AC02-06CH11357 by the UChicago Argonne, LLC.

### 2:00 PM

### (ICACC-S1-021-2025) Development of a Silicon Carbide Composite Receiver for Concentrated Solar Power

F. Mohammadi\*<sup>1</sup>; J. Halfinger<sup>1</sup>; K. Armijo<sup>2</sup>; N. Schroeder<sup>2</sup>; T. Daspit<sup>3</sup>; M. Anderson<sup>4</sup>

- 1. Ceramic Tubular Products, LLC, USA
- 2. Sandia National Laboratories, USA
- 3. University of Virginia, USA
- 4. University of Wisconsin-Madison, USA

In the past several years, silicon carbide (SiC) fiber-reinforced composites have been extensively investigated for high temperature applications especially in the areas of solar-thermal energy. Its excellent mechanical, thermal, and optical properties at high temperatures make SiC very attractive for the use in "Gen 3" concentrated solar power (CSP) plants, as a solar receiver or as a heat exchanger coupled to an sCO2 Brayton cycle power conversion system. In this work, the performance of multilayer SiC fiber composites made by a polymer infiltration and pyrolysis (PIP) process was investigated. The composites were manufactured using Hi-Nicalon and Nicalon-CG silicon carbide fibers infiltrated with a silicon carbide matrix. The multilayer SiC tubes showed stable solar absorptance and emittance of 0.97 and 0.91, respectively, at 800 °C. The hoop tensile strength of the composites revealed no loss of mechanical strength due to the thermal shock up to 1100 °C. In addition, the joined SiC components showed significant corrosion resistance to molten chloride salt at 800 °C. This work is focused on addressing the properties of multilayer SiC fiber composites manufactured by PIP process relevant to high temperature requirements of Gen 3 CSP plants. The manufacturing and properties of multilayer SiC tubes such as mechanical, thermal, and solar optical performance will be discussed in this paper.

### 2:20 PM

## (ICACC-S1-022-2025) Compatibility of metallic phase change materials with SiC and with SiC/SiC joints

C. Malinverni\*2; M. Salvo2; C. Prentice1; M. Farnham1; V. Casalegno2

- 1. Archer Technicoat Ltd, ATL, United Kingdom
- 2. Politecnico di Torino, Italy

Ceramic matrix composites are materials that exhibit superior oxidation stability at elevated temperatures compared to metals and enhanced toughness compared to monolithic ceramics. The SiC/ SiC composites exhibit high temperature performance in terms of thermo-mechanical properties, corrosion resistance and low density. The objective of the research was to develop a joining technology that would use SiC/SiC composites and their joints in concentrated solar power (CSP) applications. This was done to promote the use of these materials as container walls for high-temperature metallic phase change material (mPCM) integrated CSP systems for thermal energy storage. It is of particular importance that these composites are capable of functioning in direct contact with mPCMs such as AlSi12 alloy and molten silicon. The joining material was selected according to a number of criteria, including the match of the coefficient of thermal expansion, good wettability, and compatibility with the selected mPCMs. The samples were characterised by scanning electron microscopy and tested with and without an outer boron nitride layer, which was used as protective coating. Finally, exposure tests between SiC/SiC samples and their joints and molten mPCMs were also performed.

### 2:40 PM

#### (ICACC-S1-023-2025) Heat exchanger additive manufacturing for CSP: Experimental and modeling studies for improving overhang stability

M. Du\*1; Q. MacKenzie1; G. Hu1; D. Singh1

1. Argonne National Laboratory, USA

Additive manufacturing (AM) technology, such as binder jetting, has been used to manufacture ceramic composite heat exchangers for concentrated solar-thermal power (CSP). The overhang design, which is critical in heat exchanger design to incorporate various fluid flows, had a challenge of low stability and consequent deformation during AM. Overhang deformation includes sagging and cracking, and has been detected in parts from the binder jetting AM process. To understand its mechanism, a design of cube part with multiple overhang cylinders at different heights was printed, and overhang deformation increased as its height increased. Printing parameters, including roller traverse speed, roller rotation, dispensed powder amount, and binder saturation, were studied for their effects on the overhang deformation. To further investigate the cause of overhang deformation, a finite element simulation program was set up for modeling the printing layer process of the overhang design, which demonstrated stress concentration at the top point of the overhang neck. To improve the overhang stability and mitigate its deformation, an innovative design, named contactless support, was incorporated into the overhang. Studies of experiments and modeling showed the effectiveness enhancement of the contactless support design as the gap height decreased.

#### 3:20 PM

### (ICACC-S1-024-2025) Rapid joining of silicon carbide through Current Activated Reactive Ultrafast Joining (CARUJ)

S. Shivakumar\*<sup>1</sup>; B. Barua<sup>2</sup>; M. C. Messner<sup>2</sup>; P. S. Chaugule<sup>2</sup>; J. Luo<sup>1</sup>; D. Singh<sup>2</sup>

- 1. University of California San Diego, USA
- 2. Argonne National Lab, USA

We propose and demonstrate a novel approach for rapid fabrication of ceramic-ceramic joint assemblies using sintered Silicon Carbide (SiC) as an initial example. Current Activated Reactive Ultrafast Joining (CARUJ) utilizes resistive heating of carbon-based materials to apply localized heat through or around the joint zone at rates of  $10^{\rm l}$  -  $10^{\rm 3}$  °C/min. A reactive interfacial precursor based on elemental silicon and carbon allows the fabrication of high strength SiC-SiC joints with a Si/SiC interface utilizing minimal pressure (1 - 2 MPa), at time scales which are an order of magnitude shorter (several minutes opposed to hours) than conventional approaches for similar systems. Optional additions of refractory metals such as Molybdenum can be utilized to introduce secondary inclusions such as MoSi<sub>2</sub> within the joint interface While CARUJ joined samples can exhibit joint strengths as high as 100 MPa in compressive shear, average strengths lie between 25 - 45 MPa. We find a careful consideration of volume changes during CARUJ is required to produce joints with minimal defects and good strengths. We further demonstrate joining tubular geometries using both reaction bonded and sintered silicon carbide via contact and non-contact heating of the joint interface. The localized and rapid heat application realizes a versatile material joining technique that could be extended to the field.

# S1- Repair, Joining, Integration and Testing of Ceramics

### Room: Coquina E

Session Chairs: Dong Liu, University of Oxford; Michael Halbig, NASA Glenn Research Center

#### 3:40 PM

### (ICACC-S1-025-2025) Robust Repair and Refurbishment (R3) Technologies for Ceramic Matrix Composites in Aerospace and Ground Based Applications (Invited)

M. C. Halbig\*<sup>1</sup>; M. Singh<sup>2</sup>; A. S. Almansour<sup>3</sup>; G. Costa<sup>1</sup>

- 1. NASA Glenn Research Center, USA
- 2. Ohio Aerospace Institute, USA
- 3. NASA Glenn Research Center, Mechanical Engineering, USA

Ceramic matrix composites (CMCs) offer high temperature capability, environmental durability, and damage tolerance. CMCs are becoming more widely considered and utilized in aerospace applications such as turbine engine components, scramjet engine combustor walls, thrusters and nozzles for launch and in-space propulsion, and heat exchangers and thermal protection systems for vehicle airframe and propulsion systems for launch and reentry vehicles. During operation, CMC components are prone to damage mechanisms which introduce component life limiting flaws such as erosion, foreign object damage, de-laminations, and cracking. The ability to repair in service and as-manufactured flaws is a mission critical need. Carbon fiber-reinforced silicon carbide (C/SiC) is a leading candidate CMC. However, the susceptibility of the carbon fibers to oxidation requires the use of protective seal coatings and matrices. Fundamental oxidation studies were conducted on C/SiC to determine the effects of temperature, environment, and stress. A flaw repair concept was developed, and its performance was assessed via testing by comparing undamaged, damaged and unrepaired, and damaged and repaired C/SiC coupons. This approach is also being applied for the repair of C/C and SiC/SiC. Also, the applicability for in-space repair will be discussed.

### 4:10 PM

## (ICACC-S1-026-2025) Ceramic to metal joining for high temperature oxygen separation applications

S. De La Pierre<sup>\*1</sup>; F. Da Prato<sup>1</sup>; P. Fedeli<sup>2</sup>; A. Cavaliere<sup>2</sup>; A. Cammi<sup>2</sup>; A. Benelli<sup>1</sup>; F. Smeacetto<sup>1</sup>; F. Drago<sup>2</sup>; M. Ferraris<sup>1</sup>

- 1. Politecnico di Torino, DISAT, Italy
- 2. Ricerca sul Sistema Energetico RSE SpA, Italy

The integration of Oxygen Transport Membranes (OTMs) in industrial processes can lead to energetic and economic advantages. Still, proof of concept membrane modules are highly necessary to demonstrate the feasibility of this technology. This study identifies

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innovative materials to be used to join ceramics to metals, with a specific focus on joining materials for the integration of OTMs in metallic modules for high temperature applications. In this work is presented the development and high temperature characterization carried out on glass-ceramic sealants selected to join ceramic membranes (LSCF) to the metallic part. First of all the glass ceramics have been produced and analyzed to evaluate their thermal properties as sealant materials for the application. Then glass-caramic pastes have been developed and tested, to be employed in a robocasting deposition technique. Furthermore the thermo-mechanical compatibility of the selected sealants, with the ceramic membrane and the metallic case, has been tested, after joining, with X-ray thermography analysis and SEM observation of the interfaces. The produced joints have been subjected to relevant condition ageing tests (800-950°C, 1 to 3 weeks) and microstructurally analyzed afterward. In the end, gas tightness tests of the joints, and scale-up to a final module configuration, have also been performed.

### 4:30 PM

## (ICACC-S1-027-2025) Developing and testing joints and surface modification techniques for CMCs for energy-intensive industries

V. Casalegno<sup>\*1</sup>; C. Malinverni<sup>1</sup>; M. Salvo<sup>2</sup>; G. Puchas<sup>3</sup>; S. Schafföner<sup>4</sup>; P. Bertrand<sup>5</sup>

- 1. Politecnico di Torino, DISAT, Italy
- 2. Politecnico di Torino, Italy
- 3. University of Bayreuth, Ceramic Materials Engineering, Germany
- University of Bayreuth, Chair of Ceramic Materials Engineering, Germany
- 5. UTBM, CNRS, Laboratory ICB, UMR 6303 CNRS, France

Ceramic Matrix Composites (CMCs) are advanced materials known for their exceptional thermo-mechanical properties, corrosion resistance, and low density, making them ideal for high-temperature applications. In the steel-making industry, CMCs offer enhanced performance and energy efficiency and they can replace metallic alloys in radiant tube furnaces. For the manufacturing of these CMC-based radiant tubes, it is necessary to develop a suitable joining technique. However, achieving robust and reliable brazed connections in CMCs remains a challenge due to their inherent characteristics, including low wettability and chemical inertness. The experimental activity presented in this work is focused on the study, development and characterization of surface modification techniques, new joining materials and processes for oxide-based ceramic matrix composites (Al<sub>2</sub>O<sub>3</sub>f /Al<sub>2</sub>O<sub>3</sub>-ZrO<sub>2</sub>) as radiant tube furnace components in the steel industry. New glass-ceramic systems and high-entropy brazing alloys have been tested as joining materials, considering high in-service joint T, no degradation during service life, compatibility with harsh environments, pressureless joining technologies. This abstract is part of the NODES project which has received funding from the MUR - M4C2 1.5 of PNRR funded by the European Union - NextGenerationEU (GA no. ECS0000036).

### 4:50 PM

## (ICACC-S1-028-2025) Glass-based sealants for joining $\alpha$ to $\beta''-Al_2O_3$ in a novel Na–Zn battery

M. Salvo<sup>1</sup>; F. D'Isanto<sup>\*1</sup>; A. Baggio<sup>1</sup>; D. Basso<sup>2</sup>; D. Gaia<sup>2</sup>; F. Smeacetto<sup>1</sup>

- 1. Politecnico di Torino, Department of Applied Science and Technology, Italy
- 2. FZSONICK S.A., Switzerland

The SOLSTICE project (European Union's Horizon 2020, grant agreement No. 963599, www.solstice-battery.eu) is developing a novel solid electrolyte Na-Zn cell, similar to the classical ZEBRA\* cell, with a working temperature of approximately 300 °C and using Na- $\beta$ "-alumina ceramic as the ion conductor. In this work, the process of producing a new sodium-zinc solid-electrolyte battery was studied by selecting and modifying a commercial silica-based, sodium-resistant glass. Furthermore, a new silica-free glass composition was designed and optimized to further reduce the sealing

temperature and consequently minimize the manufacturing costs associated with the new battery. The two glass-based sealant systems were extensively characterized through thermal, chemical, and morphological analyses. The sintering behavior of these systems and their wetting characteristics on alumina were evaluated. The microstructural analysis confirmed good thermo-mechanical compatibility between the glass-based sealants and the alumina components. The sealant deposition process was automated via robocasting, and the ink recipe was optimized for this technique. The optimized compositions were applied to join  $\alpha$ - and  $\beta$ -alumina components in the cells, resulting in a lower sealing process temperature compared to the state-of-the-art solution. The cells were then tested under operating conditions.

## <u>S2 Advanced Ceramic Coatings for</u> <u>Structural/Environmental & Functional</u> <u>Applications</u>

### **S2- CMAS-type recession and mitigation strategies II** Room: Coquina C

Session Chair: Kuiying Chen, National Research Council Canada

### 1:30 PM

# (ICACC-S2-018-2025) The effect of soda additions on the degradation of gadolinium zirconate by CMFAS (Invited)

C. S. Holgate\*1; N. Basilyan1; C. G. Levi1

1. University of California, Santa Barbara, Materials, USA

The degradation of thermal barrier coatings (TBCs) by molten silicates (CMFAS) represents a significant challenge toward improving engine efficiency and decreasing their emissions. The key issue relates to the penetration of the TBC by CMFAS, which induces premature failure through thermomechanically-induced stresses. This penetration can be arrested through partial TBC dissolution and reaction with the CMFAS; however, the success of this mechanism utimately depends on the balance between the kinetics of penetration vs. reaction. In principal, this balance could be shifted by the presence of soda (NaO<sub>0.5</sub>), which should worsen CMFAS penetration by lowering the solidus and melt viscosity without being incorporated substantially into typical reactive phases (e.g., apatite). Despite this, few works have studied sytematically the effect of soda additions on TBC-CMFAS interactions. Herein, we report a combined computational and experimental investigation of Gd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> and two CMFAS melts with 0, 5, and 10 mol% NaO<sub>0.5</sub> incorporated. Thermo-Calc calculations elucidate the expected role of soda on liquid and apatite stability. Experiments on Gd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> pellets reveal that, counterintuitively, soda additions reduce pellet consumption and penetration, likely due to enhancing the kinetics of reactive crystallization.

### 2:00 PM

# (ICACC-S2-019-2025) A Core-Shell Thermal Barrier Coating with Strong Resistance to Molten Silicate Attack and Fracture

Z. Li\*1; G. Brewster2; L. Isern3; C. Chalk3; J. Nicholls3; P. Xiao1; Y. Chen1

- 1. The University of Manchester, Department of materials, United Kingdom
- 2. Rolls-Royce Plc Marine, United Kingdom
- 3. Cranfield University Surface Engineering and Precision Institute, United Kingdom

Calcia-magnesia-alumina-silicate (CMAS) attacks greatly reduce thermal barrier coatings (TBCs) lifecycles. While some current alternative TBC materials such as gadolinium zirconate (GZO) show excellent CMAS resistance, its low fracture resistance sacrifices TBC durability. To address this issue, we present a new TBC design featured a core-shell microstructure, where each building block of the TBC consists of tough yttria-stabilized zirconia (YSZ) core surrounded by a CMAS-resistant shell. To demonstrate this design, we chose alumina, an established CMAS-resistant ceramic, as the shell material. The core-shell TBC was successfully fabricated by first synthesizing "YSZ core-alumina shell" powder using the sol-gel method, and then thermally spraying the powder to deposit the core-shell coating. However, thermal spray leads to some melting and mixing of alumina and YSZ, forming alumina-alloyed zirconia, with alumina concentration increasing from the core to the shell. The alumina-rich shell promotes the self-crystallisation of CMAS at infiltration front, resulting in CMAS penetration depth in the coreshell TBC an order of magnitude lower than that in the industrial benchmark YSZ TBC. Meanwhile, the YSZ-based core ensures high fracture resistance due to the ferroelastic toughening mechanism. This innovative microstructure design achieves both robust CMAS and fracture resistance.

#### 2:20 PM

# (ICACC-S2-020-2025) Chemical and mechanical properties of modified $Yb_2Si_2O_7$ environmental barrier coatings corroded by molten CMAS

- G. Costa\*1; M. J. Presby2; A. S. Almansour3; R. I. Webster1; K. Lee1
- 1. NASA Glenn Research Center, USA
- 2. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA
- 3. NASA Glenn Research Center, Mechanical Engineering, USA

Corrosion of coatings based on Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> (YbDS) by molten silicate debris composed of CaO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (CMAS) is a longstanding environmental degradation mode of Environmental barrier coatings (EBCs). The corrosion of the coatings initiates when silicate debris particles based on CMAS composition enter with the intake air of gas turbines, then stick, melt, and react with ceramic coatings at high temperatures, resulting in premature failure In this study, the chemical and mechanical properties of plasma-spray-modified Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> environmental barrier coatings were investigated after corrosion by a low CaO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (CMAS) melt surface concentration at 1,315 °C for 1 h. X-ray diffraction, simultaneous thermal analysis, electron probe microanalysis, electron microscopy, and nanoindentation testing were used to probe coating samples. Garnet was favored to form over apatite in coatings with alumina content higher than 1 to 2 mol%. Garnet formation arrested corrosion through removal of the melt components. The corroded and heat-treated coatings exhibited a higher overall percentage of enhancement to the Young's modulus and hardness results when compared to as-deposited coating samples.

#### 2:40 PM

### (ICACC-S2-021-2025) Progressive Development of Deposits of CMAS Arriving as Individual Minerals

- E. H. Jordan\*<sup>1</sup>; H. D. Diaz<sup>1</sup>; S. P. Jordan<sup>2</sup>; B. Jun<sup>3</sup>
- 1. University of Connecticut, Mechanical Engineering, USA
- 2. Google, Quantum, USA
- 3. University of Connecticut, Materials Science, USA

In actual turbines and in the UConn gradient rig CMAS is delivered as individual particles with multiple different compositions and melting points. In this type of deposition, the initial deposits are discontinuous set of individual splats. Due to random arrival locations full coverage requires much more splat area that the sample area to be covered. Monte Carlo verified analytical formulae for coverage fraction is presented. A second formulae is presented and verified where it is assumed that un-melted particles only stick if they land on melted one. For the specific minerals in test CMAS AFRL-03 the melting points of all combinations of minerals are determined and it is clear that many combinations can melt when the constituent minerals do not. Some melt combinations that melt do not contain all the elements of CMAS but might be damaging. This raises the question if TBC enemy #1 CMAS is the only enemy? A few example turbine deposites that are not CMAS will be noted.

#### **S2- CMAS-type recession and mitigation strategies III** Room: Coquina C

Session Chair: Seongwon Kim, Korea Institute of Ceramic Engineering and Technology (KICET)

#### 3:20 PM

## (ICACC-S2-022-2025) Thermochemistry of Yttrium, Ytterbium, and Gadolinium CMAS Glasses

R. Bogle<sup>2</sup>; B. Aberra<sup>3</sup>; R. I. Webster<sup>1</sup>; N. P. Bansal<sup>1</sup>; M. J. Presby<sup>4</sup>; G. Costa<sup>\*1</sup>

- 1. NASA Glenn Research Center, USA
- 2. Purdue University, USA
- 3. Arizona State University, USA
- 4. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA

Rare-earth CaO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (RE-CMAS) glasses are considered one the major molten silicate-induced corrosion products of ceramic coatings applied on hot-section components of military and commercial gas-turbine engines. Evaluation of the thermochemical properties of rare-earth CMAS glasses provide important insights for understanding their thermochemical stability in the phase equilibria with ceramic coatings. In this work, high-temperature oxide melt drop solution calorimetry in molten 2PbO-B<sub>2</sub>O<sub>3</sub> solvent at 800 °C was used to measure the enthalpies of formation and reaction of RE-CMAS (RE = Y, Yb, and Gd) glasses. In addition, glass transition temperatures and enthalpies of fusion of the RE-CMAS samples were measured by differential scanning calorimetry. Spheroid samples were synthesized by laser-beam heating and melt quenching in a High Temperature Conical Nozzle Levitation (HT-CNL) instrument. All synthesized samples were characterized by X-ray diffraction, vibrational spectroscopy, and elemental composition analysis. Trends in the enthalpies of reaction, formation, and fusion as well as glass transition temperatures are discussed in terms of their chemical and compositional parameters as well as the implications for thermal and environmental barrier coatings with CMAS glasses.

#### 3:40 PM

#### (ICACC-S2-023-2025) Mechanistic Insights in the Degradation of Thermal/Environmental Barrier Coatings by Mixtures of Calcia-Magnesia-Aluminosilicate Glass & Salt/Sulfates

C. J. Louzon<sup>\*1</sup>; N. P. Padture<sup>1</sup>

1. Brown University, School of Engineering, USA

Worldwide increases in pollution have led to high concentrations of sulfate/salt particulates around major cities. Gas-turbine engines on airplanes can ingest environmental particulates, which form calcia-magnesia-aluminosilicate (CMAS) deposits in the engine hot-section. Thermal and environmental barrier coatings (TBCs and EBCs) are used throughout the hot-section to defend against degradation by such deposits. Substantial research has investigated the degradation of TBCs/EBCs by single-particulate deposits, but few studies have focused on complex, mixed deposits. To that end, a systematic study was conducted to understand the synergistic mechanisms active in the degradation of TBC/EBC ceramics by mixed CMAS-sulfate/salt deposits. Extensive characterization indicates significant variations in degradation behavior correlated with deposit composition. The Calculation of Phase Diagrams (CalPhaD) approach was used to model relevant equilibrium conditions corresponding to these reactions. Recent experimental results will be discussed in conjunction with these models. Insights from this work can guide the development of next-generation protective ceramic coatings to resist attack from mixed-particulate deposits.

### Abstracts

#### 4:00 PM

#### (ICACC-S2-024-2025) Influence of Cation Size on Calcium-Magnesium-Aluminosilicate Interactions with Binary Rare Earth Disilicate Coatings

L. A. Doumaux\*1; E. Opila2; R. Golden3

- 1. University of Virginia, Materials Science and Engineering, USA
- 2. University of Virginia, USA
- 3. Rolls-Royce Corp, USA

Rare-earth disilicate environmental barrier coatings are the current industry standard for application on SiC-based ceramic matrix composite hot section turbine engine components. Rare-earth disilicate coatings are desirable due to their increased stability with water vapor, thermal stability, and compatible elastic moduli and coefficients of thermal expansion with the SiC substrate. Siliceous debris, such as sand and ash, can be ingested into engines and deposit as molten calcium-magnesium-aluminosilicate (CMAS) glass on these hot section components, which can lead to premature coating failure. This study focuses on the influence of average rare earth cation size on CMAS resistance for binary rare-earth disilicate coatings. Binary rare-earth disilicates were exposed to a CMAS loading of 3 mg/cm<sup>2</sup> for 48h at 1316°C in a stagnant air box furnace. These reactions were then characterized via SEM, EDS, and XRD. These observations are critical for the optimization of CMAS resistant rare-earth disilicate environmental barrier coatings.

#### 4:20 PM

# (ICACC-S2-026-2025) Spherical CMAS-type particles for controlled, sequential exposure of thermal/environmental barrier coatings

P. Mechnich\*1; G. Alkan1

1. Deutsches Zentrum fur Luft- und Raumfahrt DLR, Germany

The interaction of thermal/environmental barrier coatings to CMAS-type deposited has been reported in many studies in the past years. Typical corrosion experiments have been performed by placing fixed amounts of CMAS powders and single heating runs. Alternative experiments were reported where liquid CMAS precursors were fed into flames of burner rigs in order to mimic a low concentration, but continuous exposure. In the present work, small spherical CMAS-type particles were processed by a dripping process and subsequent sintering. Due to the low weight scattering of CMAS spheres, a highly reproducible and scalable dosage of CMAS on coating surfaces is possible. Moreover, the approach is well suitable to simulate multiple exposition scenarios. Various CMAS stoichiometries were tested with standard coating variants such as YSZ, GZO, YAG, and Y2O3.

### <u>S3 22th Intl Symp on Solid Oxide Cells</u> <u>Materials Science & Technology</u>

#### S3- Metal supported cells

Room: Ballroom 4 Session Chair: Prabhakar Singh, University of Connecticut

#### 1:30 PM

### (ICACC-S3-014-2025) Metal-supported solid oxide electrolyzers for high temperature electrolysis (Invited)

B. Hu\*1; Z. Zhu1; F. Shen1; G. Lau1; M. Tucker1

1. Lawrence Berkeley National Laboratory, Energy Storage and Distributed Resources, USA

Metal-supported solid oxide electrolyzers (MS-SOEs) have demonstrated highly efficient conversion of steam to hydrogen or carbon dioxide/methane to syngas via electrolysis using electricity with many advantages of rapid start-up, dynamic operation, mechanical ruggedness, and low-cost materials. The symmetric MS-SOC architecture developed at Berkeley Lab, utilizes infiltrated catalysts deposited inside the pores of the zirconia electrode backbone and stainless-steel MS. Protective coatings on the metal support provide an effective mitigation approach of Cr evaporation. Compared to cells without protective coatings on MS, cells with protective coatings have shown significant improved cell stability during 1kh steam electrolysis. Catalyst optimization has greatly improved cell performance and stability. The catalyst porosity and layer thickness, which is controlled by precursor concentrations and number of infiltration cycles greatly affects mass transport and catalyst loading. Pure phase catalysts were obtained by selection of proper firing temperature using high-temperature (HT) X-ray diffraction, resulting in high performance and durability. Nano-size catalysts are prone to particle coarsening during HT electrolysis. A combined approach with physical and chemical methods has shown effective mitigation of particle coarsening. Degradation mechanisms will be discussed with posttest analysis results.

#### 2:00 PM

### (ICACC-S3-015-2025) Durable and robust steam electrolysis in Metal Supported Cells

J. Zamudio Garcia\*1; B. Sudireddy1; P. Hendriksen1; A. Hagen1

1. Technical University of Denmark, DTU Energy, Denmark

Solid oxide electrolyzer technology has a high potential to play a critical role in energy conversion devices for large-scale power-to-X applications. Recently, Metal-supported solid oxide cells (MS-SOC) have attracted great attention due to their cost-effectiveness and enhanced mechanical robustness in comparison to the traditional fuel electrode-supported configuration, leading to an expected longer lifetime under dynamic operating conditions. The present study investigates the long-term durability of MS-SOCs in electrolysis mode, operating under galvanostatic conditions (-0.5 A cm<sup>-2</sup>) for 7000 h at 650 and 700 C, showing degradation rates below 2%/kh. In order to study the performance under different operation conditions, testing parameters were changed stepwise progressively, aiming at higher electrolysis efficiency. Specifically, the H<sub>2</sub>O/H<sub>2</sub> ratio was increased from 50/50 to 90/10 %, the current density from -0.5 to -1.1 A cm<sup>-2</sup> and the gas utilization from 27 to 90 %. Stable cell voltage over time were observed in each segment lasting 500 h, even under the harshest conditions. The EIS analysis conducted under load unveiled that the principal increase in total resistance was attributed to polarization contributions, while only a minimal increase in ohmic resistance was observed. Cross-sectional SEM characterization was performed to evaluate the impact of the longterm operation in the microstructure of the cell.

#### 2:20 PM

#### (ICACC-S3-016-2025) Large-Area Metal Supported BZCY Proton Conducting Electrolysis Cell

Z. Zhuang\*1; L. Mastropasqua1

1. University of Wisconsin-Madison, Mechanical Engineering, USA

In the low-temperature electrochemical production of hydrogen, the hydrogen evolution reaction faces a significant challenge due to its high overpotential, necessitating the use of electrocatalyst materials. Photon-conducting solid oxide electrolysis offers a promising alternative, capable of converting high-temperature vapor directly into dry hydrogen without relying on noble metal catalysts. A proposed solution involves using a chemically stable perovskite material, specifically BaZrxCeyY1-x-yO3 (BZCY), as the solid electrolyte. To enhance the mechanical strength of the cell and withstand the pressure differentials required for hydrogen separation and compression, a 20 µm dense membrane and a 50 µm porous composite cathode are coupled with a robust porous metal support. The hot laminated thin layers of the electrode and electrolyte are applied to this support using a tape casting technique to achieve large area cells of at least 5×5 cm2. The pure BZCY powder is successfully synthesized using a sol-gel method, and a defect-free thin half-cell is fabricated via

successive hot lamination, and atmosphere-controlled sintering at 1475 °C. The metal support is bonded to the half-cell post-sintering using a cathode slurry and calcined at 900 °C. A 5  $\mu$ m uniform layer of nickel is electrochemically plated onto the stainless-steel support to prevent dissolution of chromium and silicon during operation.

#### 2:40 PM

#### (ICACC-S3-017-2025) Evaluation of Electrochemical Properties on Controlled Microstructure by Infiltration Method for Solid Oxide Fuel Cell Cathode

R. A. Budiman\*1; T. Namigawara1; K. Yashiro2; T. Kawada1

- 1. Tohoku Daigaku, Graduate School of Environmental Studies, Japan
- 2. Shimane Daigaku, Faculty of Materials for Energy, Japan

Reducing solid oxide fuel cell (SOFC) operating temperature without sacrificing performance remains a critical challenge, particularly in improving SOFC cathode performance. Various approaches have been proposed to enhance cathode performance, one of them is by controlling the microstructure. The use of nano-sized particles in the cathode has been shown to improve performance by increasing the surface area. In this study, the microstructure of the SOFC cathode by fabricating a porous Ce<sub>0.9</sub>Gd<sub>0.1</sub>O<sub>1.95</sub> (GDC) electrolyte layer on top of a dense GDC electrolyte, followed by the infiltration of  $La_{0.6}Sr_{0.4}CoO_{3-\delta}$  nanoparticles into the porous layer were prepared. Despite a significant enhancement in electrochemical performance, compositional analysis revealed the presence of impurity phases in the infiltration electrodes, indicating the need for optimization in the fabrication process. Additionally, while performance improvements were observed, the underlying mechanisms of the enhancement were not well understood. Here, we employed the transmission line model to simulate electrode reactions and identify the key factors responsible for the improved performance of the infiltration electrodes. Thus, both the optimization of the fabrication process and the factors governing performance enhancement in SOFC cathodes are discussed.

#### **S3- Air Electrode**

Room: Ballroom 4 Session Chair: Jakub Kupecki, Institute of Power Engineering

#### 3:20 PM

#### (ICACC-S3-018-2025) Microstructural Engineering of Innovative Nanostructured Oxygen Electrodes for Solid Oxide Cells (Invited)

E. Djurado\*1; O. Celikbilek2; N. Khamidy1; R. Sharma1

- 1. Universite Grenoble Alpes Phelma, LEPMI, France
- 2. Universite Grenoble Alpes, CEA LITEN, France

This talk aims to design novel optimized oxygen electrodes with improved mixed ionic-electronic properties to be used as more efficient oxygen electrodes in SOCs operating at ≈700°C. Indeed, it is of high importance to control the electrode microstructure and composition to obtain large surface areas. These properties are essential to increase the number of active sites for the ORR/OER and to enhance the ionic transfer at the electrode/electrolyte interface. Recent advances in the design of the state-of-the-art  $\rm La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta},$  $La_{2,x}Pr_{x}NiO_{4+\delta}$ , with  $0 \le x \le 2$ , and  $Pr_{6}O_{11}$  oxygen electrodes are reported with grain size and porosity at the nanometer length scales. These active functional layers are fabricated using electrostatic spray deposition, a unique bottom-up method capable of depositing films with porous morphologies by a nano-texturing approach. The latest electrochemical performance results of these innovative oxygen electrodes will be shown investigating the role of the nanostructure and the electrode/electrolyte interface. The correlation between microstructure, composition, grain size, interfaces, and electrochemical properties is discussed in detail. To conclude, the suitability of these mixed ionic and electronic conductors (MIEC) with innovative and controlled microstructure as durable air electrodes for SOECs has been proven to be promising.

#### 3:50 PM

#### (ICACC-S3-019-2025) Enhancing Low-Temperature SOFC Performance and Durability via Surface Modification and Scaling High Power Cells (Invited)

E. D. Wachsman\*1

1. University of Maryland, USA

Low temperature operation ( $\leq$ 650 °C) enables high surface area nano-catalysts with enhanced activity and high durability. A number of nano-catalysts were evaluated with PrO<sub>x</sub> being the best. The activity was in fact so high that SOFCs fabricated with a GDC scaffold and impregnated with PrO<sub>x</sub>, without a separate "cathode" phase, obtained exceptionally high-power densities at low temperature. This high-power density is demonstrated not only in button cells, but due to readily scalable processing in full format commercial scale cells.

#### 4:20 PM

#### (ICACC-S3-020-2025) Development of Heterostructured Cr-Resistant Oxygen Electrodes for Solid Oxide Electrolysis Cells (SOECs)

Y. Zhong<sup>\*1</sup>; G. Liu<sup>1</sup>; A. Kalu<sup>3</sup>; C. Klemstine<sup>2</sup>; S. Yang<sup>1</sup>; W. Li<sup>3</sup>; E. M. Sabolsky<sup>2</sup>; X. Liu<sup>2</sup>

- 1. Worcester Polytechnic Institute, Mechanical and Materials Engineering, USA
- 2. West Virginia University, Mechanical & Aerospace Engineering, USA
- 3. West Virginia University, Chemical and Biomedical Engineering, USA

This project aims to design, test, and validate oxygen electrode materials for Solid Oxide Electrolysis Cells (SOECs) that maintain high performance and low degradation rates in the presence of chromium (Cr)-containing gas impurities. Utilizing an innovative approach combining Integrated Computational Materials Engineering (ICME) and lab-scale testing, researchers from Worcester Polytechnic Institute and West Virginia University are developing LCO-based perovskites to create a heterostructured oxygen electrode with an LNO backbone. The primary objectives include comprehensive simulation of phase stabilities and point defect chemistry, experimental validation, and electrochemical testing of button cells. This research addresses critical challenges in SOEC technology, focusing on enhancing current density and mitigating long-term degradation, particularly in the presence of Cr-containing impurities. The findings will contribute to the development of more efficient and durable SOECs, potentially revolutionizing clean hydrogen production and energy storage technologies.

#### 4:40 PM

### (ICACC-S3-021-2025) Structure and Electrochemical Behavior of Praseodymium Oxide Thin Film Oxygen Electrode

B. Lemieszek<sup>1</sup>; S. Molin<sup>\*1</sup>

1. Department of Functional Materials Engineering, Faculty of Electronics, Telecommunications and Informatics, Poland

One of the primary challenges in SOC development is creating an efficient oxygen electrode, especially as the industry trends towards lower operating temperatures of 600°C or even 500°C. Praseodymium oxide has emerged as a promising alternative to current state-of-the-art materials like LSC or LSCF for SOC cathodes. Despite its high oxygen affinity and low electrode conductivity, praseodymium oxide's potential as an oxygen electrode material remains largely unexplored. This study investigates praseodymium oxide as a high-performance oxygen electrode for intermediatetemperature SOCs. The research aims to better understand this complex compound's properties and transformations across various temperature ranges, positioning it as a leading cobalt-free, nextgeneration SOC material. The experimental process involved applying the oxygen electrode to a CGO barrier layer using spincoating. Structural parameters were analyzed using XRD, HT-XRD, and HT-Raman spectroscopy from 400°C to 1000°C. Conductivity

was measured using the Van der Pauw method, while electrochemical properties were assessed through electrochemical impedance spectroscopy on symmetrical samples. Acknowledgements This research has been supported by National Science Centre (NCN) DAINA 2 project number UMO-2020/38/L/ST8/00513: "Porous metal supported micro-scale solid oxide fuel cells: fundamentals, fabrication and testing".

#### 5:00 PM

# (ICACC-S3-022-2025) Study of the Reversible Solid Oxide Fuel Cell's performance with $PrNi_{0.5}Co_{0.5}O_{3\cdot\delta}$ Oxygen Electrode and 10ScCeSZ Electrolyte

S. A\*1; S. S1; A. St1

1. CSIR-National Aerospace Laboratories, Bengaluru, Surface Engineering Division, India

Future stationary and mobile applications could benefit significantly from reversible solid oxide cells' energy conversion and storage capabilities (RSOCs). When using LSM as an air electrode, there was some delamination in the air electrode mainly due to internal precipitation due to molecular oxygen, over-sintering of electrode concerning electrolyte, disintegration into nanoparticles, etc., which could have been avoided with the help of another promising oxygen electrode with a higher electronic conductivity. From the experiment, the  $\text{PrNi}_{0.5}\text{Co}_{0.5}\text{O}_{3\cdot\delta}$  perovskite oxygen electrode has an electronic conductivity of 300 Scm<sup>-1</sup> at 750°C. It also work as a better triple conducting oxygen electrode with proton conducting electrolytes, but the electrochemical performance in the RSOFC mode was comparatively poor due to water and CO<sub>2</sub> absorption on electrolyte surface. The cell delivered a power density of 76 mWcm<sup>-2</sup> at 800°C while using 8 mol% Yttria stabilized zirconia (8YSZ) as electrolyte. However, in this work, the cell performance was studied using 10 mol% Scandia stabilized zirconia (10ScCeSZ) as an electrolyte to have more ionic conductivity than 8YSZ.

#### 5:20 PM

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### (ICACC-S3-023-2025) Cu-doped La<sub>2</sub>NiO<sub>4</sub> oxides as Oxygen Electrodes for Solid Oxide Electrolysis Cells

- S. B. Karki<sup>+1</sup>; L. M. Seymour<sup>2</sup>; L. Le<sup>2</sup>; R. Springer<sup>2</sup>; T. Liu<sup>2</sup>; C. A. Coyle<sup>2</sup>; O. A. Marina<sup>2</sup>
- 1. Pacific Northwest National Laboratory, Energy and Environment Division, USA
- 2. Pacific Northwest National Lab, USA

Copper doped La<sub>2</sub>NiO<sub>4</sub> electrodes for oxygen evolution reaction (OER) in solid oxide electrolysis cells (SOEC) were fabricated and tested using Ni-YSZ electrode-supported cells. Strontium free oxygen electrodes are of high interest because it could eliminate the strontium segregation and reactivity issues observed in the stateof-the-art LSC and LSCF oxygen electrodes. When Sr segregates to the LSC or LSCF surface, it suppresses the OER activity and readily reacts with the volatile impurities, such as sulfur from air and Cr from the metallic interconnect.  $La_2Ni_{1-x}Cu_xO_4$  (x=0.1-0.2) were synthesized using glycine nitrate combustion method. The electrochemical performance of the La2Ni1-xCuxO4 electrodes was studied using small and large active area (1.5-13 cm<sup>2</sup>) cells and compared to that of cells with LSC and LSCF-GDC electrodes. Short- and longterm tests were conducted at 650, 750, and 800°C with the Ni-YSZ hydrogen electrode exposed to 50-90% steam in hydrogen. Scanning electron microscopy with electron diffraction spectroscopy was used to analyze the electrode microstructure before and after testing. Compared to the Sr-containing electrodes, the La2Ni0.8Cu0.2O4 demonstrated lower degradation rate at 1.3V resulting in over 1 Acm<sup>-2</sup> at 750°C for at least 1000 hours of testing. La<sub>2</sub>Ni<sub>0.8</sub>Cu<sub>0.2</sub>O<sub>4</sub> appeared to be most active as well as most stable in both button and large size cells.

### S4 Advanced Materials for Thermoelectric and Thermionic Energy Conversion

#### **S4-** Theoretical and experimental approaches to thermal and electrical transport mechanisms in thermoelectric/thermionic materials Room: Coquina D

Session Chairs: Yinan Liu, Colorado School of Mines; Shuo Chen, University of Houston

#### 1:30 PM

# (ICACC-S4-008-2025) Electron Transport in Hierarchical Ceramic Composites (Invited)

J. Bahk\*1; M. Jackson1

1. University of Cincinnati, Mechanical and Materials Engineering, USA

Recent advances in additive manufacturing have enabled the use of binder solutions to selectively bond ceramic powders and create strong 3D ceramic parts with no or low-temperature heat treatment. During this process, conducting micro/nano-scale materials can be dispersed in the binder solution, and be jetted into the space between powder particles to create hybrid hierarchical ceramic composites while preserving the powder microstructure. These secondary filler materials can form percolation networks around the ceramic particles to create electrically conducting pathways in the composite. In this work, we combine experimental and theoretical study to investigate the electron and thermoelectric transport through the networks of nanomaterials embedded in binder-jetted hybrid ceramic composites. Nanocarbon materials such as carbon nanotubes and graphene nanoplatelets are used as the conducting secondary materials embedded in silica powders to create macroscale conducting ceramic materials. We investigate the variation of transport properties such as electrical conductivity, thermal conductivity, and thermopower of the composites with varying filler concentration in several different binder solutions to study the microstructure-property relationship. Electron tunneling at the junctions between the nanomaterials is considered to explain the electron transport properties in the composites.

#### 2:00 PM

#### (ICACC-S4-009-2025) In-Plane Thermal Conductivity Measurements of 2D Layered Materials Using Heat Diffusion Imaging (Invited)

M. Maliat\*1; F. Tonni1; M. Zebarjadi1

1. University of Virginia School of Engineering & Applied Science, Electrical & Computer Engineering, USA

The precise measurement of in-plane thermal exploritivity of 2D flakes is pivotal for the integration of 2D materials in future microelectronics, optical devices, and thermal and there y conversion and storage systems. Heat diffusion imagins (HDI), a technique that integrates the heat spreader method with thermoreflectance imaging, presents an accurate and relative methodology for measuring thermal conductivity in supported thin films. This approach addresses the limitation exconventional techniques such as the  $3\omega$  method and bridg tec inque eliminating the need for multiple thermometers fabricative or film suspension. HDI offers high spatial (300nm) and temperal (~0.1K) resolution for direct temperature mapping and the side of the flake is Joule-heated, and the resulting lateral heat dissipation is captured through variations in the surface reflectivity of the flake, allowing the extraction of in-plane thermal conductivity. Studies of silicon thin films were used to validate the reliability of the HDI measurements. Here, we present HDI measurements performed on several 2D layered materials with a focus on InSe, CoTa<sub>3</sub>S<sub>6</sub>, and VTa<sub>3</sub>S<sub>6</sub>, where thickness and temperature-dependent thermal conductivities have been studied in 40 K to 800 K, making HDI a versatile tool for thermal measurements.

#### 2:30 PM (ICACC-S4-010-2025) Applying the Wiedemann-Franz Law in Thermoelectric Ceramics

S. Akhbarifar\*1

1. The Catholic University of America, Physics, USA

The Wiedemann-Franz law (WFL) is a fundamental principle in solid-state physics that describes the relationship between electrical and thermal conductivities of metals. Limits of applicability have been encountered for ceramics at cryogenic temperatures and more recently at room temperature in  $\dot{VO}_2$ , a metal-like ceramic. In Pb- and Pb-Y-ruthenate defect structures the lattice thermal conductivity  $(k_1)$  became negative in some compounds. Significant deviations from the degenerate limit of Lorenz number (L) are known for non-degenerate semiconductors with Kane band structures. L can be  $1.5 \times 10^{-8}$  W $\Omega/K^2$  or lower due to acoustic phonon scattering. The literature shows that L can be calculated using measured Seebeck coefficients (S), if band structure and scattering mechanisms are not known. This would provide significantly improved estimates of k<sub>L</sub>. However, in our study, S measurements failed to provide meaningful k<sub>L</sub> values for Pb and Pb-Y-ruthenates. We will present a new approach to overcome the limitations of the WFL in these materials. By using the atomic positions and the unit cell composition, we calculate both electron and phonon band structure. With these band structures and using the Boltzmann Transport theory, the electrical contribution to the thermal conductivity and k<sub>1</sub> can be calculated independently. This approach allows for the design of novel Pb-ruthenate compounds with enhanced thermoelectric efficiency.

#### 2:50 PM

#### (ICACC-S4-011-2025) Thermoelectric Properties of ScN Thin Films Controlled by Ion Implantation

C. Poterie<sup>\*1</sup>; H. Bouteiller<sup>1</sup>; R. Burcea<sup>1</sup>; S. Dubois<sup>1</sup>; A. le Febvrier<sup>2</sup>; P. Eklund<sup>2</sup>; T. Cabioch<sup>1</sup>; J. Barbot<sup>1</sup>

- 1. PPRIME Institute, France
- 2. Uppsala Universitet, Department of Chemistry, Sweden

Scandium nitride (ScN) thin films are of high interest for thermoelectric applications due to their large power factor. When incorporated during deposition, oxygen substitute nitrogen in the lattice which creates a donor defect causing the films to be in a degenerate n-type state. However, its large thermal conductivity  $(\kappa \sim 12 \text{ W.m}^{-1}.\text{K}^{-1})$  is a drawback for industrial use and defects engineering and/or doping using ion implantation has recently been considered to improve its thermoelectric properties. We studied the implantation at high damage regime of oxygen ions into ScN thin films to control their electrical properties and experiments are underway to better assess the structural disorder induced. Two types of defects have been identified through the characterisation of resistivity, carrier concentration and Seebeck coefficient. The first type involves interstitials which modifies the conduction mechanism. The second type, more stable, is assumed to be of the  $(V_{sc}-yO)$  complex type, as DFT calculations have shown. Both types act as acceptors enhancing the Seebeck coefficient but increasing the resistivity. These results will be compared with defects induced by argon and helium implantation, where the thermal conductivity was reduced to 3 and 7 W.m<sup>-1</sup>.K<sup>-1</sup> respectively, leading to an increase of the zT. Hence, finding the best conditions using oxygen implantation will allow to further improve the zT.

# S4- Advanced Materials for thermoelectric and thermionic energy conversion II

Room: Coquina D

Session Chairs: Bin Xu, Tokyo Daigaku; Jan-Willem Bos, University of St Andrews

#### 3:30 PM

#### (ICACC-S4-012-2025) Advancing Thermoelectric Performance with Solution-Based Synthesis of Defect-Tuned Silver Selenide (Invited)

N. Jakhar\*'; T. Kleinhanns'; Y. Liu²; S. Xu¹; A. Lawal¹; F. Milillo¹; S. Horta¹; M. Ibáñez¹

- 1. Institute of Science and Technology Austria, Austria
- 2. Hefei University of Technology, China

Thermoelectric (TE) applications face challenges due to high costs of rare elements, complex synthesis methods, and low efficiencies. A promising solution is using abundant elements in solution-based synthesis, enabling control over properties like defect type and density, chemical composition, and particle morphology before sintering, offering multidimensional optimization potential. In this talk, we focus on silver selenide (Ag<sub>2</sub>Se) as an alternative to Bi<sub>2</sub>Te<sub>3</sub>-based alloys. However, replicating high TE performance near room temperature is challenging due to its mixed ionic-electronic conduction, which leads to variable compositions and defects at elevated synthesis temperatures, causing inconsistent transport properties. Here, we present solution-based methods that allow precise control over composition and defects, ensuring consistent transport properties. We also introduce a method for synthesizing TE powders at room temperature, providing opportunities to explore phase transitions during sintering. By optimizing sintering, we achieve a thermoelectric performance above the state of the art, with a stable figure of merit ( $zT_{ave} = 1.1$ ) from room temperature to 100°C. Finally, we demonstrate the use of these powders to 3D print thermoelectric legs for a 32-pair cooling device, achieving DT > 50 K below room temperature.

#### 4:00 PM

### (ICACC-S4-013-2025) High-Performance Thermoelectric Polymers with zT > 1

J. Ouyang\*1

1. National University of Singapore, Department of Materials Science & Engineering, Singapore

Thermoelectric materials can be used in thermoelectric generators to directly harvest waste heat into electricity and in Peltier coolers for localized cooling. Thus, they are significant for sustainable development because of the abundant waste heat on earth and energy saving by localized cooling. The traditional thermoelectric materials are inorganic materials like Bi<sub>2</sub>Te<sub>3</sub> and its derivatives. Although they can have high thermoelectric properties, they have problems of high cost, toxic/scarce element(s) and low mechanical flexibility. Organic thermoelectric materials emerged as the next-generation thermoelectric materials because of their merits including low cost, common elements, high mechanical flexibility and low intrinsic thermal conductivity. But their thermoelectric properties must be greatly improved for practical application. Here, I will present some of our research works on developing high-performance thermoelectric polymers. We invented several methods to significantly enhance the conductivity and/or the Seebeck coefficient thus the power factor of conducting polymers

### Abstracts

#### 4:20 PM

#### (ICACC-S4-014-2025) Novel conjugated polymers decorated with radical pending units for thermoelectric applications

E. Orgiu<sup>\*1</sup>

1. Universite du Quebec, Institut national de la recherche scientifique (INRS), Canada

With world's reserves of fossil fuels being depleted rapidly, researchers are working towards the quest for new and more environmentally friendly sources of energy. Further, it is estimated that >60% of the energy is lost in the form of waste heat, resulting in useless dissipation and environmental pollution. Hence, it appears clear that recycling waste heat is of utter importance, and for this reason, more attention is being paid to thermoelectric materials. I would like to give a few examples on how to use conjugated polymers to make organic thermoelectric generators. First, I will talk about the versatility of inkjet printing technology with a commercial PEDOT:PSS ink to evaluate the thermoelectric performances of films deposited on different substrates (polyimide foils, glass, and silicon oxide). In particular, a relatively high Seebeck coefficient of 10 mV K<sup>-1</sup> was achieved along the direction parallel to the printing direction on the silicon oxide substrate. Moreover, to investigate the thermoelectric performances of a fully inkjet-printed flexible thermoelectric device, we compared the role of e-beam evaporated vs. inkjet-printed electrodes. In addition, I will present a novel polymer with a joint polaronic and radical conductivity which brings to a higher conductivity which is pivoltal to achieving a high thermoelectric figure of merit.

#### 4:40 PM

#### (ICACC-S4-015-2025) Reproducing Cassini-era SiGe Using Vacuum Casting and Mechanical Alloying (Invited)

H. Wang\*1

1. Oak Ridge National Laboratory, USA

SiGe has been used to power NASA's radioisotope thermoelectric generators (RTG) since the 1970s. The last production of SiGe in the US was in the 1988 for four spacecrafts: Galileo (1989), Ulysses (1990), Cassini (1997) and New Horizon (2006). Because of its flight-proven history and performance at 1000°C hot-side temperature, SiGe has been selected by the NextGen program for missions beyond 2030s. After a brief review of SiGe, the effort to reproduce the heritage materials at ORNL will be discussed. Traditional vacuum induction melting, and chill casting has been used to produce 40-gram ingots of both n-type and p-type SiGe as well as doped Si. The ingots were pulverized by Shatterbox and hot-pressed at 1300°C. Transport properties were measured to calculate the figure of merit, zT, which was reproducible compared with the handbook values. Boron and phosphorus doped SiGe were also produced by mechanical alloying (MA) in a high-energy ball mill. The MA powders were hot-pressed under the same conditions as the heritage materials. Transport properties also showed similar zT. Microscopic analysis on SiGe produced via different routes showed distinct features in microstructure and compositions. Different processing methods present an opportunity to improve the transport properties and understand the long-term performance of SiGe.

#### 5:10 PM

#### (ICACC-S4-016-2025) Building Thermoelectric Modules for **Nuclear Battery Applications**

- H. Bouteiller\*1; T. Muth1; A. May1; D. Hoelzer1; H. Wang1
- 1. Oak Ridge National Laboratory, USA

Nuclear batteries are isotope-based devices that provide stable and long-term power supply for various applications such as underwater vehicules, airplanes, or satellites. Among these, Radioisotopes Thermoelectric Generators (RTGs) leverage the direct conversion of heat, produced by a decaying radioactive source, into electricity by thermoelectric (TE) materials. Such devices have been used in the past decades to power space exploration mission, including the Voyager spacecraft and the Curiosity and Perseverance Mars rovers for instance. To extend the number of potential applications, the development of reliable, low-cost and high efficiency thermoelectric devices is essential. In this presentation, the manufacturing of skutterudite-based thermoelectric devices will be presented, from the processing routes of TE material to the device design and performance optimization. Key challenges encountered in improving energy conversion efficiency will be addressed, with a focus on microstructural and transport properties characterizations. Special attention will be given to interfacial properties and their impact on overall efficiency.

### S6 Advanced Materials and Technologies for **Rechargeable Energy Storage**

#### S6- All-solid-state batteries III

Room: Coquina B

Session Chairs: Wan Si Tang, Underwriters Laboratories Inc; Mahalingam Balasubramanian, Oak Ridge National Lab

#### 1:30 PM

#### (ICACC-S6-015-2025) Development of High-Performance All-Solid-State Lithium-Sulfur Battery (Invited)

M. Jeong<sup>1</sup>; M. Kindle<sup>1</sup>; J. Wu<sup>1</sup>; D. Jin<sup>1</sup>; U. Kim<sup>1</sup>; H. Xu<sup>1</sup>; D. Lu<sup>\*1</sup>

1. Pacific Northwest National Laboratory, USA

All-solid-state lithium-sulfur batteries (ASSLSBs) hold great promise for delivering safe, high-energy density, and cost-effective battery technologies for vehicle and aviation electrification, as well as grid energy storage. Achieving high specific energy in ASSLSBs (e.g., >400 Wh kg<sup>-1</sup>) requires sulfur cathodes with high areal capacity (>6 mAh cm<sup>-2</sup>) to compensate for the relatively low working voltage of the elemental sulfur cathode. This requires high mass-loading sulfur cathodes by maximizing both the sulfur content in the entire electrode and the sulfur utilization rate to minimize parasitic weight. However, due to the non-flowable nature of the solid components, achieving maximum contact between the sulfur/solid electrolyte/ carbon triple phases presents a significant challenge. Our study explores sulfur host microstructures and their impact on the triplephase contact in ASSLSB systems. Specifically, we elucidate sulfur host selection principles, sulfur infiltration, and spatial distribution, and their impacts on sulfur utilization and cycling stability. Advanced characterization and computational tools are employed to elucidate the key parameters for high sulfur utilization in high sulfur loading cathodes. The detailed findings of this study will be presented and discussed at the meeting.

#### 2:00 PM

#### (ICACC-S6-016-2025) High Performance Solid-State Batteries with Solvent-Free Processing (Invited)

- Y. Lin\*1; J. Su1; V. Yamakov2; J. Kang1; D. Dornbusch3; R. P. Viggiano3
- 1. NASA Langley Research Center, Advanced Materials and Processing Branch, USA
- 2. Analytical Mechanics Associates, USA
- 3. NASA Glenn Research Center, Materials, Chemistry, and Physics Branch, USA

The non-flammable nature of solid-state batteries make them ideal candidates for applications that require ultimate safety and reliability, such as electric aviation. Significant progress has been made to address many related challenges with regard to improving energy, power, cyclability, scalability, and sustainability of the solidstate batteries for them to be more practically viable. Compared to conventional Li-ion batteries, solid-state batteries provide a unique opportunity for solvent-free processing because all battery components are solids. However, organic solvent-based electrode and

electrolyte fabrication methods are still being widely used in solidstate battery research because the resultant products usually exhibit low porosity and consistent performance. Solvent-free processing, on the other hand, would be much less costly and more environmentally friendly, despite challenges in battery performance. In this presentation, we discuss our explorations of the use of holey graphene, a unique carbon nanomaterial, that assists in the solvent-free processing of various components in high performance solid-state batteries. The dry compressibility of holey graphene, not available in any other carbon materials, is key for the successful solvent-free approach that may be conveniently scalable for practical use.

#### 2:30 PM

### (ICACC-S6-017-2025) Anode-free solid-state batteries based on 3D-printed metal-carbon composite interlayers (Invited)

S. Risal<sup>\*1</sup>; Z. Fan<sup>1</sup>

1. University of Houston, USA

Recent advances in battery technology have sparked the emergence of all-solid-state Li metal batteries (ASSLMBs) with high energy density lithium (Li) metal anodes, superior ionic conductive solidstate electrolytes (SEs), and composite cathodes. Importantly, the next-generation ASSLMBs present unparalleled opportunities for a growing number of high power and energy applications and are specifically garnering the interest of the electric vehicle (EV) community. Rapid deterioration of performance at the thermodynamically metastable interfaces between the Li anode and SE has, however, hindered the breakthroughs introduced by ASSLMBs. Studies suggest that the current performance issues could be addressed by the development of innovative metal-carbon-based mixed ionic-electronic conductive (MC-MIEC) interlayers with self-regulated Li diffusion. This work reports the introductions of non-noble metal involved metal-carbon composite interlayers into sheet-type solid-state cells (overall width < 100 µm). The interlayer enables alleviated mechanical strain and improved strip/plate homogeneity, thereby addressing the lithium metal dendrite growth between the Li metal anode and the solid electrolytes. The sheet-type cells with the interlayer achieve an average Coulombic efficiency of 99.5% over 100 cycles.

#### S6- Solid electrolytes for batteries I

Room: Coquina B

Session Chairs: Wan Si Tang, Underwriters Laboratories Inc;

#### 3:20 PM

### (ICACC-S6-018-2025) Developments of Air-Stable Sulfide Solid Electrolytes (Invited)

M. Otoyama\*1; K. Kuratani1; H. Kobayashi1

1. National Institute of Advanced Industrial Science and Technology, Japan

Sulfide all-solid-state batteries have attracted much attention because of high ionic conductivity and deformability of sulfide solid electrolytes (SEs). However, sulfide SEs have an issue of  $H_2S$  gas generation when they are exposed to air due to the low air-stability. To put sulfide all-solid-state batteries into practical use, air-stable sulfide SEs should be developed. The stability of sulfide SEs against moisture in air can be explained by hard and soft acids and bases theory. Based on the theory, sulfide SEs with softer acids such as Sn show higher air stability than those with harder acids such as P because the former can prevent the replacement of soft base S in sulfide SEs with hard base O in air. Therefore, Sn-based sulfide SEs such as Li<sub>4</sub>SnS<sub>4</sub> show higher air stability than P-based sulfide SEs such as Li<sub>3</sub>PS<sub>4</sub>. In this study, we developed xLi<sub>4</sub>SnS<sub>4</sub>-(1-x)Li<sub>3</sub>PS<sub>4</sub> glasses/glass-ceramics and investigated a relationship between their structure, ionic conductivity and air stability systematically.

#### 3:50 PM

# (ICACC-S6-019-2025) Mechano-electrochemical Phenomena in Ceramic Ion Conductors (Invited)

#### J. Sakamoto<sup>\*1</sup>

1. University of California Santa Barbara, Materials, USA

The recent emergence and discovery of new ceramic ion conductors (CIC)s with fast ionic conductivity creates the opportunity to push the frontiers of electrochemical energy conversion and storage. The ability to replace traditional liquid or polymer electrolytes with ceramics has the disruptive potential to improve safety and enable next generation technologies including solid-state batteries with metal anodes, impermeable membranes to prevent crossover in redox flow batteries for long-duration energy storage (LDES). Enabling the next generation of electrochemical conversion and storage, however, requires fundamental research to understand and control the emergent mechano-chemical environments that arise when CIC materials are interfaced with other dissimilar materials. The United States Department of Energy is supporting the collaborative and interdisciplinary project Mechano-chemical Understanding of Solid Ion Conductors (MUSIC). The overarching scientific mission of MUSIC is to reveal, understand, and model, and ultimately control the chemo-mechanical phenomena underlying the processing and electrochemical dynamics of CICs for clean energy systems. This presentation will consist of highlights from MUSIC to include topics such as stress corrosion cracking, Li/Na free manufacturing, and composite cathode analyzed using complementary experimentation and computation.

#### 4:20 PM

## (ICACC-S6-020-2025) Composite Electrolytes for High-Energy Lithium Batteries (Invited)

D. Bresser\*

1. Karlsruher Institut fur Technologie, Helmholtz Institute Ulm (HIU), Germany

Li-ion batteries are presently the technology of choice to power electric vehicles and portable electronic devices. This great success is also the result of the development of high-performance liquid organic electrolytes providing a high ionic conductivity and wide electrochemical stability. When targeting a further improved safety, however, solid-state electrolytes are anticipated to provide significant advantages owing to their commonly higher thermal stability and reduced flammability in combination with an inhibited leakage issue - especially when transitioning from classic graphite-based anodes to high-capacity alternatives such as silicon or lithium metal. Nonetheless, all solid electrolyte systems come with their own challenges, which are, though, frequently complementary. Thus, there is a tremendous interest in smartly combining different electrolyte classes to finally achieve a real breakthrough towards safer high-energy and high-performance lithium batteries. Herein, several different composite (frequently referred to as "hybrid") electrolyte systems will be presented, starting from the reasoning for the given design and selection of components, highlighting the potential and eventual benefits and remaining challenges, and finally discussing some very recent in-depth insights into the charge transfer across the different phase boundaries, which are essential for the meaningful design of such multiphase systems.

### Abstracts

### <u>S7 19th Intl Symp on Functional</u> <u>Nanomaterials & Thin Films for Sustainable</u> <u>Energy Harvesting</u>

### S7- Nanomaterials for energy conversion, storage and

catalysis- IV

Room: Flagler C Session Chair: Muhammet Toprak, KTH Royal Institute of Technology

#### 1:30 PM

(ICACC-S7-017-2025) Organoferrous Photosensitizers for DSSC Applications: A Promising Future? (Invited)

C. Cebrian Avila<sup>\*1</sup>; P. C. Gros<sup>2</sup>

1. Universite de Strasbourg, France

2. Universite de Lorraine, France

Precious metal complexes have long been used in research areas such as optoelectronics, solar energy conversion and photocatalysis due to their ideal photophysical and electrochemical properties. However, the scarcity of these metals has prevented large-scale commercial applications. Interestingly, during the last decade, photosensitizers based on abundant first-row transition metals have emerged as a result of judicious ligand design combined with original approaches. In particular for iron(II) complexes, strong ligand fields have proven essential to limit the ultrafast deactivation of their metal-to-ligand charge transfer (MLCT) states by low-lying metal-centered (MC) states. In our group, we have demonstrated that iron complexes comprising N-heterocyclic carbenes (NHC) and azine moieties can efficiently sensitize the TiO2 semiconductor in dye-sensitized solar cells (FeSSCs), resulting in photocurrent generation. In this contribution, we will present a rational approach to improve the power conversion efficiency in FeSSCs up to 2%. In addition, alternative complex designs to further enhance their electronic and photophysical properties will be discussed.

#### 2:00 PM

# (ICACC-S7-018-2025) Tailoring Microstructure of Polyvinyl Chloride Films via BaTiO\_3 Nanowires to Achieve Improved Electrical and Mechanical Performance

S. Dadashov\*1; B. Göl4; S. Kinden3; E. Suvaci2

- 1. Eskisehir Teknik Universitesi, Chemical Engineering, Turkey
- 2. Eskisehir Teknik Universitesi, Material Science and Engineering, Turkey
- 3. Eskisehir Teknik Universitesi, Electric Electronics Engineering, Turkey
- 4. Eskisehir Teknik Universitesi, Material Science, Turkey

This research investigates the fabrication of a Polvinyl Chloride (PVC)/BaTiO<sub>3</sub> nanowire based hybrid nanogenerator combining triboelectric and piezoelectric properties using an alternative fabrication approach for wearable microdevices and sensors. To achieve high piezoelectric effect even at low deformations, flexible BaTiO<sub>3</sub> nanowires were synthesised by hydrothermal synthesis method and incorporated into PVC matrix as piezoelectric filler. It also aims to comprehensively investigate how different PVC/BT compositions affect the porosity, pore structure and consequently the electrical performance. Furthermore, the critical porosity ratio of the PVC/BT composite structure will be determine to produce a nanogenerator with high electrical performance and sufficient mechanical strength. The findings of this research are expected to contribute significantly to the design and development of advanced nanogenerators, especially in areas such as wearable technology and sensor systems where flexible, high-performance energy solutions are increasingly in demand.

#### 2:20 PM

#### (ICACC-S7-019-2025) Enhanced Oxygen Evolution and Zinc-Air Battery Performance via Electronic Spin Modulation in Heterostructured Catalysts

L. Yang\*1; R. He1; A. Cabot1

1. Institut de Recerca en Energia de Catalunya, Spain

Modulation of the electronic spin configuration is an effective strategy, often overlooked, to boost activity and selectivity in a range of catalytic reactions, including the oxygen evolution reaction (OER). This electronic spin modulation is frequently accomplished using external magnetic fields, which makes it impractical for real applications. Herein, spin modulation is achieved by engineering Ni/MnFe<sub>2</sub>O<sub>4</sub> heterojunctions, whose surface is reconstructed into NiOOH/MnFeOOH during the OER. NiOOH/MnFeOOH shows a high spin state of Ni, which regulates the OH<sup>-</sup> and O<sup>2</sup> adsorption energy and enables spin alignment of oxygen intermediates. As a result, NiOOH/MnFeOOH electrocatalysts provide excellent OER performance with an overpotential of 261 mV at 10 mA cm<sup>-2</sup>, a high open circuit potential of 1.56 V, and exceptional stability for zinc-air batteries of more than 1000 cycles. This outstanding performance is rationalized using density functional theory calculations, which show that the optimal spin state of both Ni active sites and oxygen intermediates facilitates spin-selected charge transport, optimizes the reaction kinetics, and decreases the energy barrier to the OER. This study provides valuable insight into spin polarization modulation by heterojunctions enabling the design of next-generation OER catalysts with boosted performance.

#### 2:40 PM

## (ICACC-S7-020-2025) Promoting Polysulfide Redox Reactions through Electronic Spin Manipulation

J. Yu\*1

1. Institut de Recerca en Energia de Catalunya, Spain

The use of defect-engineered catalysts, with tunable surface electronic properties and chemistry, as a cathode additive in lithiumsulfur batteries (LSBs) is a promising strategy to accelerate the polysulfide reduction reaction and thus promote LSB performance. In contrast to earlier research that predominantly concentrated on how defects influence the electronic density of states, this study explores the impact of defects in modulating electronic spin. It is also demonstrated here how these changes in electronic spin can subsequently adjust the macroscopic adsorption properties and activity of the catalytic additive. We showcase this effect with the introduction of Co vacancies on the surface of ultra-thin CoSe nanosheets. As demonstrated both experimentally and through theorectical calculations, the presence of vacancies increases the number of unpaired electrons on the nanosheet surface, changes the electron spin state distribution, and induces their parallel alignment. This local electronic rearrangement enhances chemical adsorption and electron transfer, thereby reducing the activation energy of chemical reactions. As a result, more uniform nucleation and growth of Li<sub>2</sub>S and an accelerated liquid-solid conversion are obtained.

### **S7- Nanotoxicity, bio-imaging, drug-delivery and tissue engineering with tailored nano-bioconjugates** Room: Flagler C

Session Chair: Jose Serrano Claumarchirant, Kungliga Tekniska Hogskolan

#### 3:20 PM

#### (ICACC-S7-021-2025) Bioconjugated Nanoparticles for Precision Drug Delivery (Invited)

S. Ilyas<sup>2</sup>; T. Fischer<sup>1</sup>; S. Mathur<sup>\*1</sup>

- 1. Universitat zu Koln Mathematisch-Naturwissenschaftliche Fakultat, Institute of Inorganic and Materials Chemistry, Germany
- 2. Institute of Inorganic and Materials Chemistry, Chemistry, Germany

Chemical processing of functional ceramics and glasses has played a key role in converging disciplines, which is especially true for biomedical applications. For example, the development of biocompatible drug-carriers that can hold back the payloads and release the drugs or antibiotics at the specific diseased area is a materials processing challenge. The selective transport and retention of drugs in sufficiently high concentrations at the target site is inhibited by various physiological barriers, which reduces or even blocks the therapeutic efficiency of molecular drugs. Therefore, advanced drug-delivery systems designed to overcome biological barriers are needed to meet the specific traits of physiological and disease-related barriers. In this context, chemically functionalized SiO2 nanoparticles act as efficient drug-carriers to transport higher amounts of therapeutic payloads to diseased sites that also reduces the undesired off-site effects. Moreover, hollow nanocarriers can incorporate more than one drug enabling theranostic and theraregenerative approaches. Finally, silica nanoparticles can be modified with surface-bound target ligands to exploit the overexpression of receptors and promote cell specific attachment of the carriers for a localized high concentration of drug around disease sites. This talk will discuss the potential benefits of silica nanoparticles towards precision drug delivery.

#### 3:50 PM

#### (ICACC-S7-022-2025) Development of Inorganic Nanoparticles for Emerging X-Ray Fluorescence Bioimaging (Invited)

M. S. Toprak\*1; G. Saladino1; B. Brodin1; H. M. Hertz1

1. KTH Royal Institute of Technology, Dept. of Applied Physics, Sweden

Nanoparticles (NPs) have found use in many areas from hybrid materials, to sensors, antiviral/antibacterial coatings and various biomedical applications, including use as contrast agents. Each application area has its own set of NP requirements that has to be complied in order to assure their successful implementation. We have been developing different families of ceramic nanoparticles for a diverse set of biomedical applications, using bottom-up solution chemical techniques. Whenever needed the individual NPs were coated, or assembled into larger micron-scale architectures by the use coupling mechanisms using their surface functionality. In this respect, it is of utmost importance to have the right surface chemistry to minimize the number of process steps, in order to reach the desired material attributes. The developed NPs were tested in-vitro, which were then refined to use for in-vivo X-Ray fluorescence bioimaging (XRF) studies. In this talk, I will present about some of the recent activities and materials dedicatedly designed for XRF bioimaging facility unique in Sweden, and among the few pioneering labs in the world. The presentation will cover the developments, starting from the first-generation NPs to the core-shell particles, and various surface functionalization schemes. Some of the recent research achievements using the developed NPs for in-vitro and in-vivo studies will be presented.

#### 4:20 PM

### (ICACC-S7-023-2025) Magnetite@mesoporous silica core-shell nanostructures: an innovative and promising theranostic material

M. Garrido Blay<sup>\*1</sup>; B. Hamawandi<sup>2</sup>; G. Saladino<sup>2</sup>; M. Marcos<sup>3</sup>; J. Ros-Lis<sup>4</sup>; P. Amorós<sup>1</sup>; M. S. Toprak<sup>2</sup>

- 1. Universitat de Valencia, ICMUV, Spain
- 2. KTH Royal Institute of Technology, Applied Physics, Sweden
- Universidad Politecnica de Valencia, Instituto Interuniversitario de Investigación de Reconocimiento Molecular y Desarrollo Tecnológico (IDM), Spain
- 4. Universitat de Valencia, Inorganic Chemistry, Spain

Nanoparticles have been designed as biomedical materials for various applications, including bio-imaging and drug delivery-coined under the term theranostics. Iron oxide is an intensively studied material, especially when the size of primary particles is in the range of ≤ 20 nm, showing a novel magnetic characteristics of superparamagnetism (SPM) -making them suited for biomedical applications. In this work, we synthesized core-shell particles where the core is made of monodisperse SPM iron oxide nanoclusters (SPION-NCs), using a polyol method combined with microwave-assisted synthesis, leading to a more eco-friendly product in a rapid and energy-efficient manner. Then, the SPION-NCs were coated with a thin silica layer, protecting them from the harsh chemical environment in subsequent steps. Afterward, a mesoporous silica layer was incorporated using the atrane method, which involves silatrane as the silicon source and CTAB as the templating agent. Surfactant removal was achieved through chemical exchange, leading to large surface-area with mesopores of around 3 nm. Finally, the pores were filled with methylene blue as a model molecule for drug, and its release was studied using PBS. The potential application of these particles in imaging and drug delivery studies and other biomedical applications open up promising avenues for future research and practical applications.

#### 4:40 PM

### (ICACC-S7-024-2025) Red to near-infrared emitting materials for biomedical optoelectronics (Invited)

M. Mauro\*1

1. Universite de Strasbourg, France

Photo- and electro-active materials are attracting a great attention due to their use in light-emitting devices as well as bio-imaging and theragnostic agents. Nevertheless, achieving bright emission in the red and near infrared (NIR) region is intrinsically highly challenging and efficient NIR emitting devices are scarce to date, despite their importance in fields such as biomedical devices for phototherapy. During the talk, our most recent results in the field will be presented. On one hand, selective management of the excited-state mixing enabled the preparation of highly emissive heterobimetallic Ir<sup>III</sup>/M<sup>I</sup> complexes. Their successful application in solution-processed light-emitting electrochemical cells (LECs) allowed to achieve external quantum efficiency up to 6%: one of the highest for red LECs to date. On the other hand, Cu(I) complexes are an attractive alternative to those based on rarer and more expensive platinum-group metals. To date, Cu(I)-based emitters typically display luminescence from blue to orange, while achieving deep-red to NIR emission is still very difficult. Finally, we will present a series of novel family of bimetallic Cu(I) complexes that display emission maxima between  $\lambda = 700$  and 790 nm. These features led successfully to the fabrication of the first examples of stable NIR LECs based on Cu(I) complexes that display electroluminescence maximum up to ca. 780 nm.

### <u>S8 19th Intl Symp on APMT for Structural &</u> <u>Multifunctional Materials & Systems</u>

# S8-Advanced composite manufacturing technologies, hybrid processes

Room: Flagler A

Session Chairs: Lalit Sharma, CSIR-Central Glass & Ceramic Research institute; Gaku Okuma, Tokyo Institute of Technology

#### 1:30 PM

## (ICACC-S8-017-2025) Alumina ceramics without sintering additives as potential substrates for integrated circuits (Invited)

K. Balazsi\*2; C. Balazsi1

- 1. Magyar Kutatasi Halozat Energiatudomanyi Kutatokozpont, Hungary
- 2. Magyar Kutatasi Halozat Energiatudomanyi Kutatokozpont, Thin Film Physics, Hungary

Aluminum nitride (AlN) is an alternative refractory ceramic material being used in various range of applications such as optics, electronics and computer circuits for its unique thermal and electrical properties. It has a really high degree of thermal stability and wear resistance while exhibiting a low density. The effect of the pressureless post-sintering in hydrogen on the structural and mechanical properties of the hot isostatic pressed alumina (Al<sub>2</sub>O<sub>3</sub>) ceramics prepared by oxidized AlN powder has been studied as the potential substrates for integrated circuits. Bulk sintered Al2O3 / AlN has been prepared by combined sintering process, the hot isostatic pressing (HIP) in N<sub>2</sub> and pressureless sintering (PS) in the atmosphere without sintering additives. AlN has been oxidized between in ambient atmosphere. The volume of Al<sub>2</sub>O<sub>3</sub> phase increased with the increasing of oxidation time of AlN powder. High temperature HIP sintering transformed  $\theta$ -Al<sub>2</sub>O<sub>3</sub> and only two major phases  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and minor AlN have been stabilized. PS post-sintering in 1800 °C for 10 h caused the phase transformation to  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> which had effect on the apparent density and hardness of PS sintered ceramics. The highest apparent densities 3.11-3.39 g/cm3 (78-85% relative densities) and highest hardness values (17-18 GPa) have been measured for PS sintered  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> prepared from base powder oxidized between 3 and 10 h.

#### 2:00 PM

#### (ICACC-S8-018-2025) High-speed growth of non-oxide composites by laser chemical vapor deposition using alkylamido compound precursors (Invited)

H. Katsui\*1; K. Shimoda2; M. Hotta1

- 1. National Institute of Advanced Industrial Science and Technology (AIST), Multi-Material Research Institute, Japan
- 2. National Institute for Materials Science (NIMS), Research Center for Structural Materials, Japan

Coatings of non-oxide ceramics such as SiC, BN, transition metal carbides and have been promising to provide the durability and longevity for structural components exposed to harsh environments. The sublimable nature and high melting points of the non-oxides are problematic to obtain dense and protective layers. CVD using alkylamido compounds as precursors is a promising route to deposit condensed non-oxides on a variety of substrates. The less-hazardous precursors including no oxygen can be decomposed and reactive in the gas phase at moderate temperatures, contributing to the high-speed deposition at locally activated reaction fields, enabling us to accelerate the exploration of non-oxide composites and solid solutions having enhanced durability and unique properties. In the presentation, we will demonstrate two cases of high-speed growth of non-oxide composites, i.e., SiC-TiCN nanocomposites and BN incorporated with C and O, by laser-assisted CVD using alkylamido compounds. Nanometric mosaic structure comprising low-crystallinity SiC and TaCN grains with high hardness and moderate elastic modulus formed at deposition rates

over 80  $\mu$ m/h<sup>-1</sup>, exhibiting superior durability in slurry erosion tests. C-incorporated BN (BCN) was grown at high deposition rates, while C- and O-incorporated BN (BCNO) phosphors formed from a single alkylamido precursor.

#### 2:30 PM

## (ICACC-S8-019-2025) Chemical vapor deposition of $HfO_2\text{-}Lu_2O_3$ and $ZrO_2\text{-}Lu_2O_3$ films and their phase relations

A. Ito\*1

1. Yokohama National University, Graduate School of Environment and Information Sciences, Japan

Materials in  $HfO_2$ -Lu<sub>2</sub>O<sub>3</sub> and  $ZrO_2$ -Lu<sub>2</sub>O<sub>3</sub> systems are expected to be applied to protective coatings and radiation-induced phosphors due to high melting point, high density, and high effective atomic numbers. These materials have fluorite-related structures; however, there are a few reports on phase relations of these materials. In the present study, we synthesized  $HfO_2$ -Lu<sub>2</sub>O<sub>3</sub> and  $ZrO_2$ -Lu<sub>2</sub>O<sub>3</sub> films doped with Eu<sup>3+</sup> ions using chemical vapor deposition and studied their phase relations in the fluorite-related structures in terms of crystallography and spectroscopy.

#### 2:50 PM

# (ICACC-S8-020-2025) Modeling study of SiC deposition into porous substrates by thermal gradient chemical vapor infiltration

N. Bessouet\*1; G. L. Vignoles1; S. Jacques1

1. Laboratoire des Composites Thermostructuraux, France

SiC/SiC ceramic matrix composites (CMCs) are emerging in the aerospace and energy industries for high temperature applications. The matrix is mainly manufactured by isothermal and isobaric chemical vapor infiltration (I-CVI), which produces a high purity silicon carbide. However, this gaseous route results in high residual porosity (10-15%). A way to develop both dense and pure SiC/SiC composites is to apply a thermal gradient in the fibrous porous preform during its gaseous infiltration using the thermal gradient CVI (TG-CVI) method with different types of heating (micro-waves, radio-frequency induction, direct contact). Models have been used to define the best conditions for approaching the existence of an optimal infiltration front in TG-CVI, progressing from the hot side to the cold side of the porous substrates. We discuss a theoretical approach that includes criteria with increasing levels of severity, all based on a specific definition of a Thiele modulus. The model shows the results of several configurations differing by the shape and amplitude of the thermal gradient, by the nature of the precursor chemical system and by the nature and structure of the porous substrate. This work has been funded by Horizon 2020 (CEM-WAVE, 958170), the Aquitaine Region (GaMA, 2019-1R10131) and Safran Ceramics.

#### 3:30 PM

#### (ICACC-S8-021-2025) Design and processing to develop multifunctional AlN-SiC and AlC-SiC based bulk, nano and microcrystalline large band gap materials (Invited)

#### N. B. Singh\*1

1. University of Maryland Baltimore County, Chemistry and Biochemistry and Computer Science and Electrical Engineering, USA

There is a strong thrust to develop multifunctional materials for electronic, optical, nuclear and chemical biological sensors, and structural applications with large bandgap, desired symmetry for substrates, large conductivity for heat spreaders, high energy radiation resistant transparent widows, and composites with lotus characteristics for ground and space applications. A great deal of research has been focused on controlling the morphology and hence performance of AlN-SiC and AlN-AlC systems by developing novel processing conditions. We have performed extensive experiment to develop these materials and develop unique structures for these multifunctional materials using reactive solution growth, physical and chemical vapor transport, Bridgman and Czochralski methods. A novel processing approach to develop AlN-SiC and AlN-AlC materials at low temperature using a combination of reactive solvent and Czochralki methods in the eutectic melt will be presented in detail. Results of the processing method, morphological evolution and transition, such as dendritic morphology into facetted long crystals and composites will be described. Low temperature 2H-SiC developed as result of AlN nucleation will be described to demonstrate that hexagonal crystals with large band gap are possible for variety of industrial applications.

#### 4:20 PM

### (ICACC-S8-023-2025) Physico-chemical studies of the preparation of SiC/BN/SiC composites

G. L. Vignoles\*1; S. Jacques2; H. Plaisantin3; J. Danet2; G. Chollon2; O. Caty1;

- Y. Lepetitcorps<sup>1</sup>; G. Couégnat<sup>2</sup>; J. Roger<sup>1</sup>; S. Denneulin<sup>4</sup>; A. Marchais<sup>4</sup>;
- N. Eberling-Fux<sup>4</sup>; G. Camus<sup>2</sup>; S. Jouannigot<sup>2</sup>; P. Fénétaud<sup>1</sup>; C. Chanson<sup>1</sup>;
- H. Delpouve<sup>1</sup>; P. Carminati<sup>1</sup>; H. Carpentier<sup>1</sup>
- 1. University Bordeaux, LCTS Lab for ThermStructural Composites, France
- 2. CNRS LCTS, France
- 3. Laboratoire des Composites Thermostructuraux, France
- 4. Safran SA, Safran Ceramics, France

SiC/BN/SiC composites are now increasingly recognized as gamechanging materials for hot parts of next-generation aircraft turbines. In conjunction with increasing efforts in TRL scale climbing, basic questions arise concerning their processing and their behavior in the envisaged environments. This talk will give an overview of recent results obtained by LCTS on SiC/BN/SiC composites foreseen for use in aircraft turbines. Fundamental physico-chemical questions on gas-route (CVI) and liquid-route (MI) processing and on the influence of the BN interphases will be addressed. Parts of this work were funded by Safran Ceramics, mostly through PhD grants to P. F., C. C., H. D., P. C., I. B. and H. C.

#### 4:40 PM

#### (ICACC-S8-024-2025) On the manufacturing of novel materials by using Corn-based Precursors

M. Fuka\*1; J. Zhang1; S. Gupta1

1. University of North Dakota, Mechanical Engineering, USA

Biomass is a an example of renewable and abundantly available raw material for designing functional materials. In this presention, we will focus on corn-based feedstocks for generating novel materials. We will provide critical insights into the effect of different manufacturing processes like cold and hot-pressing on the properties of corn-based materials by integrating it with different addtives like sand and aggregates. Thereafter, detailed microstructure and property characterization of different composites will be presented. It is expected that these materials can be used for different functional applications.

#### 5:00 PM

#### (ICACC-S8-025-2025) Design and Development of Multicomponent Polymeric Blends for Enhanced Performance

A. Islam\*1; A. Thorne1; S. Gupta1

1. University of North Dakota, Mechanical Engineering, USA

In this study, polyvinylidene fluoride (PVDF), polyether ether ketone (PEEK), and polytetrafluoroethylene (PTFE) blends were synthesized via hot pressing to explore their mechanical, thermal, and tribological properties for advanced material applications. A systematic study was done to understand the compressive strength of these new-generation polymers. Among all polymers, PVDF and PVDF75-PEEK25 showed plastic behavior. The tribological behavior of the polymers against alumina ball, 5 N load, and 2000-meter run was also explored, and the data analysis revealed a low wear rate (~10-6 mm3/Nm) for four polymers. Differential Scanning Calorimetry (DSC) was employed to investigate the thermal transitions. The DSC was used to investigate the thermal behavior of the blends. A detailed microstructure of these polymers was also studied in this work. In addition, a wettability experiment was also performed that showed all polymers have hydrophobic characteristics.

### <u>S9 Porous Ceramics Novel Developments and</u> <u>Applications</u>

### **S9-** Porous Ceramics- Novel Developments and

#### Applications

Room: Ballroom 1-2 Session Chair: Tobias Fey, Friedrich-Alexander University Erlangen-Nürnberg

#### 1:30 PM

#### (ICACC-S9-018-2025) Shaping tomorrow using robocasting: Fabrication of periodic and non-periodic porous ceramic structures (Invited)

L. Wahl\*1; M. Weichelt1; N. Travitzky1; T. Fey1

1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

Porous ceramics are a widely studied material class due to their unique combination of properties, such as low density, high-temperature resistance, and thermal insulation. Their properties make them suitable for various applications, e.g., filtration or insulation, which can be expanded by varying pore size distribution or the used material. Cellular ceramics, on the other hand, are periodic porous ceramics with more organized and larger-scale pore networks. The broader use of such advanced ceramic-based materials depends on the availability of industrial processing routes to fabricate parts with required geometries. Since traditional methods cannot produce complex-shaped ceramic parts with the desired microstructures and properties, additive manufacturing is becoming increasingly important. Robocasting is one of these additive manufacturing processes where a highly filled ceramic paste is printed layer-wise into the desired shape. It allows the production of oxide and non-oxide ceramics, a significant advantage over other additive manufacturing processes. Another feature of this process is the multi-material printing ability to combine materials and their properties in one sample, either in a layered or core-shell structure. In this talk, an overview of the possibilities for manufacturing lightweight cellular and porous structures using robocasting is given.

#### 2:00 PM

### (ICACC-S9-019-2025) Comparing Robocasting and Injection Molding: A Study on Auxetic Structures and Material Behaviour

M. Weichelt\*<sup>1</sup>; D. Köllner<sup>1</sup>; T. Fey<sup>1</sup>

1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

Robocasting and Injection molding are two advanced techniques for manufacturing cellular ceramics, each with unique strengths. They allow the use of many different materials and controlled geometric complexity with high precision. Robocasting, a direct additive manufacturing process, creates complex 3D structures and enables multi-material fabrication. Ceramic injection molding uses VPP printed positive molds for 2D structures, resulting in fine ceramic parts with high geometric precision. This study investigates both processes for the production of auxetic structures, which have a negative Poisson's ratio, allowing lateral expansion when stretched, enhancing toughness and energy absorption. Combined with perovskite materials like BT or BCZT, these structures offer variation in the mechanical properties and novel functionalities.

### Abstracts

Optimized auxetic structures were fabricated using both methods, with theoretical adjustments to reduce mechanical stress peaks. The electromechanical performance and the impact of surface material properties were characterized for both standard and optimized structures.

#### 2:20 PM

#### (ICACC-S9-020-2025) Keep it simple: Kelvin Cells via Liquid Crystal Display-Stereolithography Printing

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The field of scaffolds for bone tissue engineering represents a promising new area of research within the broader discipline of materials science. Cellular ceramics are a particularly promising candidate, as properties such as interconnected pore networks with high tortuosity and tailorable pore shapes, combined with appropriate strength, are of great importance. Nevertheless, the direct imitation of human tissue structures remains challenging using conventional cellular ceramic processing methods such as freeze-drying, sacrificial templating, or gel casting. In this study, we investigate the direct printing of complex parts with high porosities via VPP LCD-based stereolithography (SLA). The network studied was that of Kelvin cells, which exhibited a periodic pattern of 2x2x6 unit cells with a thin and fine structure, as well as strut thicknesses of 0.20 mm or less. Alumina samples were printed with a powder mass percentage of 53% and 70%, investigating two different ceramic resin compositions. Ultrahigh porosities between 89.5% and 97.2% and a maximum compressive strength of  $1.84 \pm 0.17$  MPa were reached due to the dense struts of the structure. LCD-based ceramic stereolithography proved to be a promising candidate for rapid and cost-effective fabrication of highly porous and complex ceramic structures with high accuracy.

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#### (ICACC-S9-021-2025) High-Resolution 3D Imaging of Porous Ceramics Using Confocal Laser Fluorescence Microscopy (Invited)

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- 2. Nagoya Institute of Technology, Advanced Ceramics Research Center, Japan
- 3. National Institute for Materials Science, Japan

A high-resolution three-dimensional observation method for ceramic porous bodies using confocal laser fluorescence microscopy (CLFM) and the liquid immersion technique is introduced. The liquid immersion technique, a preprocessing step for the samples, utilizes the principle that light scattering does not occur at interfaces with equal refractive indices. By infusing a liquid that matches the sample matrix's refractive index into a porous sample with open pores, light scattering is eliminated, resulting in a transparent sample. Before soaking the sample in the immersion liquid, dissolving a fluorescent agent in the liquid allows the fluorescent material to adhere to the sample's inner walls. When the prepared sample is observed with CLFM, the optical system enables the acquisition of cross-sectional images at any depth within the transparent sample. Furthermore, the matrix and pore structures can be distinctly separated from the fluorescent observations. By continuously acquiring and stacking these images, a three-dimensional representation of the sample structure is created. The method allows for the observation of three-dimensional pore structures with a resolution of approximately 1 micrometer, which is higher than that of conventional X-ray computed tomography systems. Examples of observations of porous hydroxyapatite and zeolite bulk bodies are provided.

#### 3:10 PM

#### (ICACC-S9-022-2025) Feature selection method based on porosity-hygroscopy correlations of geopolymer matrices for the prediction of the Moisture Control Capacity

E. Kamseu<sup>\*1</sup>

1. MIPROMALO, Research, Cameroon

Geopolymers are sustainable materials offering advantages as thermal comfort components. Understanding the variables that influence the matrices as hygroscopic material is important. This paper presents T-MOFS-RRGA, a hybrid feature selection technique based on a multi-objective algorithm with RreliefF combining the advantages of filter and wrapper methods. This machine learning approach is used to reduce the size of the feature by automatically selecting the most important ones. After evaluating the hybrid method on the dataset collected in laboratory, the results demonstrated superior performance with RMSE = 0.8491, MSE of 0.72 and MAE = 0.6179 who represent the difference between the actual and predicted hygroscopy values. These values outperform some existing methods. These highlight the importance of intrinsic parameters such as porosity, tortuosity, and pore diameter as well as temperature and humidity.

### <u>S12 Design and Applications of</u> <u>Nanolaminated MAX and MAB Phases Solid</u> <u>Solutions and 2D Counterparts</u>

### S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and

**2D Counterparts** Room: Ponce de Leon

Session Chair: Sylvain Dubois, PPRIME Institute

#### 1:30 PM

## (ICACC-S12-016-2025) Behaviour under ion irradiation of $\rm Cr_2AlC$ (Invited)

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Cr<sub>2</sub>AlC MAX phase presents great mechanical properties and oxidation resistance which can be of interest for nuclear reactor applications To study its behaviour under ion irradiation Cr<sub>2</sub>AlC polycrystalline thin films and single crystal were implanted with He<sup>+</sup> ions. The effects of the fluence and implantation temperature on the microstructural state of Cr<sub>2</sub>AlC, as well as post-implantation annealing, were characterized by XRD, TEM and resistivity measurements. These experiments allowed understanding the progressive formation of the disorder gamma-Cr<sub>2</sub>AlC phase and the associated strain mechanisms. For room temperature (RT) implantations, we observe a fast formation of Cr/Al antisites without associated strain but with a strong modification of the resistivity. XRD measurements interpretation show that strain meanly originates from C Frenkel pair formation. We also found a He threshold concentration for bubble formation. For the higher fluence, nano cracks are formed in the implanted region as well as surface blistering, relaxing the accumulated stress. The absence of single crystal amorphisation even at the higher damage amount (30 dpa) suggests a significant effect of grain boundaries on this transformation. When the implantation temperature increases, the defects saturation leading to the disordered phase is reached at higher fluences. Moreover, our results suggest that the phase transition is favoured by the presence of He.

#### 2:00 PM

### (ICACC-S12-017-2025) The effect of microstructure on the radiation response of MAX phase ceramics (Invited)

K. Lambrinou\*1; I. Ehikhioya1; N. Goossens2; T. Lapauw3; B. Tunca3;

S. Huang<sup>4</sup>; G. Greaves<sup>1</sup>; J. A. Hinks<sup>1</sup>; J. Vleugels<sup>3</sup>; P. Persson<sup>5</sup>

- 1. University of Huddersfield, School of Computing and Engineering, United Kingdom
- 2. Empa, High Performance Ceramics, Switzerland
- 3. Katholieke Universiteit Leuven, Department of Materials Engineering, Belgium
- 4. KU Leuven, Materials Engineering, Belgium
- 5. Linkopings universitet, Department of Physics, Chemistry and Biology, Sweden

The nanolaminated MAX phases have a remarkable ability to annihilate radiation-induced defects at temperatures >600°C, which makes them promising candidate materials for Gen-IV lead-fast reactors (LFRs). Their hexagonal crystal structure leads to anisotropic swelling under irradiation, with unit cell expansion along the c-axis and contraction along the a-axis. Moreover, phase-impure MAX phase ceramics tend to fail due to differential swelling under irradiation. This work reports on the radiation response of MAX phase ceramics for select Gen-IV LFR applications (i.e., pump impellers, anticorrosion coatings), which was monitored in-situ in the TEM by means of helium irradiation (6 keV He<sup>+</sup>, 10<sup>14</sup> ions/cm<sup>2</sup>s) in the 350-800°C range to a maximum dose of 10 dpa. MAX phases of different chemical complexity were irradiated, from ternary MAX phases (e.g., Zr<sub>2</sub>AlC) to complex solid solutions with up to 5 elements on the M-site (Zr, Ti, Hf, Nb, V/Ta) and two elements on the A-site (Al, Sn). This work discusses the effect of microstructure on the radiation response of MAX phase ceramics, in particular radiation-induced swelling, and the two approaches used to control it, i.e., making ceramics with high phase purity and/or strong textures. High-purity MAX phase ceramics can be produced by using metal hydride starting powders, whilst strong textures are easily achieved in coatings deposited by magnetron sputtering.

#### 2:30 PM

#### (ICACC-S12-018-2025) In Situ high temperature neutrondiffraction studies of loaded MAXTHAL bars and FASTsynthesized $Cr_2AIC$ Brazilian-discs

- A. A. Coleman\*1; J. Kelleher1; R. Springell2
- 1. Rutherford Appleton Laboratory, ISIS, United Kingdom
- 2. University of Bristol, Physics, United Kingdom

MAX-Phases have been proposed as potential structural bulk materials for Gen-IV nuclear reactors, requiring an in-depth understanding of their mechanical deformation behavior under high pressure and temperature. Time-of-flight (ToF) neutron diffraction (ND) is ideal for such studies, as it allows for in situ whole-sample diffractograms to be captured during loading. A series of experiments at the ToF ND instrument Engin-X at the ISIS have been performed on MAXTHAL and Cr<sub>2</sub>AlC. Evolutions in microstructure, including particle size and planar disorder were investigated by ND across a range of temperatures and pressures; Macroscopic changes were concurrently captured using Digital Image Correlation (DIC) and whole-sample strain measurements. Modes of stress response were characterized for uniaxial-bar-loading and tensile Brazilian-disc-loading regimes. Observations of in situ surface formation of alumina were characterized by DIC, SEM-EDX of postloading fractured surfaces. While this alumina formation has been described as a "self-healing" mechanism for small-scale cracks, there is currently little experimental research on the potential for re-intercalation of the A-layer over nuclear-application-relevant conditions and time periods. Together these studies will further build our framework of understanding of MAX-phase behavior in a nuclear environment.

### S12- On the Design of nanolaminated ternary transition metal carbibes/nitrides (Max Phases) and Borides (MAB Phases), Solid Solutions thereof and

2D Counterparts

Room: Ponce de Leon Session Chairs: Ankit Srivastava, Texas A&M University; Christina Birkel, Arizona State University

#### 3:10 PM

### (ICACC-S12-019-2025) MAX and MAB phase single crystals and their 2D derivatives (Invited)

T. Ouisse\*1; T. Ito2; H. Pazniak1; F. Wilhelm3; A. Sharma1

- 1. Grenoble INP, France
- 2. Nagoya University, Nagoya University Synchrotron Radiation research Center, Japan
- 3. ESRF, France

MAX and MAB phases are nanolamellar and highly anisotropic. Therefore, the availability of single crystals is key for a better understanding of their electronic and physical properties. We will present a collection of results issued from single crystal experiments, mainly conducted on large scale instruments. We will show how these results, when combined with theory and ab initio calculations, do not only shed light on some specific aspects, but also allow one to draw general and unifying considerations about the physics of MAX/MAB phases and their 2D derivatives.

#### 3:40 PM

#### (ICACC-S12-020-2025) Surface electronic structure of the Zr3SnC2 MAX phase studied by angle-resolved photoemission spectroscopy

T. Ito\*<sup>1</sup>; T. Ouisse<sup>2</sup>; M. Mita<sup>3</sup>; K. Tanaka<sup>4</sup>; L. Jouffret<sup>5</sup>; H. Pazniak<sup>2</sup>; S. Quessada<sup>2</sup>

- 1. Nagoya University, Nagoya University Synchrotron Radiation research Center, Japan
- 2. Grenoble INP, France
- 3. Nagoya University, Graduate School of Engineering, Japan
- 4. Bunshi Kagaku Kenkyujo Kyokutan Shigaiko Kenkyu Shisetsu, Japan
- 5. Université Clermont Auvergne, CNRS, ICCF, France

MAX phase compounds, such as Mn+1AXn, have attracted significant attention for their potential to be converted into MXenes, two-dimensional materials formed by removing the A atoms. In this study, we have performed angle-resolved photoemission spectroscopy (ARPES) on Zr3SnC2 to directly investigate the electronic structure of this system. We found that Zr3SnC2 single crystals exhibit nonreconstructed surfaces after mechanical cleavage, with distinct surface state bands characterized by well-defined energy dispersions. Just after cleavage, the contribution of those surface bands to the ARPES signal largely prevails over the bulk one. Those surface state dispersions can be satisfactorily retrieved and explained by density functional theory (DFT). Since the lack of surface reconstruction was also observed on other 211 MAX phases, this result can probably be generalized to many MAX phases. The result suggests the feasibility of studying surface topological properties using DFT for various MAX phases, assuming non-reconstructed surfaces as observed in Zr3SnC2.

#### 4:00 PM

# (ICACC-S12-021-2025) Synthesis of high temperature MAX phase in the Nb-Al-C, V-Al-C and Ta-Al-C system by molten salt shielded synthesis (Invited)

A. Dash\*1; C. Roy1

1. Danmarks Tekniske Universitet, Department of Energy Conversion and Storage, Denmark

The synthesis of MAX phases like Nb<sub>2</sub>AlC, V<sub>4</sub>AlC<sub>3</sub>, Ta<sub>2</sub>AlC needs a high temperature exceeding 1500°C. Recently, the synthesis of MAX phases are demonstrated by a molten salt shielded synthesis (MS3)

route where molten salt is used both as a reaction medium and for the protection of the oxidation prome materials against oxidation. A very common choice of salt is pottasium bromide (KBr) as it can be compacted to high density at room temperature and can form a gas tight cladding around the reaction mixture of MAX phase. This strategy protects the MAX phase reactants from oxidation at a temperature below the salt melting point (734°C for KBr). Upon melting, the salt forms a melt pool which is impervious to oxygen from ambient atmosphere and the sample being submerged in the salt melt pool is protected from oxidation at synthesis temperatures (1000-1300°C). The boiling point of KBr is 1435°C, which limits the synthesis temperature above 1400°C due to the high vapor pressure and evaporation of salt leaving behind the exposed MAX Phase resulting in complete oxidation. There is a need to have a different salt system to synthesize high temperature MAX phase in the temperature interval of 1400-1600°C. Here, we have demonstrated the synthesis of Nb<sub>2</sub>AlC, V<sub>4</sub>AlC<sub>3</sub> and Ta<sub>2</sub>AlC with the aid of KCl-CaCl<sub>2</sub> eutectic salt mixture with a low vapor pressure and high boiling point (≈1900°C).

#### 4:30 PM

### (ICACC-S12-022-2025) Synthesis and Characterization of $Mo_2NiB_2$ Ceramics

G. Ngige\*1; M. Malusky1; J. Zhang1; S. Gupta1

1. University of North Dakota, Mechanical Engineering, USA

There is an urgent need for high performance ceramics for extreme environment applications. MAX and MAB phases are some examples of ternary carbides and borides system which have shown excellent potential for usage in complex and extreme environments. In this presentation, we will present the recent progress in synthesis and characterization of novel Mo2NiB2 based ceramics. Detailed analysis of microstructural and mechanical property will be presented.

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### (ICACC-S12-023-2025) First-principles investigation of the phase stability and mechanical properties of 2D MXenes

N. D. Oyeniran\*<sup>1</sup>; C. Hu<sup>1</sup>; P. Ganesh<sup>2</sup>; J. Jakowski<sup>3</sup>; P. Kent<sup>3</sup>; B. Sumpter<sup>2</sup>; J. Huang<sup>2</sup>

- 1. The University of Alabama, Aerospace Engineering and Mechanics, USA
- 2. Center of Nanophase Materials Sciences, Oak Ridge National Laboratory, USA
- 3. Computational Sciences and Engineering Division, Oak Ridge National Laboratory, USA

Two-dimensional (2D) transition-metal carbides and nitrides, also known as MXenes, have attracted significant attention due to their exceptional physical and mechanical properties. In this talk, we present our recent first-principles studies on the phase stability and mechanical properties of a broad range of MXenes. First, our studies reveal that although 2D MXenes are typically derived from their precursor MAX phases, their core structures correspond to bulk phase counterparts in a manner akin to the relationship between graphene and graphite. The intriguing relationships between 2D MXenes and their corresponding 3D bulk phases offer valuable insights into the phase stability of 2D MXenes. Second, we found that the mechanical properties of MXenes are strongly influenced by their coordination environment and thickness. Specifically, a gradual increase in octahedral coordination environments enhances the mechanical properties of TiC-based MXenes, while the same coordination environments are detrimental to the mechanical performance of MoN-based MXenes. Interestingly, the mechanical properties tend to stabilize as the number of MXene layers increases, reaching a plateau at four layers. These findings offer new perspectives on optimizing materials through structure-property correlations and underscore the potential for structural designs within the MXenes family.

#### 5:10 PM

### (ICACC-S12-024-2025) Design and Characterization of PEEK-based Composites for Tribological Applications

M. Malusky\*1; S. Gupta1

1. University of North Dakota, Mechanical Engineering, USA

Polymer matrix composites (PMCs) have emerged as important class of materials for structural and functional applicatons. There is an industrial need for additives which can increase the mechanical and functional properties (for example, lubrication, thermal conductvity etc.) of the composites. MAX or MAB phases are an important class of nanolayered materials which has the potential to be an effective reinforcing additive in composites. In the presention, we will present our research on functional composites by using MAX or MAB based additives. Initially, we will present a process of manufacturing PMCs by using different fractions of MAX or MAB phases additives. Thereafter, detailed tribological and microstructural characterization will be presented.

### **<u>S14 Crystalline Materials for Electrical</u> <u>Optical and Medical Applications</u>**

#### **S14- Scintillator II**

Room: Coquina A

Session Chairs: Hiroaki Furuse, National Institute for Materials Science (NIMS); Yasushi Sato, Okayama University of Science

#### 1:30 PM

### (ICACC-S14-017-2025) Synthesis and characterization of translucent $(Gd_{0.894}La_{0.1}Ce_{0.006})_3Al_3Ga_2O_{12}$ ceramics (Invited)

S. Kim<sup>1</sup>; M. Zhuravleva<sup>2</sup>; C. Melcher<sup>2</sup>; J. Glodo<sup>1</sup>; Y. Wang<sup>1</sup>; M. Müller<sup>\*1</sup>

- 1. Radiation Monitoring Devices Inc, Ceramics, USA
- 2. University of Tennessee, Scintillation Materials Research Center, USA

Customs and Border Protection utilize non-destructive high-energy X-rays to screen incoming cargo in search for contraband. Single crystal scintillators are widely employed in radiation detectors, but come with certain drawbacks, including high costs and difficult production on a large scale. Although single crystals are more common, ceramics can be produced at lower temperatures, with faster processing cycles, and lower costs. Also, polycrystalline scintillators show a more homogenous dopant distribution and can be fabricated in complex shapes and forms reducing waste and processing effort. Garnets are of great interest due to their cubic crystal structure, tunable composition, variety of suitable dopants as well as their chemical and mechanical stability. To this end, ceramics with the composition (Gd<sub>0.894</sub>La<sub>0.1</sub>Ce<sub>0.006</sub>)<sub>3</sub>Al<sub>3</sub>Ga<sub>2</sub>O<sub>12</sub> were produced through reversed coprecipitation followed by hot-isostatic pressing. Phase purity and microstructure were evaluated using X-ray diffraction and scanning electron microscopy. The optical properties were characterized through photo and radioluminescence spectroscopy as well as pulse-height analysis. The ceramics were translucent and showed the <sup>5</sup>d-<sup>4</sup>f emission of Ce<sup>3+</sup> with an energy resolution of 12% at 662 keV and a light yield of 23900 photons/MeV. This work was supported by the U.S. Department of Homeland Security under Grant Award Number 20CWDARI00037.

#### 2:00 PM

# (ICACC-S14-018-2025) Scintillation Properties of Transparent Rare-Earth Ions Doped $PbF_2$ Crystals Prepared by Spontaneous Melt Crystallization (Invited)

N. Kawaguchi<sup>\*1</sup>; T. Kunikata<sup>1</sup>; T. Kato<sup>1</sup>; D. Nakauchi<sup>1</sup>; T. Yanagida<sup>1</sup>

1. Nara Institute of Science and Technology, Japan

Scintillation materials are applied for radiation detectors in medical, industrial, and scientific fields. Transparent single crystalline scintillators by the Czochralski method and Bridgman–Stockbarger method are widely utilized due to their uniform light output and high emission intensities. However, single crystal growth generally requires a long production time, and there is a potential need for simpler fabrication methods. In this study, we focused on the production of transparent crystals by spontaneous melt crystallization, in which inorganic compounds are melted and solidified in a stationary crucible. We have previously succeeded to prepare transparent crystals of BaF2 and CaF2-based materials by this method, and we represent the results of applying it to PbF2-based materials. Although PbF2 shows a structural phase transition at a high temperature, transparent crystals were obtained with rapid cooling process. Scintillation properties of the obtained crystals under X-ray irradiation were investigated.

#### 2:30 PM

#### (ICACC-S14-019-2025) Eco-friendly Organic Metal Halide Hybrids for X-ray Scintillation and Detection (Invited)

B. Ma<sup>\*1</sup>

1. Florida State University, Chemistry and Biochemistry, USA

X-ray scintillators and detectors are crucial for medical diagnostics, security, and industrial inspection. Traditional inorganic materials, though widely used, have limitations in performance, versatility, and cost, prompting the search for eco-friendly alternatives. In this talk, I will present our recent work on developing sustainable X-ray scintillation and detection materials based on zero-dimensional (0D) organic metal halide hybrids (OMHHs). These hybrid materials consist of co-crystallized organic and metal halide ions, forming ionically bonded single-crystalline systems with remarkable structural and property tunability. X-ray scintillators based on 0D OMHHs offer many advantages over traditional inorganic materials, including (i) simple, low-cost fabrication via room-temperature wet chemistry, (ii) tunable visible emissions with near-unity photoluminescence quantum efficiency, and (iii) higher light yields and shorter decay times than inorganic scintillators. For direct X-ray detection, the isolation of metal halides by organic cations in 0D OMHHs ensures excellent stability and reduces current drift by limiting ionic migration. Using semiconducting 0D OMHHs with molecular sensitization, we have developed highly efficient detectors with high sensitivity, low detection limits, and exceptional stability, making them promising for medical, security, and scientific applications.

#### S14- Piezoelectric/Ferroelectric Material

Room: Coquina A

Session Chairs: Mariola Ramirez, Universidad Autonoma de Madrid; Tetsuo Tsuchiya, National Institute of Advanced Industrial Science and Technology (AIST)

#### 3:20 PM

#### (ICACC-S14-020-2025) High-Performance Domain-Engineered Tunable Dielectrics for Efficient Sensing (Invited)

#### J. E. Spanier<sup>\*1</sup>

1. Drexel University, Mechanical Engineering and Mechanics, USA

Realization of tunable materials that are multifunctional and maintain high performance in dynamically changing environments is a fundamental goal of materials science and engineering. Tunable dielectrics are promising for sensing devices and require breakthrough performance improvement to enable next-generation technologies. Engineering the ferroelectric polarization energy landscape offers intriguing new opportunities for tailoring properties. I will present our recent collaborative work to design and model the domain structure-property relationships of film materials that exhibit exceptionally large tunable dielectric response over a wide temperature range, and tunability that itself can be modulated. These results suggest that domain engineering is a powerful approach for achieving unprecedented modulation of functional properties in ferroelectric films, and for promising application, including in Smart Grid technologies. Work supported by the U.S. Army Research Laboratory under Cooperative Agreement W911NF-24-0100.

#### 3:54 PM

### (ICACC-S14-023-2025) Tuning the properties of magnetoelectric nanoparticles to enable multiplexed brain stimulation

A. Milojkovic\*1; K. Kozielski1

1. Technische Universitat Munchen, Germany

Neural devices can be used to treat neurological disorders but their need for surgical implantation causes complications that limit widespread patient use. To approach less invasive neural stimulation, we propose injectable, wirelessly powered nanoparticles. However, the wireless powering of nanomaterials is poorly understood, and thus the ability to rationally design nanostimulators for a desired outcome is currently not possible. Here we show magnetoelectric nanoparticles (MENPs) with tunable magnetic properties for better control of neural stimulation. These MENPs consist of magnetostrictive cobalt ferrite (CFO) and a piezoelectric barium titanate (BTO) coupled by a common interface to induce magnetic-to-electric coupling. We hypothesized that tuning the magnetic properties of the MENPs would allow us to control their signal response, and thus enable multiplexing. We observed a rising trend in the coercivity and magnetic saturation of the CFO as temperature increased while EDXS elemental maps confirmed the interfacial coupling. We showed that by controlling the magnetic properties, we can tailor the magnetoelectric properties and tune the performance of MENPs as neural stimulators. Our findings show that the signal response of these nanoparticles can be tuned by basic chemistry. We report MENPs with tunable properties as a promising approach to multiplexed neural stimulation.

#### 4:14 PM

### (ICACC-S14-024-2025) Ultra-low dielectric permittivity in $Li_2O\text{-}B_2O_3\text{-}SiO_2$ glass-ceramics

J. Qiu\*1; C. Tu2; K. Feng3

- Ming Chi University of Technology, International Ph.D. Program in Innovative Technology of Biomedical Engineering and Medical Devices, Taiwan
- 2. Fu Jen Catholic University, Physics, Taiwan
- 3. Ming Chi University of Technology, Department of Mechanical Engineering, Taiwan

The demand for miniaturized low-profile communication devices with energy efficiency and high-frequency application has attracted extensive interest in advanced material research. Low-temperature co-fired ceramics (LTCC) of  $xLi_2O-B_2O_3-SiO_2$ ,  $x = 6 \sim 12$  wt% (xLBS) glass-ceramics have emerged as promising candidates due to their exceptional high-frequency properties. In this study, B<sub>2</sub>O<sub>3</sub> and Li<sub>2</sub>O were added into the SiO<sub>2</sub> matrix to form the xLBS glass-ceramics. The XRD patterns and Raman spectra revealed a primary quartz phase at 900 °C with a secondary phase Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>, that partially transformed into Li<sub>2</sub>SiO<sub>3</sub> at 950 °C. As the quartz phase diminishes, Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub> and Li<sub>2</sub>SiO<sub>3</sub> begin to develop. The SEM and TEM analyses revealed dense microstructures and well-formed crystalline grains in xLBS glass-ceramics. The quality factor Q\*f value was primarily affected by grain size and density. In addition, Li<sub>2</sub>SiO<sub>3</sub> in the xLBS glass-ceramics can aid to reduce dielectric permittivity ( $\varepsilon_r$ ) and Q\*f, particularly at higher frequencies. In this report, a low  $\varepsilon_r$  of 4.7–5, a high Q\*f of 2600 GHz, and a hardness of 249 MHV were achieved in the 900 °C sintered xLBS (x= 12 wt%). These xLBS glass-ceramics exhibit significant potential for LTCC applications in high-frequency communication devices.

### **S17 Advanced Ceramic Materials and Processing for Photonics and Energy**

# S17- Advanced Ceramic Materials and Processing for Photonics and Energy II

Room: Coquina H

Session Chairs: Rafik Naccache, Concordia University; Federico Polo, Ca' Foscari University of Venice

#### 1:30 PM

#### (ICACC-S17-008-2025) Chiral metal complexes for enhanced photo- and electrochemically-induced circularly polarized luminescence (Invited)

M. Mauro<sup>\*1</sup>

1. Universite de Strasbourg, France

The design of enantiomerically pure circularly polarized luminescence (CPL) emitters would enormously benefit from the accurate and in-depth interpretation of the chiroptical properties by jointly photophysical measurements and state-of-the-art theoretical investigation. These CPL-active compounds find fashinating application in energy-efficient CP-optoelectronics and photonic devices. During the talk, our most recent results in the field will be presented. The computed and experimental (chiro-)optical properties of a series of enantiopure phosphorescent Re(I) tricarbonyl complexes will be systematically compared in terms of electronic circular dichroism and CPL. The compounds display dissymmetry factor|gLum|up to  $4 \times 10^{-3}$ . On the other hand, the generation of emissive excited states may take place via alternative ways, e.g. electrochemical pathways (ElectroChemiLuminescence, ECL). ECL occurs when radical ion species electro-generated at the electrode|solution interface undergo highly exergonic electron transfer reactions yielding to an excited state that radiatively relaxes to the ground state. In the second part of the talk, a novel series of enantiopure heterobimetallic cyclometalated complexes of general formula  $Ir^{III}-M^{I}$  ( $M^{I} = Cu^{I}, Au^{I}$ ) will be disclosed that display efficient and stable Circularly Polarized ElectroChemiLuminescence (CP-ECL) with gLum up to 3×10<sup>-3</sup>.

#### 2:00 PM

#### (ICACC-S17-009-2025) Rational design of inorganic nanomaterials with tailored morphology as efficient photocatalysts (Invited)

E. Moretti<sup>\*1</sup>

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1. Ca' Foscari University of Venice, Department of Molecular Sciences and Nanosystems, Italy

Nowadays, one of the main technological challenges that we are facing is the ability to provide a sustainable supply of clean energy and, among all renewable sources, solar energy displays the greatest potential. Recently, the development of novel synthetic strategies has led to the preparation of nanostructured materials displaying unique properties compared to the bulk counterpart systems, with controlled and tunable morphologies able to enhance the activity and selectivity of a catalytic process. In particular, nanostructured materials synthesized via the bottom-up approach present an opportunity for future generation manufacturing of devices. This talk will focus on the importance of tuning the morphological features of a catalyst as a strategy to the photocatalytic activity, focusing on how rationally designing inorganic materials at the nanoscale can lead to morphologies and structures suitable to enhance the catalytic performance of industrially and environmentally important processes. The talk will discuss some energy and environmental applications that can be addressed by multi-component oxide systems synthesized via the bottom-up approach, highlighting their structure-reactivity relationship. Photocatalytic H2 production and purification and drugs degradation will be presented as a successful case history.

#### 2:30 PM

#### (ICACC-S17-010-2025) Novel Catalysts for Water Splitting: Strategies for Performance Enhancement (Invited)

#### T. A. Shifa\*1

1. Ca' Foscari University of Venice, Department of Molecular Sciences and Nanosystems, Italy

The generation of clean energy from water electrolysis is a feasible solution to overcome the problems of energy crisis. However, this viable route depends on the utilization of Pt, which is scarce and expensive. In this regard, 2D materials (layered or non-layered), and transition metal phosphides have got copious attention. Here, we present strategies to enhance the catalytic performance of these materials giving a particular emphasis for transition metal chalcogenides, transition metal phosphorus trichalcogenides and metal phosphides. We discuss the advantages of these materials for catalysis and the different routes available to tune their electronic states and active sites. Experimental results show that doping and hybrid material formation play a significant role in optimizing the free energy of hydrogen adsorption and desorption Another compelling issue is about solving the sluggish kinetics of the other half reaction (i.e OER) in water splitting catalysis. We discuss the mechanism behind the very good performance of Ni5P4 and CrOx-CuS toward electro-catalysis of OER. The metal phosphides or sulfides are not the true catalysts, rather in-situ generated metal oxides at the vicinity of phosphides/sulfides are. Moreover, We highlight the emerging layered MPX<sub>3</sub> (M= Mn, Ni, Fe, Cu/In) nanosheets as promising materials for photocatalytic water splitting.

#### 3:20 PM

#### (ICACC-S17-011-2025) Innovative Approaches in Theranostics: The Role of Luminescent Rare Earth Doped Nanoparticles (Invited)

F. Vetrone\*1

1. INRS, Université du Québec, Centre Énergie, Matériaux et Télécommunications, Canada

Luminescent nanomaterials that can be excited, as well as emit, in the near-infrared (NIR) have been investigated for use in a plethora of applications related to human health and biology. They have received considerable attention for theranostic (therapy and diagnostic) platforms where light is used as an external trigger. NIR light can penetrate tissues much better than high-energy light especially when these wavelengths lie within the three biological windows where tissues are optically transparent. At the forefront of NIR excited nanomaterials are rare earth doped nanoparticles (RENPs), which due to their 4f electronic energy states can undergo conventional (Stokes) luminescence and emit in the three NIR biological windows. However, unlike other nanoparticles, they can also undergo a multiphoton process (known as upconversion) where the NIR excitation light is converted to higher energies resulting in anti-Stokes luminescence spanning the UV-visible-NIR regions. Due to the versatility of their optical properties, it now becomes possible to generate high-energy light (UV or blue) in situ to trigger other light activated therapeutic modalities while using the NIR emission for diagnostics. Here, we present the synthesis of diverse RENPs and demonstrate how their luminescence properties can be exploited for potential use in diverse biomedical applications.

#### 3:50 PM

# (ICACC-S17-012-2025) Sodium: the journey of a "diffusion catalyst" from the surface to the bulk of $Cu(In,Ga)Se_2$ (Invited)

D. Colombara\*1

1. Universita degli Studi di Genova, Italy

Cu(In,Ga)Se2 (CIGS) is the most efficient commercial thin film photovoltaic (PV) material. Yet, its polycrystalline microstructure is full of potential recombination centers. Additionally, CIGS has a high density of oppositely charged point defects, a condition known as compensation. Compensated semiconductors yield a photoluminescence emission that is red shifted compared to the optical absorption onset. The shift is due to charge carrier thermalization, a source of performance losses that results from an electronic band structure affected by electrostatic potential fluctuations. Despite these challenges, CIGS technology thrives thanks to the presence of sodium. Even trace amounts of it can boost CIGS solar cell efficiency from a few percent to over 23%. But what exactly does sodium do? Sodium's role in improving CIGS optoelectronic properties involves complex effects at surfaces, grain boundaries, and grain cores. Unraveling these effects has taken over 30 years of research. My work reveals sodium's ability to (i) catalyze the diffusion of matrix atoms within the material, and (ii) modulate oxygen incorporation at surfaces and grain boundaries. These processes reduce electrostatic potential fluctuations and parasitic recombination of charge carriers. Sodium, thus, acts not as a simple dopant but as a "diffusion catalyst," a concept that could be applied to other chalcogenide materials.

#### 4:20 PM

#### (ICACC-S17-013-2025) Nano-Catalyst Formation by Exsolution: Applications For Electrochemical Fuel Production (Invited)

S. Barnett<sup>\*1</sup>

1. Northwestern University, USA

Exsolution occurs when an oxide material is exposed to reducing conditions, such that a minority cation is reduced and nucleates as metallic nanoparticles on the oxide surfaces. Oxides with exsolved nanoparticles have been used as catalysts and as electrodes in electrochemical cells such as fuel cells and electrolysers. This talk will focus on the latter application - when electrolysis cells are powered using renewable electricity, efficient energy storage and production of renewable fuels can be achieved. This talk will first review the fundamentals of the exsolution process, including the factors that determine exsolve particle composition and size distribution, phase changes that may occur in the host oxide during exsolution, and the long-term stability of exsolved nanoparticles. The focus will then turn to how exsolution impacts the electrochemical performance of the oxide electrode, particularly during electrolysis cell operation. Results on Sr(Ti,Fe)O<sub>3</sub>-based electrodes will be highlighted. Here, small amounts of Ni or Ru substituted on the B-site result in the formation of Ni-Fe or Ru-Fe nanoparticles, respectively, during exposure of the electrode to a reducing fuel during cell operation. The results suggest that exsolved metal nanoparticles enhance electrochemical performance by promoting hydrogen dissociation on electrode surfaces, resulting in reduced electrode resistance.

#### 4:50 PM

## (ICACC-S17-014-2025) Design of CeO $_2$ -based nanocomposites for production of Liquid Hydrogen Carriers (Invited)

T. Montini\*1

1. Universita degli Studi di Trieste, Department of Chemical and Pharmaceutical Sciences, Italy

The emergence of hydrogen economy with the current scenario of the need to switch to cleaner and greener forms of energy sources is seen to be inevitable. Despite many possibilities in hydrogen production, its transport and capillary distribution could present important challenges in terms of safety and costs. In this context, Liquid Hydrogen Carriers (LHC) represent an interesting alternative to compressed hydrogen. LHC are non-toxic, low molecular weight and water-soluble molecules that can be easily converted in H<sub>2</sub>-rich gas mixtures. LHC, such as HCHO and HCOOH, can be produced by different processes, such as valorisation of biomasses or  $CO_2$  reduction. In this talk, the most interesting results obtained in our research group regarding the design of  $CeO_2$ -based nanocomposite materials to be used for LHC production will be presented.  $CeO_2/g-C_3N_4$  nanocomposites was tested for LHC production by photocatalytic partial oxidation of biomasses leading to HCHO with very high selectivity. On the other hand,  $CeO_2/MWCNT$  nanocomposites demonstrated promising performance as electrocatalyst for  $CO_2$  reduction to HCOOH. The employed nanocomposite materials were prepared by a bottom-up approach and deeply characterized in terms of structural, morphological and functional properties.

### **<u>S18 Ultra-High Temperature Ceramics</u>**

#### S18- Processing-Microstructure-Property Relationship

#### Room: Coquina F

Session Chairs: Kun Wang, Alfred University; Vinothini Venkatachalam, University of Birmingham

#### 1:30 PM

# $(ICACC-S18-017-2025)\ Near\ net\ shape\ processing\ of\ high\ \&\ ultra-high\ temperature\ ceramic\ matrix\ composites\ (Invited)$

V. Venkatachalam\*1; J. Binner2

- 1. University of Birmingham, Metallurgy and Materials, United Kingdom
- 2. University of Birmingham, Ceramic Science & Engineering, United Kingdom

High and ultra-high-temperature ceramic matrix composites (CMCs) are advanced materials designed for use in extreme environments, such as aerospace and space applications, as they possess outstanding chemical stability, high thermal conductivity, high strength and high melting points. Amongst various processing routes, polymer-derived ceramics (PDCs) and chemical vapour infiltration (CVI) are two advanced techniques promising to create near-net-shape, high-performance ceramic matrix composites (CMCs). This preliminary work brings the perspectives of PDC and CVI methods to fabricate carbon fibre-reinforced CMC components with superior thermal and mechanical properties. PDCs are produced by the pyrolysis of an inexpensive commercially available polysilazane offering an amorphous SiCN phase. On the other hand, CVI involves the infiltration of gaseous precursors, methyl trichlorosilane (MTS), into a porous preform, followed by in-situ chemical reactions to deposit a silicon carbide (SiC) ceramic matrix. The present work uses a radio frequency-assisted CVI (RF-CVI) technique to improve efficiency and processing time without compromising the properties. Furthermore, this research explores how the synergistic use of PDC and CVI processes can optimise the microstructure and performance of CMCs, making them suitable for demanding high-end applications.

#### 2:00 PM

#### (ICACC-S18-018-2025) Polymer Derived Ultra-High Temperature Ceramic Matrix Composites

A. Advincula<sup>\*1</sup>; S. Angelopoulos<sup>1</sup>; W. Meador<sup>1</sup>; J. Ponder<sup>1</sup>; J. Delcamp<sup>1</sup>; M. B. Dickerson<sup>1</sup>; T. Pruyn<sup>1</sup>

1. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Vehicles for extreme environments can experience exceptionally high heat fluxes resulting in high temperatures in oxidizing environments. Materials selection for such hot structures is limited to the most refractory systems, such as carbon/carbon composites coated with ultra-high temperature ceramics (UHTCs) or UHTC matrix composites (UHTCMCs). Recent Air Force Research Laboratory efforts have been focused on the synthesis, scale-up, and characterization of precursor polymers that can enable the production of UHTCMCs. This presentation will introduce and discuss new preceramic polymers (termed Air Force Preceramics (AFPCs)) capable of producing UHTC materials, such as zirconium carbide (ZrC). The invention of these new AFPCs is significant as these polymers have properties (e.g., low viscosity, high ceramic yield, and compositional tunability) attractive for producing UHTCMCs. Specifically, AFPCs excel in infiltrating fiber tows allowing for densification of continuous UHTC matrix around individual carbon fibers on the micron-length scale, a desirable UHTCMC feature challenging to achieve with historical approaches (e.g., slurry methods). In this presentation, AFPC-based production of UHTCMCs will be discussed, as well as the thermal/mechanical characterization and performance-testing of the finished composites. Knowledge from this work will enhance future capabilities for flight in extreme environments.

#### 2:20 PM

### (ICACC-S18-019-2025) Group IV (Zr, Hf) Metal Carbide Whisker Synthesis

P. Loughney<sup>\*1</sup>; L. M. Rueschhoff<sup>1</sup>

1. Air Force Research Lab, Materials and Manufacturing Directorate, USA

Ultra-high temperature ceramic matrix composites (UHTCMCs) are attractive materials for use in extreme aerospace environments, in which a UHTC matrix (ZrB<sub>2</sub>, HfB<sub>2</sub>) is reinforced with a secondary fiber phase such as C<sub>f</sub> or SiC<sub>f</sub>. However, C and SiC are limited by oxidative degradation and incompatible coefficient of thermal expansion with UHTC matrix materials, challenging their processibility and operable temperature windows. UHTC fibers or whiskers such as group IV transition metal (Zr, Hf, etc.) carbides are of particular interest as reinforcements because of their robust thermal and mechanical properties, as well as compatible CTEs with diborides. Whiskers, although providing less reinforcement than continuous fibers, have been shown to improve mechanical properties over monolithic ceramics while also allowing for enhanced processibility over continuous fibers with additive manufacturing. UHTC fibers and whiskers, however, remain largely unavailable on the commercial scale and common synthesis techniques lack scalability and morphological control. Carbothermal reduction is a viable synthesis technique for producing whiskers in high yields, however methods that successfully tune aspect ratio while achieving sizeand shape-control need more development. This work explores the morphological control and scalability that can be achieved in carbothermal reduction of ZrC and HfC whiskers.

#### 2:40 PM

### (ICACC-S18-020-2025) Sintering of Arc-Melted Carbon-rich Carbides

A. Patel\*1; A. Celik1; Z. Ayguzer Yasar1; R. A. Haber1

1. Rutgers The State University of New Jersey, Material Science and Engineering, USA

In this study, carbon-rich carbide ( $B_4C$  and ZrC) ingots were synthesized via the arc-melting process using commercially available carbide powders and Carbon Lampblack. The arc-melted ingots were milled into fine powders and sintered via SPS. Microstructural analyses and mechanical property measurements were performed on both arc-melted and densified samples. Amorphization from indentation was measured using Raman spectroscopy. Submicron carbon islands were observed throughout the ZrC arc-melted samples.

#### 3:20 PM

#### (ICACC-S18-021-2025) Development of Advanced High Temperature Testing of Ceramic Materials (Invited)

B. Allen<sup>\*1</sup>

1. Dynamic Systems Inc., USA

Dynamic Systems Inc. (DSI) has expanded its Gleeble thermalmechanical testing capabilities to include high-temperature mechanical testing of non-conductive ceramic materials. With expertise in high-temperature testing, DSI now offers three- and four-point bend tests for ceramics in controlled atmospheres at up to 2500°C. The system ensures precise heating, cooling, and temperature control, allowing for accurate and repeatable results. It supports ASTM standards for flexural strength, modulus, fracture toughness, and slow crack growth. With rapid thermal cycling, the system enables high throughput of 8 to 12 tests per day, benefiting industries like aerospace, energy, and advanced manufacturing.

#### 3:50 PM

# (ICACC-S18-022-2025) Densification, mechanical and thermal properties of zirconium diboride ceramics

Y. Zhou\*1; W. Fahrenholtz1; G. Hilmas1

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

Zirconium diboride (ZrB2) ceramics were fabricated by hot-pressing. Two batches of starting powders were prepared, one with 0.5 wt% carbon and the second with 0.5 wt% carbon plus 4.7 wt% zirconium hydride (ZrH2). The carbon was added as phenolic resin, which was used to promote densification. ZrH2 was used to react with and remove graphite and B4C impurities from the final microstructure. Starting powders were densified at temperatures from 1750 - 2150°C under 32 MPa for 10 minutes. The cross-section morphologies were observed by scanning electron microscopy. Mechanical and thermal properties of both compositions were measured and compared. Strength, fracture toughness, hardness, and elastic modulus were measured at room temperature. Thermal diffusivities were measured from room temperature to 1500°C. Keywords: zirconium diboride, densification, mechanical properties, thermal properties.

#### 4:10 PM

# (ICACC-S18-023-2025) Influence of fibre architecture on the fracture behaviour of 2D $C_{f^-}ZrB_2$ -SiC ultra-high temperature ceramic matrix composites: A 3D image analysis

- A. R. Mishra\*1; V. Singh2; D. Kumar2; M. Patel2; R. Mitra1
- 1. Indian Institute of Technology Kharagpur, Metallurgical and Materials Engineering, India
- 2. DRDO Defence Metallurgical Research Laboratory, India

The world is witnessing a surge in developing novel processing and characterization methods for UHTCMCs. This study examines the fracture behaviour of 2D Cf-ZrB2-SiC UHTCMCs, fabricated via slurry infiltration and hot pressing, using 3D imaging of crack patterns after mechanical testing. The influence of fibre architecture on fracture behaviour has been analysed, revealing non-brittle failure across all architectures. 3D crack propagation analysis shows that cracks initiated below the notch reduce their opening as they propagate towards the compressive end, irrespective of fibre architecture. The UD-0/0° composite has a moderate crack surface area but the highest crack volume, indicating thicker cracks. It shows highly tortuous cracks with mixed-mode failure, fibre pull-out, and matrix spalling, resulting in the highest WOF (~2032.7 J/m<sup>2</sup>). The UD-0/90° composite has the smallest crack surface area and volume, with linear propagation through 90° laminae. The 8H-SW composite exhibits a large crack surface area and moderate volume, with confined crack propagation due to the interlaced fibre architecture, leading to a unique failure mode involving defect-fibre interactions and compressive buckling for fibres.

#### 4:30 PM

#### (ICACC-S18-024-2025) Microstructural Evolution in a One-Directional Phase Changing UHTC-Metal-Composite

- M. J. Large\*1; B. Taylor4; J. Rosales4; C. R. Weinberger2; G. Thompson3
- 1. The University of Alabama, Materials Science, USA
- 2. Colorado State University, Department of Mechanical Engineering, USA
- 3. University of Alabama, Metallurgical & Materials Engineering, USA
- 4. NASA Marshall Space Flight Center, USA

Ultrahigh temperature ceramics (UHTCs) are characterized by their high melting temperatures and high hardness. However, this hardness is accompanied by these materials being brittle. In this work, we have added Zr metal laminates to improve the toughness of ZrC. While the addition of a metal phase can improve the durability at low temperatures, it will also lower the operating temperature as the metal has a much lower melting point. To mitigate this issue, the laminate composite is designed to phase transform into a single phase sub-stoichiometric carbide. Here, a series of laminate composites were made fabricated by processing ZrC powder in-between Zr metal foils which were then collectively direct current sintered into a consolidated composite. Subsequent annealing was then performed to drive the diffusional transformation as carbon depleted from ZrC and converted Zr into ZrCx. During this transformation, a gradient in de-cohesion in the initial ZrC grain boundaries was observed as the lattice parameter contracted in response to the carbon depletion. Furthermore, at the reaction front, Zr laths precipitated out of the ZrC<sub>x</sub> upon cooling because of a change in carbon solubility. The as-fabricated, partially transformed, and fully transformed composite structures were mechanical tested to assess the fracture toughness at these various stages of transformation.

#### 4:50 PM

# (ICACC-S18-025-2025) Effect of $B_4C$ on sintering behavior and induced self-healing of SiC-based ceramics prepared by solid-state synthesis

M. Park\*1; S. Jung1; W. Kwon1; S. Lee1

1. Korea Institute of Materials Science, Extreme Materials Research Institute, Republic of Korea

Silicon carbide (SiC) and boron carbide ( $B_4C$ ) are both engineering ceramics notorious for their difficulty in sintering; on the other hand, they promote each other's sintering. However, the sintering behavior of SiC with B<sub>4</sub>C remains controversial between solidstate sintering (SSS) and liquid-phase sintering (LPS). Additionally, applying sintering additives requires caution as it easily compromises SiC's high-temperature properties. This is particularly important because SiC-based materials have been succesfully applied for high-temperature applications, such as commercial aircraft engines. In this study, we synthesized SiC and SiC-B<sub>4</sub>C filler via mechanochemical synthesis using high-energy planetary milling. Green bodies were produced using either a colloidal process or cold isostatic pressing (CIP) of the fillers, before integration through FAST/SPS. The specimens then underwent precursor impregnation and pyrolysis (PIP) for densification, without harming their high-temperature properties. By incorporating small amount of B<sub>4</sub>C, ranging from 1 vol% to 7 vol%, into the filler, we observed the effect of  $B_4C$  on the microstructure of the matrix, as well as on the thermo-mechanical properties. This also provides insights into the sintering mechanism of SiC-B<sub>4</sub>C systems and methods for improving both high-temperature properties and productivity of SiC-based products.

### **<u>S19 Molecular-level Processing and Chemical</u>** <u>Engineering of Functional Materials</u>

# S19- Precursor-derived ceramics for high-temperature applications

#### Room: Ballroom 3

Session Chair: Günter Motz, University of Bayreuth

#### 1:30 PM

#### (ICACC-S19-018-2025) Preceramic Polymers and Hybrid Systems for the Fabrication of Nanoscale High-Temperature Ceramics (Invited)

M. B. Dickerson\*<sup>1</sup>; J. Ponder<sup>2</sup>; J. J. Bowen<sup>1</sup>; T. Pruyn<sup>1</sup>; J. Delcamp<sup>1</sup>

- 1. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
- 2. Air Force Research Lab, USA

Polymer-derived ceramics have several desirable properties, including high-temperature stability and chemical resistance. In our work, we have applied several soft-matter processing methodologies to PCPs, including block copolymer (BCP) templating and nanoparticle surface grafting, to yield high-temperature nanostructures. The ability to fabricate nanofeatured high-temperature ceramics and composites with features below the critical crack length improves mechanical loading responses and therefore fracture toughness as well as crack resistance. BCPs can be used to direct PCPs by selective swelling of one block leading to tailorable morphologies through control of the ratio of the polymers. BCPs can be burned out during pyrolysis, resulting in nanofeatured ceramics. As PCPs suffer from substantial shrinkage between casting and pyrolysis, incorporation of nanoparticles can be used to aid in reducing contraction. Nanoparticles' propensity to flocculate makes them challenging to work with and to evenly disperse, but this can be overcome by synthesis of a polymer layer on the surface to produce polymergrafted nanoparticles (PGNPs).

#### 2:00 PM

### (ICACC-S19-019-2025) Thermal Stability of Yttrium-modified Polymer-Derived Ceramics

R. Shiva Kumar\*1; R. Prasad1

1. Indian Institute of Technology Ropar, Metallurgical and Materials Engineering, India

The main aim is to study the thermal stability of yttrium-modified silicon oxycarbide ceramics at high temperatures up to 1600 °C. Yttrium-modified silicon oxycarbide (SiOC) ceramics were synthesized via pyrolysis of polymethylsilsesquioxane (PMS) with the modification of yttrium acetate from 1000 to 1600 °C. Microstructural anlaysis of resulting ceramics were done using characterization techniques such as FTIR, Raman, XRD and FESEM. FTIR analysis revealed the vibrational bonds in polymer and removal of organic groups from the polymer to form SiOC ceramics at 1000 °C. Raman spectroscopy shows a decrease in the intensity of the D and G bands with increase in pyrolysis temperatures. XRD analysis of SiOC ceramics shows predominant peaks of amorphous silica, with phase transitions occurring as temperature increases, leading to crystallization of silicon carbide. XRD analysis of Y-modified SiOC ceramics reveals yttrium oxide peaks at 1000 °C, transitioning to yttrium silicate formation at 1100 °C. FESEM/EDS analysis reveal spherical particles of SiOC ceramics with the presence of yttrium silicate on the surface. Yttrium-modified SiOC ceramics exhibited significantly less weight loss compared to unmodified SiOC ceramics at 1600 °C indicating the increased thermal stability of yttrium-modified SiOC ceramics.

### Abstracts

#### 2:20 PM

### (ICACC-S19-020-2025) Polymer-derived HfSiCO monolithic ceramics and fibers using Starfire's SHP-199

K. Hendrix\*1; P. Kroll<sup>2</sup>

- 1. The University of Texas at Arlington, Chemistry and Biochemistry, USA
- 2. University of Texas, Arlington, USA

SHP-199 is a hafnium-2-butynyl-bis-alkoxide polymeric precursor. Annealing to 1000 °C under inert atmosphere converts the precursor into hafnia (HfO2) and residual carbon. Further annealing to 1600 °C under exclusion of oxygen yields crystalline hafnium carbide (HfC). The thermal processing of SHP-199 goes along with high volume shrinkage, hampering its application in ceramics engineering. We developed different chemical routes to modify SHP-199, making it suitable for shaping and fiber drawing. Reacting SHP-199 with silane precursors yields HfSiCO resins that can be converted to monolithic ceramics. After annealing to 1600°C and holding for multiple hours, one such formulation displays hafnon (HfSiO4), hafnia (HfO2), and silica (SiO2) in the presence of graphitic carbon. Tuning of reaction conditions yields a viscous liquid suitable for drawing HfSiCO-fibers. The phase development of these fibers after annealing to 1600 °C for multiple hours will be discussed.

#### 2:40 PM

### (ICACC-S19-021-2025) Solution processing of metal carbide composites (Invited)

G. Westin<sup>\*1</sup>

1. Uppsala University, Sweden

Metal carbides and their composites with various binder phase metals are due to their tunable hardness and toughness of great importance for a wide range of applications, such as metal machining, rock excavation, and low friction durable coatings for automotive industry. Solution based processing of carbides and offer great flexibility in the material compositions and makes deposition on complex surfaces possible. Herein, solution based routes to W,Nb and Zr carbides and solution based routes to coated carbide powders for improved sinterability are described, as well as their effect on the microstructures and properties. The improved sinterability of the nano-dot coated powders allowed for hard composites with excellent mechanical properties. Oxidation behaviour in liquid lead will be described.

### S19- Pyrolysis and precursor-derived ceramic fibers

Room: Ballroom 3

Session Chair: Matthew Dickerson, Air Force Research Laboratory

#### 3:30 PM

#### (ICACC-S19-022-2025) Novel Multifibrillar Carbon/Ceramic Hybrid Fibers Consisting of Thousands of Individual Nanofibers (Invited)

G. Motz\*1; J. Denk2; S. Schafföner2; X. Liao4; S. Agarwal3

- 1. University of Bayreuth, Ceramic Materials Engineering, Germany
- 2. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany
- 3. Universitat Bayreuth, Macromolecular Chemistry II, Germany
- 4. Tianjin University, School of Materials Science and Engineering, China

For the development of new technologies, more and more materials with very unusual and tailor-made properties are required. In the past, carbon and ceramic fibers were initially developed for extreme conditions in aerospace and military applications. However, these are now used on a large scale for civil applications such as  $CO_2$ -free energy generation (wind turbines), in transport or in sports. Typically, carbon or ceramic fiber bundles and fabrics consisting of several thousand 10 and 15 µm thick individual fibers. In this context, we have developed a strategy to produce continuously novel multifibrillar carbon/ceramic nanofibers. The process starts with the synthesis of the polyacrylonitrile/polysilazane blend, followed by electrospinning, curing and final pyrolysis. This novel multifibrillar C/SiCON bundle with a diameter of 15 to 20  $\mu$ m consists of thousands of individual fibers with diameters in the nanometer range. This would enable the production of multifibrillar fibers with extremely high strength in the future, because of the strongly reduced diameter if sticking of the nanofibers together can be avoided. The large surface area of the fibers should guarantee for a much better interaction to polymer matrices, so that the resulting fiber-reinforced plastics could achieve much better mechanical properties with a reduced fiber content.

#### 4:00 PM

### (ICACC-S19-023-2025) Alumina-YAG and Alumina-Zirconia fiber precursors: from synthesis to oxide ceramic conversion

F. Vergnaud\*1; E. De Sousa1; J. Jouin1; G. Delaizir1; S. Bernard1; P. Thomas1

1. Institut de Recherche sur les Ceramiques, France

Oxide ceramic matrix composites are important strategic materials. However, their key raw materials, oxide ceramic fibers, are mainly produced in the United States. The InVECOF project seeks to develop a European production chain for ceramic oxide fibers, including next-generation oxide (NGO) fibers with improved thermo-mechanical properties. To increase creep resistance at high temperatures, fiber composition or microstructure must be finely tuned. The addition of YAG or ZrO<sub>2</sub> to α-Al<sub>2</sub>O<sub>3</sub> showed great results due to their ability to inhibit grain growth and provide their inherent creep resistance to the high-strength alumina. However, Y and Zr precursor amount and nature can affect the mechanisms occurring during the precursor synthesis and further heat treatments. One of the challenges of NGO fiber development is the understanding of these different mechanisms to obtain the desired ceramic nature (crystal phases) and microstructure (grain size, densification). Al<sub>2</sub>O<sub>3</sub>-YAG and Al<sub>2</sub>O<sub>3</sub>-ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub> fiber precursors were prepared by sol-gel method. The effects of the Y and Zr precursor amount and nature (molecular precursor or oxide colloid) on thermal behavior and final properties (crystallization, grain size, densification) were investigated by structural (XRD, FTIR), microstructural (SEM), and thermal (TGA-DTA) analyses. Dense multiphased fibers were obtained for both compositions.

#### 4:20 PM

## (ICACC-S19-024-2025) Synthesis of tailored preceramic polymers for the design of SiAlON fibers

B. Tolve Granier\*2; S. Beaudet-Savignat1; P. Hourquebie1; S. Bernard2

- 1. CEA Le Ripault, France
- 2. CNRS, IRCER, France

Ceramic matrix composites (CMCs) reinforced with ceramic fibers are of great interest due to their high-temperature resistance, thermal shock resistance, and low density, making them ideal for aerospace, automotive, energy, and defense applications. The performance of CMCs is closely tied to the properties of the reinforcing fibers, which present ongoing scientific and technological challenges. These fibers are expected to exhibit specific dielectric, mechanical, and thermal properties for high-temperature applications. To address these challenges, we aim to develop oxynitride fibers using the Polymer-Derived Ceramics (PDCs) route. This approach involves synthesizing preceramic polymers with tailored rheological properties suitable for melt-spinning, followed by converting the spun fibers into ceramic fibers through appropriate curing and thermal treatments. In this presentation, we will focus on the synthesis of preceramic polymers suitable for melt spinning and the formation of oxynitride fibers, such as SiAlON fibers. The evolving materials will be characterized at each stage of the elaboration process. Thus, this work highlights the close relationship between precursor chemistry, its rheology, and the composition and structure of the derived fibers.

#### 4:40 PM

## (ICACC-S19-025-2025) Computational Pyrolysis of SMP-10 and SHP-199 (Invited)

P. Kroll\*1

1. The University of Texas at Arlington, Department of Chemistry and Biochemistry, USA

We present results of ab-initio Molecular Dynamic (aiMD) simulations for the pyrolysis of two polymer precursors. Models of SMP-10 cross-linked through allyl-groups are thermalized at elevated temperatures, and several fundamental reactions are observed. We discern the role of hydrogen in facilitating bond breaking and formation. Through the adjustment of elimination rates of gaseous species, we simulate reactive environments and study their impact on chemical composition. SMP-10 is transformed into amorphous SiC(:H), and a pyrolysis under hydrogen reduces the amount of bonds between carbon. SHP-199 rapidly transforms into amorphous HfO<sub>x</sub>:C<sub>p</sub> with a large fraction of excess carbon. We generate hybrid co-polymers with SHP-199 and indicate pathways to new systems.

### Poster Session A

Room: Ocean Center

#### 5:00 PM

#### (ICACC-PA001-2025) Enhancing Energy Output in Piezoelectric Nanodevices: A Focus on Electrode Selection

B. Göl\*1; G. Yüksel2; S. Dadashov4; S. Kinden3; E. Suvaci2

- 1. Kahramanmaras Sutcu Imam Universitesi, Electrical and Electronics Engineering, Turkey
- 2. Eskisehir Teknik Universitesi, Materials Science and Engineering, Turkey
- 3. Eskisehir Teknik Universitesi, Electrical engineering, Turkey
- 4. Eskisehir Teknik Universitesi, Chemical Engineering, Turkey

The increasing importance of piezoelectric energy harvesters in wearable electronics and self-powered sensors highlights the need to improve energy conversion efficiency. However, current piezoelectric systems often do not perform optimally due to limitations in electrode design. To enhance electrical output, it is essential to carefully select and configure the electrode materials within the device structure. The research objective of this study was investigate the use of different electrode materials to optimize the energy conversion efficiency of ZnO nanowalls and BaTiO<sub>3</sub> nanowires in piezoelectric applications. These materials were integrated into a sandwich-like structure with the piezoelectric layer to maximize power output under mechanical stress. The piezoelectric response was measured using key metrics such as output voltage, current density, and power density. The results show that the careful selection and arrangement of electrode materials can significantly improve electrical power generation, emphasizing the importance of electrode design in improving overall device performance. This research contributes to the development of more efficient, self-powered nanodevices, which can be applied in wearable electronics.

#### (ICACC-PA002-2025) Beyond Earth for Earth: Innovating Sensors with 3D-Printed Lunar Regolith Composites

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In-space manufacturing, while recognized for its microgravity advantages, presents broader technological possibilities by exploiting in-situ resource utilization (ISRU). We explore this sustainable avenue to develop 3D-printed lunar regolith composite sensors by investigating manufacturing processes and compositions with the goal of achieving enhanced Raman or Luminescence sensitivity in response to external stimuli. Experiments quantifying the relationship between spectral emissions and various volume fractions of regolith simulants, manufactured using additive approaches are \*Denotes Presenter **49th International Conference 8**  presented. The findings offer a pathway to the use of in-situ lunar resources for the design of functional materials, while advancing sensor technology for terrestrial applications. The outcomes are aimed at reducing the impact of payload and launch resources while protecting assets deployed beyond Earth as well as for Earth.

#### (ICACC-PA003-2025) Closing the loop in recycling: Car2Car

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The poster will present the research and development project "Car2Car," funded by the German Federal Ministry for Economic Affairs and Climate Action (BMWK). The goals of climate protection and the risks associated with global supply chains for raw materials pose particular challenges for the automotive industry. To address these challenges, experts from the automotive, scientific, and recycling sectors are collaborating on sustainable recycling concepts for key material groups in the automotive industry, including steel, aluminum, glass, plastics, and copper. The consortium is evaluating solutions for automated disassembly and improved separation and processing of high-quality, type-pure secondary resources. The poster will focus on the meltability and quality of crucible-melted glasses made from various streams of post-consumer cullet.

### (ICACC-PA004-2025) Recycling and circular economy with clay waste: trends and challenges

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Clays and clay minerals, known as marginal wastes in road construction, present an interesting opportunity for low-cost geothermal pavements due to their properties such as thermal conductivity, heat absorption, and mineral adsorption. This work compiles the results of numerous publications that describe a wide range of mechanisms for encapsulating inorganic and organic functional guests between the layers of clay minerals. Processes like acid activation, inorganic cation exchange, intercalation, and pillarization aim to establish new applications for clay-based materials, paving the way to a nanometric world that enables the synthesis of new materials and applications.

# (ICACC-PA005-2025) Vibrational spectroscopies of modified ytterbium di-silicate environmental barrier coatings reacted with a Ca-Mg-Al-Silicate melt

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This work reports the vibrational spectroscopic properties of Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> (YbDS) environmental barrier coatings (EBCs), when reacted with low concentrations of calcium-magnesium-aluminosilicates (CMAS). Raman and Fourier Transform Infrared Spectroscopies were conducted through the cross-sections of these plasma-sprayed EBCs, which had been reacted with CMAS on the surface at 1315 °C for 1 hour. The modified YbDS coating compositions include 98YbDS-1Al<sub>2</sub>O<sub>3</sub>-1TiO<sub>2</sub>, 98.61YbDS-1.39Mullite-2.33YAG, 98.61YbDS-1.39 Mullite, 94 YbDS-6 Al2O3, 98YbDS-2Al2O3, and 99YbDS-1Al<sub>2</sub>O<sub>3</sub>. The concentration of CMAS reacted on the surface of the YbDS coatings were 0 to 10 mg/cm<sup>2</sup>. This builds upon previous structural and elemental characterization of the same EBCs reacted with CMAS, including X-ray diffraction, simultaneous thermal analysis, electron-probe microanalysis, electron microscopy, and nanoindentation. The EBCs reacted with CMAS did not show changes in molecular vibrations in the YbDS chemical bonds, although additional phases were detected, and were shown to have an increased hardness and larger Young's modulus. These findingsshow that solubilization of Ca<sup>2+,</sup> Mg<sup>2+,</sup> Al<sup>3+</sup>, or Si<sup>4+</sup> ions into the YbDS crystal lattice have no significant effect on the coating's local range order indicating that YbDS maintains good phase stability when exposed to low concentrations of CMAS.

#### (ICACC-PA006-2025) High Purity Lanthanum and Yttrium-Based Materials Analysis by Astrum ES Glow Discharge Mass Spectrometry

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High purity lanthanum and yttrium-based materials are important materials and additives to emerging and high-tech industries, including solar energy, optoelectronics, lithium batteries, and biomedicine. Direct analysis of these materials by glow discharge mass spectrometry (GDMS) provides consistent, reproducible, low detection limits, while avoiding the complexities and contamination introduced by wet chemistry. The Astrum ES is a forward-geometry, cryo-cooled, low pressure direct current GD source, magnetic sector instrument. Analysis of nonconductive materials pose a challenge to analysis by GDMS. Since the sample acts as the cathode, it needs to be conductive. The solution to that is utilizing conductive holding electrodes, often composed of high purity tantalum. It supports the plasma and assists sputtering the material being analyzed. It is imperative to ensure that this difference in sputtering mechanism and bond strength (as compared to conductive metals) provides repeatable and reproducible data. In this study we analysed high purity lanthanum and yttrium-based reference samples across multiple days and analysts on the Astrum ES. Utilizing certified and consensus values, we are able to monitor multiple different impurities present in these materials and calculate the statistics to demonstrate the Astrum ES repeatability and reproducibility analyzing these materials.

### (ICACC-PA007-2025) Investigating Durability of 8YSZ via Wear and Erosion Testing for Lunar Applications

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As the number of missions to land on the Moon with and without crew continues to increase, there are a plethora of factors to consider that could affect aerospace structures. Lunar dust, or lunar regolith, composed of small rock fragments, glass beads, and minerals, is formed by years of meteorite impacts. Lunar dust is quite corrosive, abrasive, reactive and adhesive, necessitating effective mitigation strategies. Ceramics have emerged as a promising material selection in the aerospace industry for structural protection due to their high strength, excellent thermal properties, and resistance to degradation. Among these ceramics, zirconia (ZrO<sub>2</sub>) is a promising material, exhibiting exceptional mechanical and thermal properties. This study evaluates the resilience of an 8-wt% yttria-stabilized zirconia (8YSZ) ceramic coating, tested against wear and erosion, to characterize its degradation over time.

#### (ICACC-PA008-2025) Thermomechanical Properties of Rare Earth Phosphates as Environmental Barrier Coatings

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Rare earth phosphates have been shown as promising materials for environmental barrier coatings (EBCs) to protect SiC-based ceramic matrix composites (CMCs) from extreme and harsh environments. Thermomechanical properties of single component and multicomponent rare earth phosphates have been studied using high throughput density functional theory (DFT) calculations. DFT computations were done with the Vienna Ab Initio Simulation Package (VASP) which has been incorporated within the AFLOW computational materials design framework. AFLOW elastic and Gibbs Library (AEL & AGL) were used for mechanical and thermal property calculations, respectively. More accurate results for the thermal properties were obtained using the Quasi Harmonic Approximation module (AFLOW-QHA). Multicomponent rare earth phosphates showed enhanced properties as they give lower thermal conductivity than those of single component phosphates, and coefficient of thermal expansion values close to that of the SiC-based CMCs. High entropy rare earth phosphates could therefore be used as a means for rapid design of EBCs.

#### (ICACC-PA009-2025) Optimizing Steam Jet Parameters for Enhanced Environmental Barrier Coating (EBC) Performance Testing in High-Temperature, High-Velocity Environments

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Ytterbium disilicate (Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>) has emerged as a key material for Environmental Barrier Coatings (EBCs) applied to silicon carbide (SiC) ceramic matrix composites (CMCs) for high-temperature turbine engine applications. These coatings protect the underlying SiC CMCs from degradation in environments reaching gas temperatures above 1414°C, where high-velocity steam, a byproduct of combustion, poses significant challenges. The interaction between Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> and steam at elevated temperatures leads to the formation of a porous ytterbium monosilicate (Yb<sub>2</sub>SiO<sub>5</sub>) surface layer and volatilized silicon-hydroxide (Si(OH)<sub>4</sub>), raising concerns about the long-term thermochemical stability of EBCs. To address these challenges, this research focuses on optimizing conditions for testing EBCs, with the goal of maximizing the uniformity and extent of the silica (SiO<sub>2</sub>) depleted area at the steam impingement site on EBC-coated SiC samples, increasing the affected surface area on tested samples by ~400% compared to current experimental setups. The study explores key parameters such as sample angle, standoff distance, capillary tube diameter, and steam mass flow rate, using computational models to guide experimental setups to achieve the improved results.

# (ICACC-PA010-2025) Synthesis Strategies for $BaCe_{0.7}Zr_{0.1}Yb_{0.1}O_{3.\delta}$ to Boost Ionic Conductivity in Solid Oxide Cell Electrolytes

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High-temperature proton-conducting ceramics can be used as electrolytes in protonic ceramic fuel cells, protonic ceramic electrolysis cells and membrane reactors. Among the others, BCZY-Yb perovskites have recently gained significant interest d. Particularly, mixed ion conductor BaCe0.7Zr0.1Y0.1Yb0.1O3-& (BCZY-Yb) is known to exhibit rapid transport of both proton and oxide ion vacancies providing enhanced ionic conductivity at relatively low temperatures (400-600°C) in comparison with other compositions. However, the synthesis of BCZY-Yb phase remains a significant challenge for the development of high density and higher conduction electrolytes. In this work different synthetic strategies have been considered to assess the viability of producing suitable BCZY-Yb electrolyte, and evaluate the impact of the production process on the microstructure and phase purity. The concurrent phase formation during solid-state reactive sintering and the use of low-energy ball milling method led to electrolytes with high porosity. Conversely, high-energy milling improved particle packing, though secondary phases at the grain boundaries persisted. The modified sol-gel synthesis has been confirmed as one of the most promising methods for producing pure, high-density electrolytes with superior conductivity properties

#### (ICACC-PA011-2025) Thickness Dependence of the Support Layer on Gas Diffusion Resistance, Electrode Performance, and Carbon Deposition in Electrode-Supported Cells

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The thickness of the Ni/YSZ support layer in electrode-supported solid oxide cells plays a crucial role in determining gas diffusion resistance, overall cell performance, and the susceptibility to carbon deposition. Thicker support layers can impede gas diffusion, potentially limiting the reactant supply to the active sites and increasing diffusion resistance. This reduction in reactant availability can negatively affect electrode performance, particularly under high current densities. On the other hand, thinner support layers may enhance gas transport but could lead to mechanical instability or inadequate support for the cell structure. In addition to affecting gas diffusion and performance, the thickness of the support layer can influence carbon deposition, especially when hydrocarbon-based fuels are used. This study investigates the effect of varying support layer thickness on gas diffusion resistance, electrode performance, and carbon deposition behavior, on the commercial cell of electrode-supported cell (Nexceris, Elcogen, and Ningbo) which is aiming to optimize the balance between efficient gas transport, and resistance to carbon deposition in electrode-supported solid oxide cells.

### (ICACC-PA012-2025) Design and processing of glass-ceramic sealants for protonic ceramic electrolysis cell SRU assembly

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In protonic ceramic electrolysis cells (PCECs), a proton-conductive ceramic electrolyte provides high conductivity at lower temperatures (400-600°C), reducing material degradation. Additionally, PCECs produce pure hydrogen at the oxygen electrode, lowering production costs. Reliable sealants are essential for scaling up commercial stacks to ensure both electrical separation and gas tightness. Glass-based materials, combined with additive manufacturing techniques such as robocasting, enhance sealant performance through uniform deposition. This study assesses the chemical and thermo-mechanical compatibility of various glass-based systems with a PCEC half-cell composed of BaZr0.7Ce0.2Y0.1O3-8 (BCZY721)/NiO-BCZY721 and ferritic stainless steel (AISI441) interconnects in dry and humidified air. Post-mortem characterizations using FESEM and XRD are presented. Furthermore, a strategy for assembling a single repeating unit (SRU) with a complete cell consisting of Ba0.5Sr0.5Co0.8Fe0.2O3-& (BSCF)-BCZY721/ BZCY622/NiO-BZCY622 and robocasted glass sealant is explored. Finally, the assembled SRU undergoes electrochemical testing to evaluate the impact of each component on overall performance

### (ICACC-PA013-2025) High temperature gas sealing properties of sericite-based self-expansion compression seals

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Both SOFC and SOEC require reliable gas seals that are durable at high temperatures and stable in hydrogen gas. Glass seals generally show high gas-sealing properties at high temperatures. Still, they are prone to cracks or delamination under continuous vibration or rapid thermal cycling. The development of advanced glass-free gas seals for high-start/stop working systems and vehicles is a promising area of research. Our work on self-expansion compression seals, which do not require high pressure and flatness of adjacent materials to prevent gas leakage, could have significant applications in high-temperature gas sealing for SOFC and SOEC. The self-expansion seals fill gaps at the interface by expanding during the heating and would improve tightness between the seals and the adjacent materials. We currently focus on sericite instead of vermiculite. Sericite is a clay material with a layered structure and low contents of transition metals. Its irreversible and anisotropic expansion during heating makes it suitable for target sealing materials. However, low mechanical strength was clarified as an unavoidable issue. The addition of appropriate alkali metal much improved the strength owing to the formation of nepheline in sericite. Evaluation of various sealing properties for the alkali-containing sericite materials revealed that the addition improved mechanical strength and gas sealing.

### (ICACC-PA014-2025) Effects of ${\rm CeO_2}$ nano-dispersion in LSM cathode on SOFC electrode properties

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Co-sintering cells or stacks would succeed in advanced compact SOFC or SOECs, which show high power density or hydrogen evolution per volume. Cathode materials generally have some drawbacks in terms of co-sintering because of relatively low heat resistance. High-temperature heating of the cathode materials quickly brings about decompositions or undesired reactions with other cell components. (La, Sr)MnO<sub>3</sub> (LSM) would be a candidate for the cathode material of co-sintered cells or stacks, but it shows low cathodic performances because of the low oxygen diffusion coefficient. We then prepared CeO<sub>2</sub> nanoparticle dispersed LSM to improve oxygen diffusion. The nanoparticle dispersion state was evaluated using the analysis of FE-SEM images, and it was dramatically changed by sintering profiles. The sintering profiles that were investigated from the viewpoint of the sinterability difference between LSM and CeO<sub>2</sub> resulted in adequate CeO<sub>2</sub>-disperse LSM, which showed the nanoparticles located in the vicinity of LSM grain boundaries. The oxygen diffusion coefficient was estimated using the electrical conductivity relaxation method. The dispersion states also changed the coefficients, and adequate dispersion significantly improved oxygen diffusion.

### (ICACC-PA015-2025) Electrophoretic deposition of MnCu based coating for reversible SOCs

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The electrophoretic deposition is a viable and effective method for depositing homogeneous ceramic coatings even on complex shapes of metallic interconnects. In this work, a spinel based on manganese and copper has been used. A design of experiments (DoE) approach was initially performed to analyse the deposition parameters (i. e. applied voltage and deposition time), followed by microstructural and thermomechanical studies to investigate the sintering and the compatibility of the coating with the 441 stainless steel substrate. Innovative sintering processes, such as the rapid thermal annealing, will be also discussed, together with the electrical characterization on the most promising coated samples. The latest results achieved in the framework of the 24/7 ZEN project, GA 101101418 co-funded by EU and Clean Hydrogen Partnership will also show the electrophoretic deposition technique as a possible strategy to obtain multi-layered protective high-quality coatings, with high reliability and scalability, whilst improving their microstructures, electrical properties and the Cr retention capability in a reversible solid oxide mode.

## (ICACC-PA016-2025) Super-theoretical capacity of cobalt oxides in lithium-ion batteries

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The rapid decline in the electrochemical performance of metal oxide-based electrodes poses a significant challenge for their commercial application in lithium-ion batteries. Therefore, developing metal oxide-based materials with enhanced lithium storage capabilities is of utmost importance. In this study, we demonstrate a facile hydrothermal method for synthesizing cobalt oxides, followed by high-temperature calcination. Fluoroethylene carbonate and vinylene carbonate were employed as additives (as low as 2 wt.%) to achieve optimal electrochemical performance. After 400 cycles at 0.5 C, the cobalt oxide anodes exhibited a significantly increased capacity, reaching a so-called super theoretical capacity of 1427 mAh g<sup>-1</sup>, compared to an initial capacity of 925 mAh g<sup>-1</sup>. This facile synthesis method, combined with the optimized electrolyte, presents a viable approach for developing improved cobalt oxide materials for lithium-ion batteries.

#### (ICACC-PA017-2025) Influence of Air Storage on Surface Changes in Stoichiometric and Li-Rich NMC811

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Lithium Nickel Manganese Cobalt Oxides (NMC) have gained significant attention due to their high energy density, performance, and long cycle life. Among the various synthesis methods, co-precipitation is favored for NMC cathode production because of its precise control over particle size and uniformity. A key challenge in synthesizing Ni-rich NMC is minimizing Li/Ni cation mixing, which affects the crystal structure. Excess lithium is often used to reduce this mixing, but unreacted lithium forms impurities on the NMC surface, impacting electrochemical performance. Our research examines the effect of excess lithium on NMC811, focusing on structural parameters, morphology, and performance before and after washing away lithium residues. While washing can resolve issues like electrolyte degradation, excessive washing risks altering the cathode's properties, including leaching of active ions. We aim to balance lithium removal with maintaining stability and performance. We investigate the effects of calendar aging on washed and unwashed samples, exploring how LiOH and Li2CO3 influence structural and electrochemical behavior. Our study provides insights into optimizing both washing and storage strategies for Ni-rich NMC materials. This work is supported by the "Excellence Initiative - Research University (2020-2026)" at the University of Warsaw (grant IDUB I.3.4, POB1: Science for the Planet).

#### (ICACC-PA019-2025) Functionalized Carbon Coating for High-Performance Pure Silicon Anode in Lithium-Ion Capacitors

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Lithium-ion capacitors (LICs) offer the potential for high power and energy density but face challenges due to kinetic mismatches between the electrodes. Here, we address this issue by developing a high-capacity pure silicon (Si) anode for LICs. However, Si suffers from rapid capacity fading and increased internal resistance during cycling. To overcome this, we introduce functionalized herringbonetype carbon nanofibers as a protective coating for the Si anode. The functional groups on the coating interact with the Si surface and binder, promoting stable electrode contact. Additionally, the conductive layer facilitates uniform Li-ion and electron transport, aiding in the formation of a stable solid electrolyte interphase (SEI) layer. We investigate the effect of this strategy on pure Si electrodes through surface morphology analysis, chemical interaction assessment, and electrochemical testing. This novel approach has the potential to significantly improve the power and energy density of LICs by overcoming the degradation issues associated with Si anodes.

### (ICACC-PA020-2025) $\rm MSnF_4$ (M=Pb, Ba)-based solid electrolytes for room temperature applications

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Recently, fluoride ion (F<sup>-</sup>) conducting ceramics attract attention as solid electrolytes to be used in the electrochemical devices, such as the room temperature-operating fluoride batteries. In the present study,  $F^{-}$  conducting behavior in MSnF<sub>4</sub> (M = Pb, Ba) with the fluorite-type-related structure prepared via mechanical milling process was investigated in order to think of a strategy for the development of fast ion conductors. A pellet was prepared by employing a mechanical milling (MM) process using  $MF_2$  (M = Pb, Ba) and  $SnF_2$ powders, followed by the post-annealing. These electrical conductivities were evaluated by an impedance method. We succeeded in obtaining the highest conductive BaSnF<sub>4</sub>. In addition, ion conducting behavior of the well-known highest F<sup>-</sup> conductor: PbSnF<sub>4</sub> was reinvestigated. We found that the low-temperature annealing was effective to enhance its conductivity. In a closer look at the XRD patterns, the relative intensity for the reflection peak of 00l planes seems to be related to its conductivity. The conductivity increases with decrease in the ratio of the peak intensity of 00l planes to that of the main peak. The reason for this needs to be clarified in the near future by using the detailed crystal structure refinement. Acknowledgement: This work was supported by a project, JPNP21006, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

#### (ICACC-PA022-2025) Sintering Enhancement of Garnet Electrolytes for All-Solid-State Li-Ion Batteries

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Garnet-type ceramic electrolytes, such as  $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$  (LLZTO), are among the most popular Li-ion conductors for highsafety solid-state Li-ion or Li-metal batteries. Nevertheless, the densification of garnet-type ceramic electrolytes to achieve good ionic conductivity is challenging. High-temperature and lengthy sintering can be used to fabricate densified structures, whereas these strict densification conditions cause loss of Li mass from the electrolyte, thereby decreasing the ionic conductivity. Herein, we used liquid metallic Ga as a sintering aid to promote LLZTO densification at comparably low temperatures (1050 °C) over short times (3 h). The densification mechanisms in the presence of liquid metallic Ga were studied and discussed, and the electrochemical performances of the electrolyte and constructed Li-ion batteries were evaluated.

### (ICACC-PA023-2025) Polymer brush applications in lithium-ion battery electrodes

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Silicon is widely recognized as one of the most promising anode materials for lithium-ion batteries due to its large theoretical capacity. However, Si material is often associated with significant volume changes and low intrinsic electrical conductivity during the lithiation/delithiation process, which ultimately results in the pulverization of active mass particles and permanent capacity fading, hindering its practical use in lithium-ion batteries. In this study, we develop a novel approach where Si nanoparticles grafted with polymer brushes are used as electrode-active material. Specifically, the Si nanoparticles are grafted with poly(methacrylic acid) brushes. The polymer brush anode demonstrates superior electrochemical performance, including a high charge capacity of 2366 mAh g<sup>-1</sup> at 0.1 C, along with improved C-rate and cycle-life performance. Compared to conventional Si anodes using styrene-butadiene rubber/carboxymethyl cellulose (SBR/CMC) binder, the Si@polymer brush composite electrodes exhibit enhanced battery performance. These findings deepen our understanding of the impact of polymer brush electrodes on battery performance, providing valuable insights for further optimization in battery design.

#### (ICACC-PA024-2025) Building a Composite Cathode for Sulfidic Solid State Na-Ion Batteries via Infiltration Method

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While lithium-ion batteries are currently widely used, sodium systems are emerging as an alternative due to their greater availability, lower cost, and improved safety. In particular, na-solid-state sodium batteries (Na-SSB) are gaining attention for their higher energy density and enhanced safety. However, there are still many challenges to overcome in order to achieve cycle-stable Na-SSB. A well-designed composite cathode (CC) consisting of solid electrolyte (SE), cathode active material (CAM), and conductive additive (CA) is essential for a cycle-stable Na-SSB. To produce a well-designed CC, the main requirement is to have a balanced ratio of CAM, SE, and CA, to ensure the optimized electronic and ionic conduction pathways. Therefore, our objective is to use the sacrificial fugitives methodology, which is well known in ceramic processes but has never been reported for developing sulfidic SSB battery electrodes, to build the CC. For this purpose, a porous composite cathode scaffold (CCS) of NaCrO<sub>2</sub> in which a conductive matrix slurry is then (Na<sub>3</sub>PS<sub>4</sub>, and C65) infiltrated was manufactured with various sizes of Polymethyl-methacrylate (PMMA, Makevale) by applying a heat treatment. This study will present the investigated process parameters (PMMA size, thermal stability, and microstructural changes) to produce CCs.

### (ICACC-PA026-2025) Ion transport across grain boundaries in CeF $_3$ -based solid electrolytes

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Lithium-ion batteries are widely used for portable devices, electric vehicles, and renewable energy storage due to their high capacity of energy storage. However, to achieve higher energy density and to improve safety, all-solid-state batteries employing the ceramics electrolyte are needed. We are focusing on all-solid-state fluoride batteries in which the F<sup>-</sup> conductors are used as a solid electrolyte. Cerium fluoride, CeF<sub>3</sub> is a candidate for the F<sup>-</sup> conducting solid electrolyte. Although CeF<sub>3</sub> has higher chemical stability than other fluoride electrolyte candidates, one of the issues for practical use is to reduce the grain boundary resistance, since the grain boundary resistance of CeF<sub>3</sub> is quite high. In this study, sintered CeF<sub>3</sub>-based solid electrolytes were prepared at first, and then pulverized and pressed to obtain pressed compacts with different grain boundary resistance. We found that the hot press method was found to be effective in reducing grain boundary resistance. The ionic conductivity evaluated with the impedance method for the hot-pressed sample at 573 K under 174 MPa for 1 h was  $6.68 \times 10^{-5}$  S cm<sup>-1</sup> at room temperature, indicating that the grain boundary resistance was largely reduced compared to the 174 MPa-compacted and 573 K-fired sample. Acknowledgement: This work was supported by a project, JPNP21006, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

## (ICACC-PA027-2025) Development of superionic conductor glass ceramic with optimized crystallization temperature

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The increasing energy demand and the push to reduce fossil fuel use have created opportunities for new technologies to support the energy transition. Solid-state batteries (SSB) arise as an alternative, as they present a safer alternative to current Lithium-ion batteries, eliminating flammable risks. The glass-ceramics route presents itself as an advantageous route for ceramic processing, owing to a better possibility of microstructure control through different heat treatments. This work focuses on the synthesis of the glass-ceramics solid electrolyte Li<sub>1.5</sub>Al<sub>0.5</sub>Ge<sub>1.5</sub>(PO<sub>4</sub>)<sub>3</sub> (LAGP) and the study on how crystallization step affects its properties, with nucleation and crystal growth stages. The synthesis was carried out by calcination of the precursors at 700°C-2h and melting at 1250°C-30 min. Further, crystallization was achieved through a two-step heat treatment: nucleation at 513°C during 1, 2 and 3 hours (N1, N2, N3), and grain growth at 800°C, for 3 and 4 hours (C3, C4). Material characterization revealed high density and ionic conductivity, especially for the N3C4 condition, which achieved 95% of theoretical density, and 4.4x10<sup>-4</sup> Scm<sup>-1</sup> total ionic conductivity at room temperature (RT), with an activation energy of 0.37eV. These findings highlight the potential of optimizing crystallization for LAGP solid electrolytes, making them strong candidates for use in solid-state batteries.

#### (ICACC-PA028-2025) Effect of Zinc Oxide Artificial Layer on Interfacial Resistance of Garnet-Based Solid Electrolyte for Lithium Metal Anode

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Solid electrolytes, particularly garnet-type oxides like Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> (LLZO), are promising candidates for lithium metal batteries due to their high ionic conductivity ( $\sim 10^{-4}$  S cm<sup>-1</sup>) and exceptional chemical stability. These materials have the potential to overcome the limitations of conventional liquid electrolytes, offering higher energy density and longer lifespan. However, commercialization faces significant challenges, such as poor interfacial wettability with lithium metal anodes and high interfacial resistance. LLZO is prone to forming passivation layers like LiOH and Li<sub>2</sub>CO<sub>3</sub> when exposed to moisture, air, or lithium, which disrupts contact and increases interfacial resistance. To address these issues and make LLZO more suitable for use with lithium metal anodes, a ZnO artificial layer was introduced between the lithium anode and the solid electrolyte. This ZnO layer improves interfacial stability, reduces contact resistance, and enhances ionic conductivity, making LLZO more compatible with lithium metal anodes. These advancements represent crucial steps toward the commercialization of all-solid-state batteries.

## (ICACC-PA029-2025) Improving Lithium-Ion Conductivity in $\rm Li_7La_3Zr_2O_{12}$ via Molten Salt Synthesis for All Solid State Battery

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All Solid-state batteries are being recognized for their potential in next-generation energy storage systems due to their high energy density and safety. Among the solid electrolytes,  $Li_7La_3Zr_2O_{12}$ (LLZO), a cubic-phase garnet, is noted for its chemical stability. This study employed the molten salt synthesis (MSS) method to enhance lithium ion conductivity. Utilizing molten salt-based LiCl-KCl allowed the formation of the cubic phase at a lower temperature and in a shorter duration compared to traditional solid-phase synthesis methods. The pure cubic LLZO phase was achieved at temperatures between 900°C and 1000°C within a calcination process of less than 4 hr. The synthesized powder was pelletized and subjected to heat treatment at 900°C for 6 hr to increase its density. Electrochemical impedance spectroscopy (EIS) was used to measure Li<sup>+</sup> conductivity, resulting in small particles of 0.8 to 1.3 microns and an ion conductivity of  $2.398 \times 10^{-4}$  S cm<sup>-1</sup>. The MSS method with LiCl-KCl molten salt proves effective in synthesizing high-purity LLZO with minimal impurities.

## (ICACC-PA030-2025) Enhanced Photocatalytic Reaction of $(TiO_2\text{-}WO_3)$ on the $Sr_4Al_{14}O_{25}\text{:}Eu,$ Dy Long-Lasting Phosphor

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(TiO<sub>2</sub>-WO<sub>3</sub>)/Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu<sup>2+</sup>,Dy<sup>3+</sup> heterojunction photocatalysts were prepared by coating (TiO<sub>2</sub>-WO<sub>3</sub>) nanoparticles onto a Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub> phosphor substrate using a hydrothermal synthesis. The photocatalytic properties were investigated with respect to various ratios of  $TiO_2$  to WO<sub>3</sub> (10:0, 7:3, 5:5, 3:7, 0:10) and heat treatment temperatures ranging from 300 to 700°C. The photocatalytic response was analyzed through the photobleaching of methylene blue (MB) dye and the decomposition of toluene gas. In the hybrid photocatalyst of (TiO<sub>2</sub>-WO<sub>3</sub>) coated on Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu<sup>2+</sup>,Dy<sup>3+</sup> long-lasting phosphor, the phosphor might act as an internal light source to accelerate or sustain photocatalytic reactivity, even in the absence of external light irradiation. The heterojunction of (TiO<sub>2</sub>-WO<sub>3</sub>) and Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu<sup>2+</sup>,Dy<sup>3+</sup> reduced the energy band gap and enhanced visible light absorption, thereby improving photocatalytic reactivity. In particular, the 5:5 ratio of TiO<sub>2</sub> to WO<sub>3</sub> on Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu<sup>2+</sup>,Dy<sup>3+</sup> showed excellent photocatalytic performance, decomposing over 67% of toluene gas within 90 min under visible-light irradiation. The photocatalytic reactivity of (TiO<sub>2</sub>-WO<sub>3</sub>)/Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>:Eu<sup>2+</sup>,Dy<sup>3+</sup> surpassed those of  $TiO_2/Sr_4Al_{14}O_{25}:Eu^{2+},Dy^{3+}$  and  $WO_3/Sr_4Al_{14}O_{25}:Eu^{2+},Dy^{3+}$ , primarily due to the synergistic interaction between TiO<sub>2</sub> and WO<sub>3</sub>.

## (ICACC-PA031-2025) Investigation of 3D-printed structures with spinel oxide catalysts for biomass utilization

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Utilizations of renewable energies are becoming more important to mitigate climate changes. Biomass, one of renewable energies, can be converted to fuel gases containing hydrogen, carbon monoxide, and tar through gasification. We have studied recently that catalysts containing NiAl<sub>2</sub>O<sub>4</sub> (NAO) or NAO added with zirconia (NAZO) have a regenerative function by red-ox and high activity for tar reforming. Catalysts are generally processed by granulation, palletization, extrusion, and so on, whereas application of 3D-printing for processing catalysts has been attracting more attention recently. 3D-printed catalysts are expected to overcome a trade-off problem between a decrease of pressure drop and an increase of surface area of catalyst bed. An objective of our study is to optimize structures using 3D-printing to solve such a contradiction problem. Several types of lattice-structured monolith were fabricated, debinded, and calcined. To prepare the catalyst layer,  $\alpha$ -Al2O4 and NAO were coated in order on the 3D-printed lattice structured monolith. Catalyst activities were examined through reforming tar from biomass gasification as well as pressure drops of the catalyst bed. These results are expected to contribute to high performance and low cost on fabricating catalysts in efficient energy conversion systems.

#### (ICACC-PA032-2025) Green Chemistry in Materials Synthesis and Thermoelectric Device Engineering: A Comprehensive Strategy for TEGs Development

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In recent years, the demand for portable electronic devices has grown significantly. Ideally, these devices should be integrated into flexible substrates, such as textiles or paper, which can be easily incorporated into clothing. Wearable devices are used in various applications, including pressure sensors, photovoltaics, supercapacitors, and wearable power generators. Their main challenge is the need for a power source, typically batteries or supercapacitors, which require recharging. Thermoelectric materials can capture and convert thermal energy into electrical energy, enabling these devices to operate without needing batteries. The development of wearable, flexible thermoelectric generators (TEGs) has been an active area of research in recent years, combining ceramic-based thermoelectric generators with printed flexible thermoelectric devices. However, most of these TEGs have low flexibility or contain heavy and toxic metals, limiting their practical use. This work demonstrates how synthesizing nanomaterials through Green Chemistry methods enables the integration of thermoelectric nanomaterials into polymer matrices, formulated into inks for direct ink printing or additive manufacturing. Furthermore, the ability to produce p-type and n-type modules using these techniques allows for designing TEGs optimized for performance.

#### (ICACC-PA033-2025) Designing the Crystal Structure of Silicon Oxide Anodes to Enhance Their Phase Stability in Lithium-Ion Batteries

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Silicon oxide (SiOx) anodes are considered highly promising for lithium-ion batteries (LIBs) due to their exceptionally high capacity and durability. However, their widespread use is limited by substantial volume fluctuations during charge and discharge cycles, as well as inherent instability, which results in mechanical and interfacial degradation, along with irreversible lithium loss that reduces capacity retention over time. We propose a straightforward phase modification approach to enhance the stability of SiOx anodes. The introduction of alkali metal salt strengthens the material's structural integrity, leading to improved mechanical robustness and reduced lithium depletion. This modification significantly extends the anode's lifespan. By employing multi-scale simulations and experimental characterizations, we investigate how these structural changes stabilize the SiOx anode. The insights gained reveal the critical role of SiOx crystal structures in influencing degradation processes. This research offers a practical method for optimizing SiOx anodes, presenting a promising solution for enhancing the performance of high-energy-density LIBs in real-world applications.

#### (ICACC-PA034-2025) Mechanisms Governing the Influence of Solvation Structures on Amorphous Solid Electrolyte Interphase Formation in Aqueous Zinc-Ion Batteries

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Electrolyte additives have proven to be highly effective in controlling dendrite growth and minimizing parasitic reactions in aqueous zinc-ion batteries (AZIBs). However, the specific impact of these additives on the formation and properties of the solid-electrolyte interphase (SEI) remains unclear. In this research, we investigate the influence of alkali metal salt additives on the solvation structure and explore how these additives promote the reduction of anions. Our cryo-transmission electron microscopy studies reveal that the SEI primarily consists of an amorphous hybrid phase. This amorphous hybrid SEI exhibits exceptional stability, mechanical resilience, and high Zn2+ conductivity, effectively suppressing parasitic reactions and improving Zn plating/stripping reversibility. Even at high current densities, the Zn anode shows notable improvements in longevity and reversibility, operating for more than 6 months at 2 mA/cm2. Furthermore, the full-battery cell maintains excellent cycling stability, performing reliably over 4500 cycles at 10 A/g. This study advances our understanding of how solvation structure adjustments lead to the formation of a stable amorphous hybrid SEI and highlights their effectiveness in enhancing the lifespan of AZIBs.

# (ICACC-PA035-2025) Dual-Functional Pre-lithiation for Optimized High-Performance $SiO_x$ Anodes in Lithium-Ion Batteries

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SiO<sub>x</sub> anodes are regarded as the promising alternative to graphite anodes for lithium-ion batteries due to their superior cycling stability in high-capacity silicon-based family. However, the formation of irreversible Li<sub>x</sub>SiO<sub>y</sub> during the first lithiation results in a significantly low initial coulombic efficiency (ICE). Pre-lithiation, as an efficient and direct method, plays a crucial role in SiO<sub>x</sub> anodes. Herein, we employed a chemical pre-lithiation strategy to improve ICE, reducing the loss of active lithium. By simply treating the electrode with the pre-lithiation solvent, the SiO<sub>x</sub> anode achieved an ICE comparable to that of graphite. And more active silicon was reduced during the pre-lithiation process by tuning the functional groups of the pre-lithiation reagent, which further reinforced the high-capacity characteristics of the anode. Additionally, we applied this strategy to pouch cells with LiFePO<sub>4</sub> cathodes, and the optimized electrochemical performance demonstrated the effectiveness and scalability of this approach.

#### (ICACC-PA036-2025) Preparation of $ZrO_2$ -CeO<sub>2</sub> solid solution based defective oxide thin films by spray pyrolysis method for electrostriction

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Ce-Zr-based defective oxide materials are emerging as promising alternatives to lead-based piezoelectric materials due to their non-classical giant electrostriction properties and non-toxic nature. This study focuses on developing uniform and crack-free Ce-based defective oxide thin films using the Spray Pyrolysis technique. The research involved depositing Ce-Zr-O oxide thin films on Quartz and Sapphire substrates. Various cation ratios (1:3, 1:1, and 3:1) and precursor volumes (0.5, 1, 2, 5, 10, and 15 ml) were explored to optimize the film properties. SEM analysis revealed that increasing the precursor volume, particularly to 10 and 15 ml, significantly improved the uniformity of the thin films. This finding suggests that higher precursor volumes contribute to better film quality and consistency.

### (ICACC-PA037-2025) YSZ thin film growth via Pulsed Laser Deposition - a case study

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Yttria-stabilized zirconia (YSZ) is widely used in applications such as
solid oxide fuel cells (SOFCs) and high-temperature sensors due to
its excellent ionic conductivity and chemical stability. Pulsed Laser
Deposition (PLD) is established method for growing high-quality
YSZ thin films, however optimization of deposition parameters still
remains crucial for achieving desired morphology and properties.
In this study, we focus on optimizing process parameters—substrate
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temperature, laser fluence, oxygen pressure, and deposition rate for YSZ thin film growth. Thin films were deposited under various conditions, and their crystallinity, surface morphology, and ionic conductivity were analyzed using various techniques, i.e. X-ray diffraction (XRD), Raman Spectroscopy and impedance spectroscopy. Our results show that careful control of these parameters significantly impacts the microstructure and performance of YSZ films. We discuss the relationship between deposition conditions and film properties, providing insights into the mechanisms influencing YSZ film growth via PLD. This research has been supported by the National Science Centre (NCN) DAINA2 project 2020/38/L/ST8/00513.

# (ICACC-PA038-2025) Exploring kinetic kynamics in buffer layer formation for improved solar cell efficiency via chemical bath deposition

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Metal oxides and heterostructures play pivotal role in advancing modern technologies e.g., photovoltaics (PV). In particular, for Cu(In,Ga)Se<sub>2</sub>-based solar cells metal oxides/chalcogenides (e.g. Zn(O,S), In<sub>2</sub>S<sub>3</sub>, Zn<sub>(1-x)</sub>Sn<sub>x</sub>O, Zn<sub>(1-y)</sub>Mg<sub>y</sub>O, etc.) serve as a buffer layer and act as safer alternatives to toxic CdS buffer currently in use. Chemical bath deposition (CBD) allows an effective surface defect passivation, preventing the charge recombination in photovoltaic device. Therefore, this method is widely used for solar cells buffer layer fabrication. This work is focused on  $Zn_{(1-x)}(Sn/Mg)_xO$  materials and understanding the kinetics of thin film formation during CBD. In several studies the aforementioned buffers show an inhomogeneous composition of the film negatively affecting the final device, step-by-step investigation of film formation would help to unravel the growth mechanism. To address this, we use dynamic light scattering (DLS) to measure the size of the growing particles as a function of temperature. In addition, elemental analysis is performed to examine the distribution of elements within the film, ensuring compositional uniformity. This study will offer a better understanding of the buffer layer fabrication process to significantly improve the PV efficiency in the future.

#### (ICACC-PA039-2025) Effect of PDC-derived porous carbon on the electrocatalytic performance of spinel and perovskite oxides for enhanced OER activity

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Various oxides including spinel oxide and perovskite oxide, are progressively used as catalysts for oxygen evolution reactions. However, the subdued electronic conductivity of the oxides limits their electrocatalytic performance. Previously, conductive carbon have been used as the additive to enhance electrocatalytic performance of such oxides. In this work carbon obtained by the HF etching of preceramic polymer derived SiOC ceramics have been used as an additive for two different oxide systems binary NiFe<sub>2</sub>O<sub>4</sub>/CuWO<sub>4</sub> spinel heterostructure and La<sub>0.5</sub>Sr<sub>0.5</sub>Co<sub>0.8</sub>Cu<sub>0.2</sub>O<sub>3-8</sub> perovskite oxide. Detailed structural and microstructural characterization of the as-prepared composite is carried out using XRD, Raman, BET, XPS, FE-SEM, and HR-TEM. The electrocatalytic performance of the carbon-containing composite system was found to be superior to their corresponding pristine oxides, with reduced onsetpotential, overpotential, and Tafel slope. Higher mass activity and specific activity with prolonged stability were also observed upon adding the conductive carbon to the oxide system. The enhanced OER performance of the prepared catalysts can be attributed to turbostratic carbon that improves electronic conductivity and mesoporous microstructure that enables fast electron-electrolyte transport by exposing a more significant number of electrochemically active sites.

#### (ICACC-PA040-2025) Innovative Magnetite@Mesoporous Silica Core-Shell Nanostructures: A Promising Theranostic Material

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Nanoparticles have been engineered as biomedical materials for various purposes, including bio-imaging and drug delivery, a combination referred to as theranostics. Iron oxide is a material that has been extensively researched, mainly when the size of the primary particles is 20 nm or smaller, as they exhibit unique magnetic properties known as superparamagnetism (SPM), making them ideal for biomedical uses. In this study, we synthesized core-shell particles with a core composed of monodisperse SPM iron oxide nanoclusters (SPION-NCs) using a polyol method in conjunction with microwave-assisted synthesis, resulting in a more environmentally friendly product produced quickly and efficiently. The SPION-NCs were then coated with a thin layer of silica to shield them from the subsequent processes. Following this, a mesoporous silica layer was added using the atrane method, which employs silatrane as the silicon source and CTAB as the templating agent. The surfactant was removed through chemical exchange, creating a large surface area with mesopores of approximately 3 nm. Finally, the mesopores were loaded with methylene blue as a model drug molecule, and its release was studied in PBS. The potential applications of these particles in imaging, drug delivery, and other biomedical fields offer promising prospects for future research and practical applications.

#### (ICACC-PA041-2025) Enhancing the Structural Stability of Layered Lithium-Rich Manganese-Based Cathode Materials through Anionic and Cationic Co-Doping

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Layered lithium-rich manganese oxide (LMNO) is a promising cathode material due to its high energy density, low cost, and reliable safety. However, its commercialization is challenged by structural instability caused by lattice oxygen loss and transition metal (TM) migration. This study addresses these issues by co-doping LMNO with anions and cations to enhance its structural stability. Anion doping improves the redox activity and reversibility of lattice oxygen and stabilizes the TM-O bonds. Additionally, cation-O bonds have higher bonding energy compared to Mn-O bonds, which helps to prevent lattice oxygen release and enhances the initial coulombic efficiency of LMNO. Anion also forms stronger TM-anion bonds compared to TM-O bonds, further reducing lattice oxygen release and improving the material's performance. Meanwhile, electrochemically inert catiion supports the structure, preventing TM migration during charge/discharge and minimizing phase transitions, thus significantly enhancing cycling stability. The incorporation of anion and cation with larger ionic radius widens the layer spacing and boosts lithium ion diffusion efficiency, leading to better performance. In summary, this study demonstrates that anion-cation co-doping can effectively improve the structural stability and commercial viability of layered LMNO-based cathode materials.

#### (ICACC-PA042-2025) Smart Interlayer Construction for Improving NASICON-type Solid Electrolyte/Li Interface Compatibility in Solid-state Lithium Metal Batteries

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NASICON-type Li<sub>15</sub>Al<sub>05</sub>Ge<sub>15</sub>(PO)<sub>4</sub> (LAGP) based-Solid state lithium metal batteries (SSLMBs) have been recognized as a promising next generation battery due to the higher safety features and great potential for high energy density and rate capability. However, some of the challenges include the solid-solid interface and unstable interface electrochemical reaction between LAGP electrolyte and lithium anode, hindered the widespread application. Therefore, a hybrid artificial interlayer is proposed to modify the LAGP/Li interface based on the polymer ionic liquid. The introduction of the polymer ionic liquid enables the intimate interface contact, the continuous Li<sup>+</sup> conductive pathways and the homogenous Li+ flux distribution, resulting in the improved electrochemical performance and cycling lifespan. DFT calculations reveal the mechanism of hybrid interphase on inhibiting the formation of dendrite Li. Moreover, the polymeric ionic liquids also exhibit excellent mechanical properties and moisture resistance when used as the cathode binder. This research shows significant potential in the development of SSLMBs with high safety, high energy density and low cost.

#### (ICACC-PA043-2025) Influence of ZnO Nanowall Morphology on the Efficiency of Flexible Piezoelectric Nanogenerators

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Flexible piezoelectric nanogenerators, which convert mechanical energy into electrical energy, have become prominent among sustainable and renewable energy systems. The research highlights the advantageous properties of zinc oxide (ZnO), such as ease of production, environmental friendliness, and inherent self-polarization, making it an ideal candidate for lead-free piezoelectric systems. The research objective of this study was investigating the influence of ZnO nanowall morphology on energy harvesting efficiency in flexible systems. ZnO nanowalls were synthesized on flexible substrates under varying hydrothermal synthesis conditions. The structural and morphological properties of the ZnO nanowall arrays were characterized using XRD, SEM analysis. Their energy harvesting potential was analyzed with AFM semiconductor parameter analyzer. The results indicate that synthesis conditions significantly affect nanowall morphology, particularly the nanowall density and inter-nanowall voids. It was observed that when the inter-nanowall voids exceeded a critical value, the compressibility and polarizability of the nanowalls improved, leading to a nearly twofold increase in output voltage. This study highlights the importance of controlling synthesis conditions to optimize ZnO nanowall structures for enhanced energy harvesting in flexible piezoelectric nanogenerators.

#### (ICACC-PA044-2025) Surface and mechanical properties of co-sputtered Silica-Silver and Zirconia-Silver antimicrobial composite coatings: a characterization study

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The co-sputtering technique is a green and versatile method that enables the deposition of composite coatings on several substrates, including those sensitive to heat or chemicals. Composite coatings consisting of a silica or zirconia matrix embedding silver nanoclusters have shown exceptional antibacterial and antiviral properties, making them promising candidates for a wide range of applications, including air filtration systems where they have been applied to polymeric fibers. This study delves into the surface and mechanical characterization of these coatings to highlight their properties and assess their potential across multiple applications. The mechanical properties of the coatings were evaluated using nanoindentation and microhardness tests and AFM was employed in tapping, conductive, and magnetic modes to examine surface topography, while FESEM provided imaging of the coating morphology. Two different composite coatings—silica-silver and zirconia-silver—were studied, with deposition times of 30 and 60 minutes to determine the influence of deposition duration on the coatings' properties. By thoroughly characterizing these materials, this study provides a comprehensive understanding of their suitability for different applications offering a pathway to more effective and sustainable antimicrobial solutions.

#### (ICACC-PA045-2025) Fabrication of magnesium- and zirconium-added alumina nanofibrous ceramic via alternating field electrospinning

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A series of nanofibrous alumina (Al2O3)-based materials in the form of up to 10 mm thick sheets have been fabricated through a high-yield, free-surface alternating field electrospinning (AFES). Various alumina precursor compositions with Mg and Zr additives were tested to optimize spinnability, process productivity, and ceramic nanofiber mass yield after the calcination. SEM/EDS, FTIR, mechanical tests, thermal XRD, and TGA were used to characterize the as-spun and resulting nanofibrous Al2O3-based materials. The polymer carrier and alumina source are found to be determinative for the thermal processing protocol and the final ceramic nanofiber microstructure and surface morphology. With respect to additives, Mg has shown a high degree of interaction with Al, and MgAl2O4 is the dominant nanocrystalline phase at higher Mg concentrations after calcination at 1200 °C. On the contrary, ZrO2 is present as a separate tetragonal nanocrystalline phase at all tested compositions and calcination temperatures up to 1200 °C. The possible effect of boric acid stabilizer in alumina precursor on the crystallization behavior of Mg- and Zr-added Al2O3-based nanofibers and role of additives in the mechanical performance of these nanofibrous ceramic materials is discussed.

# (ICACC-PA047-2025) Investigating a simplified dip-coating technique for the development of $\rm C_f/hBN/SiC$ composites

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The present study systematically investigates a simplified dip-coating technique to introduce hBN interphase on carbon fibres for processing interfacial-engineered C<sub>f</sub>/SiC composites. Boric acid and urea are used as organic precursors for forming hBN to replace the conventional but complex chemical vapor deposition method for interphase deposition. Precursors ratios, dipping duration and cycles, heating temperature and atmosphere are investigated for optimising the dip-coating technique. FTIR analysis of coated fibres confirms the successful formation of B-N bonds in nitrogen atmosphere. XRD analysis of fibre bundles coated with 1:3 ratio of BN precursor solution indicates hBN formation. The composite is processed via slurry impregnation of SiC matrix and spark plasma sintering. SEM-EDS analysis of the composites reveals SiC matrix throughout fibre bundles indicating efficient impregnation of SiC slurry. Among investigated fibres, T800-3K fibres are identified as effective for the preparation of integral and dense C<sub>f</sub>/SiC composite. The research focuses on the significance of processing strategy by highlighting challenges, offering valuable insights for further advancements while targeting the economical and sustainable development of fibre-reinforced SiC composites for high-temperature structural applications.

#### (ICACC-PA048-2025) Usage of 3D Optical Microscopy for Understanding Defects in Composites

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Composites are an important class of materials for various defense and civilian applications. It is vital to understand the microstructure and physical properties of composites. Defects play a critical role in determining mechanical and physical properties of the composites. Novel non-destructive methods should be developed for understanding defects in composites. In this poster, we will present detailed analysis regarding the usage of 3D optical microscopy for evaluating different types of defects in advanced composite structures.

#### (ICACC-PA049-2025) Fabrication and Laser-Assisted Machining (LAM) of Fused Silica-Based Ceramic Composites Reinforced with Nanoparticles

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The fabrication and laser-assisted machining (LAM) of nanoparticle-reinforced fused silica-based ceramic composites represent a key advancement in producing high-precision components for defense and industrial applications. This study investigates the effects of ND:YAG laser parameters on machinability and surface integrity. Nanoparticles are homogeneously dispersed in the fused silica matrix, and the composite is fabricated using the gel casting process, followed by sintering. After fabrication using the gelcasting process, during the laser assisted machining, a high-power Nd:YAG laser preheats the ceramic composite, optimizing cutting conditions to improve material removal and minimize sub-surface damage. The continuous-wave laser heats the workpiece, which is then machined using a polycrystalline diamond cutting tool. Parameters like laser power, feed, depth of cut, and speed are analyzed for their impact on machinability. SEM and TEM reveal that laser assisted machining (LAM) significantly enhances machinability, reduces tool wear, and improves surface finish. Preheating reduces brittleness, enabling smoother cuts, while laser assistance mitigates issues like microcracking. This study advances LAM techniques for nanoparticle-reinforced composites, offering a reliable method for high-precision components with superior surface integrity.

#### (ICACC-PA050-2025) Preparation and characterization of lightweight SiC frameworks by connecting SiC fibers with SiC joints

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The increasing energy challenges and the rapidly developing astronautic technology require thermal insulators with low density and thermal conductivity, high-temperature thermal, chemical and mechanical stabilities. Herein, highly porous SiC frameworks were fabricated through procedures of assembling SiC fibers and formation of SiC joints by carbothermal reduction, which were named as SiC-bonded SiC fiber (SBSF) composites. The porosities were controlled in the range of 76-93% by varying aspect ratios of the SiC fibers. The SBSF composites exhibited outstanding corrosion resistance, oxidation resistance, and high-temperature thermal stability, as the inherent advantages of SiC ceramics. High strength and reversible compressibility were obtained in the out-of-plane compression load tests, and low thermal conductivity of 0.036-0.102 W/mK at 25-800 °C was achieved. The results of this study suggest that the SBSF composites are a good candidate for high temperature thermal insulators.

# (ICACC-PA051-2025) Processing of Nb/Ta-Al\_2O\_3 composites by FAST/SPS and investigation of 3D-microstructure

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Field-assisted sintering technology (FAST), also known as spark plasma sintering (SPS), offers rapid heating and cooling rates for pressure-assisted densification within short processing times. This method has been explored for the ability to produce conductive composites, applicable for high temperature applications, composed of fine- or coarse-grained alumina and the refractory metal niobium or tantalum. It is intended to create a conductive network with a minimum metal content. To elucidate, which structural characteristics are conducive to these networks and conductivity paths, this project employs X-ray based investigation methods like  $\mu$ CT. By adjusting the porosity of the composites in a targeted manner, the relationship between processing parameters, 3D-microstructure and the critical percolation threshold for conductive composites is investigated. Furthermore, the influence of raw materials and processing parameters on mechanical and electrical properties is discussed.

#### (ICACC-PA053-2025) Effect of Mg- Doping on the Structural, Dielectric and Impedance Properties of Lithium Titanate

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The objective of the investigation is to improve the dielectric and impedance properties of lithium titanate by doping with some ratios of magnesium.  $Li_{4-x}Mg_xTi_5O_{12}$  (LTO) with x= 0, x= 0.02, x= 0.04, and x=0.06 are synthesized by solid state method and labelled as  $M_1$ - $M_4$ . The prepared samples are characterized by XRD, SEM, and FTIR. Their diffraction peaks of the samples are sharp and strong. Their patterns are in good harmony with cubic spinel LTO. There are not the secondary peaks depending to MgO. The SEM images are shown the Ti and Mg are uniformly distributed in the samples. The dielectric and impedance research of the samples are carried out in the frequency range from 1 kHz to 1 MHz. Mg<sup>2+</sup>doping into Li sites can take place the reduction of Ti<sup>4+</sup> to Ti<sup>3+</sup> for the balance the change. As a result of this, Ti<sup>3+</sup>ions in LTO can conspicuously increase the electrical conductivity. Their impedance spectra are composed of one semicircle at higher frequencies followed by linear part at lower frequency end. As a result, Mg2+doping improves the dielectric and impedance performances of the samples.

# (ICACC-PA054-2025) The Effect of Groundnut Shel Addition on the Dielectric Properties of Lithium Titanate Ceramics

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Nowadays, the commercial value of waste materials such as peanut shells can be increased by utilizing them as additives in ceramic production. Therefore, the present study investigates the possibility of utilizing peanut shells as additives in the production of ceramic capacitors for electronics industry. (100- x) Lithium titanate (Li2TiO3)- (x) Peanut shell ash (GSA) (x= 0, 2, 4, 6 and 8) samples were prepared by conventional solid state reaction method. The obtained samples were characterized by XRD, SEM and FTIR spectroscopy. XRD pattern shows that the synthesized samples are crystalline. Lithium titanate and dolomite minerals can be seen in the SEM images of the doped GSA+ LTO samples. From the investigation, the greater the percentage of groundnut shell ash on LTO is shown the greater the value of the ac electrical conductivity of the samples. When adding the different percentages of groundnut shell ash to the LTO sample, the dielectric properties varies practically with respect to the LTO sample.

#### (ICACC-PA055-2025) Activation of volcanic ash as support for FeOx gliding arc plasma deposition and application in the catalytic oxidation

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This study reports the tailoring of volcanic ash (AV) to promote the subsequent anchoring of FeOx by glidarc plasma-assisted deposition and obtain a catalyst for the degradation of Rhodamine 6G in aqueous solution. The obtained materials were characterized by Fourier- Transform Infrared transmission spectroscopy (FTIR), X-ray diffraction (XRD), Thermogravimetric analyses, Energy Dispersive X-ray spectroscopy (EDX) and Nitrogen Physisorption. The acid activation of volcanic ash for 2h (AM-2) followed by gliding arc plasma assisted hydrolytic precipitation of iron dramatically increased by two orders of magnitude the total pore volume as well as the specific surface area. EDX analysis attested the incorporation of Fe within the activated volcanic ash framework. The analyses also show that iron oxides in the different materials are contained as Augite for supported material (AM-FeOx-30/0), sodium Diopside for supported and aged material (AM-FeOx-30/4), and Goethite for both materials. Catalytic activity of the different materials was evaluated for decolorization of Rhodamine 6G and revealed degradation degrees of 31, 95, 79, and 80% respectively for VA, AM-2, AM-FeOx-0/2 and AM-FeOx-30/4 in the optimum condition (t=20 min, pH=7, [catalyst]=3g/L, [Rh6G] = 25mg/L, 1mL of H<sub>2</sub>O<sub>2</sub> at 30%, run 1. Leaching tests confirmed stable catalytic activity

# (ICACC-PA056-2025) Development of carbon fibre-based continuous MAX-Phase fibres and corresponding coatings

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The demand for materials that can endure extreme temperatures and oxidative environments has exposed the limitations of current high-performance fibers, such as carbon and silicon carbide (SiC), in high temperature applications. These materials, while mechanically robust, degrade at temperatures exceeding 1400 °C due to oxidation. As aerospace, energy production, and hypersonic technologies advance, new, resilient fiber materials are critically needed. Within the ERS MAX-Fibre research project, continuous carbon fibres are initially coated with a Ti3SiC2 phase using a reactive coating process in order to create an integral oxidation protection layer on the carbon fibre and thus increase its resistance in oxidative atmospheres. In addition, the complete transformation of carbon fibres into MAX-phase continuous fibres is being investigated in a further step. These modified and transformed carbon fibres are suitable for demanding applications, including energy technologies in gas turbines, thermal protection systems, and high-temperature sensors for aerospace and electronic applications. This presentation will discuss the synthesis processes, material properties, and potential applications of these advanced fibers, highlighting their significant potential to enhance performance in high temperature environments and establish new standards in material science and engineering.

### (ICACC-PA057-2025) Turbostratic-Layering Disorder in MAX-Phases

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The presence of turbostratic disorder significantly influences the micromechanical and structural properties of bulk MAX-phase materials. Currently, the detection of turbostratic layering is limited to nanoscale sampling, where successful identification relies on obtaining a TEM Moiré pattern that coincidentally captures turbostratic disorder in the stacking of two layers. This disorder typically

resides within the bulk material, particularly at the interfaces of crystallographic domains where adjacent crystallites are rotationally misaligned, as evidenced by the broadening of peaks in diffractograms. Bulk MAX-Phases show crystallographic complexity in their multi-phase structures and anisotropic particle size broadening, which is due to prevalent needle or lenticular grains. This, in addition to their unit-cell anisotropy, makes it challenging to take precise measurements of broadening variation. NbSe<sub>2</sub> is thus used as a proxy, with similar layered structure and symmetry (SG 194 P6<sub>3</sub>/mmc) and therefore presents an analogous challenge in accurate Rietveld refinement. This study characterizes the diffractogram features of NbSe<sub>2</sub> and maps them onto MAXTHAL and high-phase purity Ti<sub>2</sub>AlC bulk samples. If these diffractogram features were statistically quantifiable, it would provide a non-destructive bulk-sample method of identifying turbostratic disorder.

### (ICACC-PA058-2025) Current Progress in Manufacturing of MAX or MAB Powders (MoAlB or $Cr_2AlC$ )

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MAX or MAB phases have become important non-oxide systems for potential structural applications. Recently, 2D structures are also derived from these ceramics. In order to further accelerate the rapid commerciaization of the production process, it is pivotal to develop new pathways for synthesizing ceramics powders. In this poster presentation, we will review and present novel design paradigm for manufacturing MAX and MAB based powders.

### (ICACC-PA059-2025) Self-Assembly of Biomolecular Piezoelectric Crystals

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Recent researches on the piezoelectric properties of various biomolecule-based materials such as bones, tendons, cartilage, ligaments, hair, skin, cochlea have been reported, and their biocompatible and bioresorbable properties have attracted great interest because they have advantages for future biomedical applications. However, since such a biomolecule based piezoelectric materials has not yet been completely discovered, it exhibits lower performance than those of conventional piezoelectric materials. In addition, the difficulty of fabricating scalable unidirectionally polarized structures and utilization of toxic organic solvent has been a major impediment to the realization of a practical bio-implantable piezoelectric device. In this presentation, recent research results of biomolecule-based self-assembling piezoelectric materials will be introduced. Controlling the polarization and orientation of in piezoelectric peptide using self-assembly method will be discussed. In addition, the development of the piezoelectric nanogenerator based on piezoelectric biomolecules will be presented.

### (ICACC-PA060-2025) Near-infrared emission characteristics of rare-earth-doped transparent ceramic materials by solar pumping

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We pumped rare-earth-doped fluorapatite (FAP) having randomly oriented non-cubic crystal grains, by solar light and investigated their near-infrared emission characteristics. The emission spectrum for Yb:FAP showed that it emitted at the 1043 nm wavelength band, which was consistent with the fluorescence wavelength of Yb:FAP pumped by a laser diode. From this result, we have succeeded in obtaining near-infrared emitted light by solar pumping from rareearth-doped fluorapatite ceramic materials. In the presentation, we will describe the detail characteristics and report on our approach in other solar pumping medium.

## (ICACC-PA061-2025) Optimized Synthesis of Polycrystalline-Based $\rm XTa_2O_6~(X=Mg,\,Cu,\,Zn)$ Semiconductors

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Single crystal semiconductors such as high-purity Ge, TlBr, and CZT have good efficiency for gamma and x-ray detection which make them suitable for radiation detection applications. The main limitations of single crystal devices are that they are often difficult to fabricate, expensive, and require precise operating conditions for peak performance. This work aims to fabricate low cost, polycrystalline-based semiconductors that can operate at ambient conditions with robust gamma detection and the ability to discriminate between gamma and neutron sources. To achieve good detection efficiency, the ceramics must be dense, phase pure, and have a uniform microstructure. Tantalates with common formula XTa<sub>2</sub>O<sub>6</sub> (X=Mg, Cu, Zn) have been outlined for this investigation based on their high densities (r <5 g/cm<sup>3</sup>), high Zeff (<60), band gap  $\sim3$  eV, and high resistivity (~10^9  $\Omega$ -cm). The goal of this work is to optimize solid-state synthesis parameters to eliminate porosity and improve microstructural uniformity of the outlined compositions. The effects of different sintering times and starting particle size on bulk density and grain size will be investigated. Fabricated ceramics will be characterized via x-ray diffraction, Archimedes density, and scanning electron microscopy.

### (ICACC-PA062-2025) Doping effects on the PTCR properties of barium titanate-bismuth sodium titanate (BT-BNT)

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Barium titanate-bismuth sodium titanate (BT-BNT) is a suitable candidate for lead-free positive temperature coefficient of resistance (PTCR) ceramics. In this application, the Curie temperature T<sub>c</sub> plays an important role, as it defines the transformation temperature of the crystal lattice and thus the transition from ferroelectric to paraelectric properties, which determines the operating point of the PTCR ceramics. The BT-BNT solid solution was selected to enhance the application potential of pure BT by increasing its T<sub>c</sub> from 130°C. Further adjustments of the PTCR behavior can be achieved through the addition of different doping elements. Donors can increase the grain conductivity, which reduces the resistivity below T<sub>c</sub>. On the other hand, the addition of acceptors at the grain boundaries can increase the resistance value above T<sub>c</sub> producing a significantly change of resistivity slope at T<sub>c</sub>. This study aims to investigate the influence of extrinsic doping elements on the PTCR effect of BT-BNT, with a focus on doping at the B-site. The samples are characterized using various analytical techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), temperature-dependent resistivity measurements and impedance spectroscopy. These techniques are used to elucidate the correlation of microstructural properties with electrical properties.

#### (ICACC-PA063-2025) New method for the exact determination of the Curie temperature using temperature-dependent X-ray diffraction on the model system barium titanate

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Barium titanate is considered a model system for lead-free PTCR ceramics. The addition of suitable solid solutions such as BNT or BKT increases the Curie temperature ( $T_c$ ), which determines the transition from the ferroelectric to the paraelectric state in PTCR ceramics. The most common method to determine the  $T_c$  is to study the relative permittivity as a function of temperature. However, this

approach is limited by the first to second order phase transformation, which leads to a diffuse transition over a wide temperature range where often no clear maximum of permittivity can be found. In this study, we present an X-ray based method to determine the  $T_C$ for materials even when an order-independent phase transformation is present and compare it to the standard method using permittivity measurements. A special feature of the presented method is the mathematical determination of the Curie temperature on the basis of lattice parameters, which are determined by means of temperature-dependent X-ray diffraction. In addition to considering the characteristic range for the tetragonal-cubic transformation, only the two reflections 200 and 002 in the 2 $\theta$  angle range of 44-48° are taken into account, which reduces the measurement time by 91%. An alternative determination of the phase transformation using dilatometry rounds off the results presented.

### (ICACC-PA064-2025) Phase identity and microstructure-property relationships in BiFeO<sub>3</sub>-BaTiO<sub>3</sub> ceramics

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In the context of lead-free piezoelectric materials, the BiFeO<sub>3</sub>-BaTiO<sub>3</sub> (BF-BT) system has gained significant attention due to its high Curie temperature (> 580°C) and environmental compatibility. However, its piezoelectric performance, characterized by a modest d<sub>33</sub> coefficient, limits its applicability in high-performance devices. Recent research efforts have focused on optimizing these properties through doping strategies aimed at enhancing domain wall mobility and ferroelectric activity. In this work the effects of Bismuth Magnesium Titanate Bi  $(Mg_{1/2}Ti_{1/2})$  O<sub>3</sub> (BMT) doping will be explored specially emphasizing on the controversial identification of tetragonal phase and lack of recognition for core-shell microstructural features. The crystal structure phases will be refined with Rietveld refinement. Atomic percentage and microstructural data will be showed with EDX analysis. Temperature-dependent dielectric loss and dielectric constant and ferroelectric loops have been measured. We aim that BMT doping not only enhance the performance of dielectric and ferroelectric response but also stabilize their performance at elevated temperatures.

### (ICACC-PA065-2025) Creation of the RbI – $SrI_2$ phase diagram to facilitate scintillator scale-up

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Scintillators absorb ionizing radiation and emit visible light. This lends them to applications of high energy (6-9MeV) X-ray imaging for national security to detect nuclear materials. Current scintillators for this application have performance limitations. To improve x-ray image quality, there is active research into discovering scintillators with high light yield and low afterglow, among other properties. Recently discovered scintillators RbSrI<sub>3</sub>:Eu and RbSr<sub>2</sub>I<sub>5</sub>:Eu exhibit promising scintillation performance, for which phase formation has not been reported. However, this information is important for growing high-quality crystals. This work investigates the full compositional relationship between RbI and  $SrI_2$  by the creation of an experimental and computational composition-temperature phase diagram. Materials were melt-synthesized in 5mol% increments of SrI<sub>2</sub>. Phase formation behavior was characterized using Differential Scanning Calorimetry (DSC), X-ray powder diffraction (XRD), and high-temperature XRD. It was found that there were eutectic points at approximately  $x(SrI_2) = 0.30$ , 0.57 and 0.80, and no more than two compounds: the perovskite RbSrI<sub>3</sub> and RbSr<sub>2</sub>I<sub>5</sub>. These results were applied to subsequent experiments to support crystal growth scale-up using the vertical Bridgman method. The effects of off-stoichiometric growths of RbSrI<sub>3</sub> and translation rates of RbSr<sub>2</sub>I<sub>5</sub> were tested.

### (ICACC-PA066-2025) Empowering advanced photovoltaic (PV) pioneers: a bilateral Italy-USA project

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In order to unlock the vast potential of clean solar energy, we need disruptive technologies capable of efficiently harvesting light on a larger scale. Available commercial PV cannot cope sustainably with the scale of this challenge. Compared to Silicon PV, thin film PV based on CdTe and Cu(In,Ga)Se2 require less energy to produce, but some of their constituents are rare. Hence, short-term sustainability is dubious. Recently, microconcentrator (MC) PV has been conceived. It exploits tenths of absorber material and is based on sunlight absorbers requiring low energy to grow. Also, semi-transparent panels could be prepared as stripes having width of ~100µm. To demonstrate such advanced PV concepts at laboratory scale, researchers used optical projection lithography (OPL). However, OPL cannot be scaled to terawatt. Industrial uptake of MCPV is only possible through both high semiconductor quality, and high throughput at cost lower than current PVs. Inspired by the research of the US partner G. Friedman, DC patented a disrupting microfabrication technique that could be scaled economically to deploy terawatts of MCPV or semi-transparent PV, as pursued in REMAP project funded by the EIC. Our intent is to leverage our know-how to empower PV pioneers and establish a lasting cooperation in this new field. Herein, we outline the progress made on the formulation of metal oxide thin films for Cu(In,Ga)Se<sub>2</sub> PV.

### (ICACC-PA067-2025) Chemical bath deposition (CBD) of ZnMgO thin films for Cu(In,Ga)Se<sub>2</sub> photovoltaics (PV)

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Recently, Cu(In,Ga)Se, PV reached an outstanding 23.6% efficiency record. However, this device exploits a CdS layer prepared with CBD whose toxicity obstacles its commercialization and whose light absorption limits the efficiency. Since CBD is among the best techniques to maximize device efficiency, following other authors, we exploited it to prepare  $Zn_{(1-x)}Mg_xO$  buffer from a reported CBD of ZnO. However, thermodynamics limits the solubility of MgO into ZnO posing a synthetic challenge. Consequently, the role of different complexing agents, Mg sources and concentrations were investigated. Citric acid (CA) improved the MMZ ([Mg]/([Mg]+[Zn])) above all when MgSO<sub>4</sub> was used as Mg source instead of MgAc2\*4H2O. Similarly to other works, CA affects also the morphology, transparency and thickness of the films. The reaction mechanism is investigated through potentiometric titrations, speciations and dynamic light scattering to understand what limits the MMZ in the film at ~ 2% preventing the ideal MMZ range 10-25%. Interestingly, the surface contains up to 24% MMZ, suggesting a remarkable depth compositional gradient. In conclusion, a novel strategy to prepare CBD ZnMgO is proposed: Mg is mainly at the surface, providing insights about the reaction mechanism and synthetic improvements. CBD ZnMgO might positively affect not only chalcogenide PV but also other fields of optoelectronics and catalysis.

# (ICACC-PA068-2025) Solid state synthesis of Er-Yb co-doped MgNb $_2O_6$ ceramics and the exploration of their up-conversion photoluminescence and photocatalytic properties

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As phosphors, rare-earth (RE) doped ceramic materials have significant potential for applications in the photon domain, especially photoluminescence, and photocatalysis due to their charge carriers. This research explores the synthesis of RE-doped MgNb<sub>2</sub>O<sub>6</sub> and the characterization of their optical and photocatalytic properties. Three different compositions of the columbite: MgNb<sub>2</sub>O<sub>6</sub>, MgNb<sub>2</sub>O<sub>6</sub>-Er, and MgNb2O6-Er-Yb were synthesized, and their crystal structures were confirmed to be orthorhombic for all three compositions. Room temperature up-conversion photoluminescence spectra of the as-sintered RE-doped ceramic bodies showed two emissions at 553 nm and 669 nm corresponding to transitions of Er<sup>3+</sup> ions from  ${}^{2}\text{H}_{11/2}$  to  ${}^{4}\text{I}_{15/2}$  and  ${}^{4}\text{F}_{9/2}$  to  ${}^{4}\text{I}_{15/2}$ , respectively. From theoretical models in the literature, the emission intensity was confirmed to be proportional to the n<sup>th</sup> power of the excitation intensity. The up-conversion photoluminescence intensity was enhanced for the Er-Yb co-doped samples, possibly due to the charge transfer process between Yb<sup>3+</sup> and Er3+ ions. The photocatalysis under UV light and adsorption studies for the decolorization of Victoria blue dye were investigated and discussed based on the influence of up-conversion photoluminescence in the RE-doped MgNb<sub>2</sub>O<sub>6</sub> Columbite.

#### (ICACC-PA069-2025) Distorted Zn and Sn-based perovskite oxide nanomaterials for piezoelectric microenergy harvesting applications

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Distorted zinc- and tin-based perovskite oxide nanomaterials with distinct crystal structural, electrical, optical, and mechanical properties have shown significant promises for piezoelectric, piezo-photronic, and piezo-tronic microenergy harvesting applications. Among these, ZnTiO<sub>3</sub> and SnTiO<sub>3</sub> nanomaterials can be synthesized using chemical vapor deposition, sol-gel processes, and hydrothermal reactions, all of which provide control over the phase purity, particle size, morphology, and shapes of the nanocrystals. Their nanoscale sizes result in more surface area, active sites, and degree of effectiveness for noncentrosymmetric properties such as piezoelectricity. We present our recent research progress on the synthesis and properties exploration of novel LiNbO<sub>3</sub> (LN) -type ZnTiO<sub>3</sub> and perovskite-SnTiO<sub>3</sub> showing piezoelectric coefficients (d<sub>33</sub>≈ 59 pm/V and 25 pm/V respectively), high dielectric constants, and tuneable band gaps. The most optimized LN-ZnTiO<sub>3</sub> compositional nanocomposites with PDMS exhibited a maximum value at 20 wt% of  $V_{\rm oc}$  ~6.1 V and optimized  $SnTiO_3$  dimensional nanocomposite bulk exhibited  $V_{oc} \sim 2.6$  V at 17 N, 5 Hz, measured using a custom-built vibration energy harvesting set-up. Results also indicated their suitability for mechanical sensors (Sensitivity~66 mV/kPa for ZnTiO3 and 40 mV/kPa for SnTiO<sub>3</sub>) applications

# (ICACC-PA071-2025) Multiphased $\rm Al_2O_3\text{-}YAG$ fiber: influence of seeding material and thermal treatment

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Oxide ceramic matrix composites (O-CMC) are important strategic materials and among the different components, the fibers are required to display improved thermo-mechanical properties. To increase creep resistance at high temperatures, fiber composition or microstructure must be finely tuned. The addition of mullite, YAG or  $ZrO_2$  to  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> showed great results due to their ability to inhibit grain growth and provide their inherent creep resistance to the high-strength alumina. YAG is reported as the most creep-resistant oxide known, has a very good compatibility with alumina up to 1700 °C. One of the challenges of NGO fiber development is the understanding of heat treatment parameters (temperature, heating rate, dwell time,) to control the different mechanisms occurring during thermal treatments to obtained the desired ceramic nature (crystal phase) and microstructure (grain size, porosity). Al<sub>2</sub>O<sub>3</sub>-YAG fiber precursors were prepared by sol-gel method. The effects of Al<sub>2</sub>O<sub>3</sub> seeding and sintering parameters on thermal behavior and final properties (crystallization, grain size, densification) were investigated by structural (XRD, FTIR), microstructural (SEM), and thermal (TGA-DTA) analyses. A dense multiphased Al<sub>2</sub>O<sub>3</sub>-YAG fiber was obtained.

# (ICACC-PA073-2025) $La_{0.5}Sr_{0.5}Co_{0.2}Fe_{0.2}Ni_{0.2}Cu_{0.2}$ $A_{0.2}O_3$ (A=V,Al,Mg) Perovskites For Medium Temperature Solid Oxide Fuel Cells

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Energy consumption has been rising with technological and industrial advances, driving the need for clean, efficient, and sustainable energy sources. Ceramic-based solid oxide fuel cells (SOFCs) stand out for their high efficiency, fuel flexibility, and environmental benefits. However, operating at high temperatures (800°C-1000°C) reduces their lifespan, making it essential to lower these to 600°C-800°C. La0.7Sr0.3MnO3 (LSM) is noted for its high electronic conductivity and stability for oxygen reduction at 800°C-1000°C, though its performance decreases at lower temperatures. In recent years, high entropy oxides, particularly ABO3-type perovskites, have attracted attention for SOFCs due to unique dielectric, ferroelectric, and catalytic properties. Although these materials improve thermal stability, magnetic properties, and catalytic activity, their application in SOFCs remains limited. This study explores the potential of La0.5Sr0.5Co0.2Fe0.2Ni0.2Cu0.2A0.2O3 (A=V, Al, Mg) perovskites in medium-temperature SOFCs.

## (ICACC-PA074-2025) Study on Property Changes Induced by Slurry Filtration in CMP Process

J. Kwon<sup>\*1</sup>; T. Kim<sup>1</sup>

1. Sungkyunkwan University, Department of Semiconductor and Display Engineering, Republic of Korea

This study examines the effects of slurry filtration on removal rates during the Chemical Mechanical Polishing (CMP) process in semiconductor manufacturing, with a focus on slurry containing Ceria abrasive. Through controlled experiments, it was observed that as filtration time increases, the proportion of larger particles in the slurry decreases, leading to a significant reduction in material removal rates. While filtration is essential to prevent slurry agglomeration and surface defects, excessive filtration can negatively impact CMP performance by altering particle size distribution (PSD). To address this challenge, the study proposes strategies such as regular monitoring of slurry filtration levels, adjusting filtration frequency, and implementing adaptive control systems. These strategies aim to balance effective filtration with the maintenance of optimal removal rates, thereby improving process stability and overall CMP quality in mass production environments.

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#### (ICACC-PA075-2025) Development of Macroporous Alumina Foams Utilizing Cellulose-Based Expanded Green Microspheres as Pore Formers

- M. Jonsson\*<sup>2</sup>; F. Akhtar<sup>1</sup>; A. De<sup>1</sup>
- 1. Lulea University of Technology, Division of Materials Science, Sweden
- 2. Nouryon AB Goteborg, Sweden

This study optimizes the gel casting process to prepare highly porous and mechanically strong alumina foam using cellulose-based pre-expanded green microspheres as pore formers. While various pore-forming methods have been explored, many rely on toxic or fossil-based ingredients. Replacing polymer-based microspheres with cellulose-based alternatives not only enhances the sustainability of the process but also improves pore formation due to the high thermal stability of cellulose, resulting in more controlled and flawless pore development during calcination. Electron microscopy of the pre-sintered foams confirmed the presence of both open and closed porosity, which was tunable by adjusting the alumina-tomicrosphere ratio and microsphere size. Mass spectrometry combined with thermogravimetric analysis further confirmed that cellulose microspheres do not release harmful byproducts during sintering, unlike polymer microspheres. The optimized foams exhibited a high compressive strength (~5 MPa) and ~70% porosity, making them promising candidates for robust applications such as catalyst supports or filtration systems.

### (ICACC-PA076-2025) Direct and Indirect Microwave Heating of SnO\_2-ZnO ceramics

P. Simonova\*1; C. Petit2; C. Meunier2; F. Valdivieso2; W. Pabst1

- 1. Vysoka skola chemicko-technologicka v Praze, Department of Glass and Ceramics, Czechia
- 2. Ecole des Mines de Saint-Etienne, Laboratoire Georges Friedel, France

Microwave (MW-) sintering is a rapid sintering technique, where the material interacts directly with the electromagnetic radiation. This leads to volumetric heating, which enables high heating rates and a uniform temperature distribution in the sample. Materials based on SnO<sub>2</sub>, ZnO and Zn<sub>2</sub>SnO<sub>4</sub> are due to its unique properties used in various applications such as gas sensors, varistors, electrodes, photoelectric devices, and others. Therefore, the investigation of their processing is important. In this contribution we present results on MW-sintered SnO<sub>2</sub>-ZnO based ceramics prepared either by direct or indirect MW-heating (i.e. without or with SiC as a susceptor). The samples were prepared by uniaxial pressing from pure SnO<sub>2</sub> and ZnO powders and their mixtures. The as-pressed samples were sintered at 1200 °C (ZnO at 1000 °C) with heating rate of 50 °C/min and a dwell time of 5 min. It was possible to heat all the samples directly by MW-heating. In the case of pure SnO<sub>2</sub> the heating initiation was faster compared to pure ZnO but on the other hand it was difficult to keep the set heating rate (compared to ZnO). In the case of the composite the behavior was a combination of these two binary oxides. Different behavior was observed on the power vs temperature curves for direct and indirect MW-heating. It is shown that the presence of SiC enhances the densification and grain growth.

#### (ICACC-PA077-2025) Processing and Characterization of Carbon Dots - Phyllosilicate Composites

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- R. T. Candidato Jr.4
- 1. Universite de Limoges, France
- 2. ENSCI, France
- 3. Laboratoire SPCTS, Chemistry, France
- 4. MSU-Iligan Institute of Technology, Physics, Philippines

Phyllosilicates and carbon dots (CDs) represent two versatile classes of materials that, when combined, form composites with remarkable potential in biomedical applications. Phyllosilicates are renowned for their layered structure, high surface area, ion exchange capacity, and biocompatibility. Conversely, carbon dots are semiconductor nanocrystals known for their unique optical properties and photostability, making them excellent tools for imaging and sensing in biological systems. The key goal of this work is to effectively incorporate functionalized CDs within the phyllosilicate structure, leveraging the strengths of both materials. The resulting hybrid composites combine the structural and chemical advantages of phyllosilicates with the optical and electronic properties of CDs. Advanced characterization techniques, including TEM, XPS, FTIR, and Raman spectroscopy, were employed to investigate the incorporation mechanisms of both materials. Their potential applications in drug delivery, tissue engineering, bioimaging, and biosensing highlights the importance of continued research and development to fully exploit their capabilities in creating innovative, effective tools for biomedical imaging and diagnostics.

# (ICACC-PA078-2025) Densification kinetics analysis of ZnO densified by Spark Plasma Sintering and Cold Spark Plasma Sintering

- N. Albar\*1; T. Herisson de Beauvoir1; C. Maniere2; E. Sanchez1;
- G. Chevallier<sup>1</sup>; C. Estournes<sup>1</sup>; A. Weibel<sup>1</sup>
- 1. Centre Inter-Universitaire de Recerche, France
- 2. Laboratoire de Cristallographie et Sciences des Materiaux, France

The study of the sintering kinetic allows to determine the predominant mechanism of densification and/or grain growth. Thanks to this, we can imagine predicting a precise microstructure depending on the sintering parameters. A modelling approach permits to predict the sintering curve and grain growth in CSP. In this work we focused on the Master Sintering Curve combined with a regression method. Activation energy Q is dependant of sintering conditions. The MSC, first introduced by Su & Johnson and based on the dilatometric study, was yet never applied to Cold Sintering. Zinc Oxide (ZnO) is known from literature to be a material that can be densified by CSP at temperatures below 300 °C. This work focuses on the study of the sintering by Cold-SPS of ZnO powder, mixed with acetic acid solution (1M). The results were compared with samples densified by SPS from the same ZnO dry powder. While the mixture is fully densified by Cold -SPS below 300°C like for CSP, it is necessary to increase the temperature at least to 500°C by SPS on the dry powder. The apparent activation energy (Q) of the ZnO powder sintered by Cold-SPS (79 kJ/mol) is 4 times lower than that of the same dry powder densified by SPS (338 kJ/mol). The low value obtained by Cold-SPS confirms the low energy surface interactions between liquid and solid phases involved in the densification mechanisms of ZnO.

#### (ICACC-PA079-2025) Mass Transport in Low-Temperature Ceramic Sintering and Printing Assisted by Pressure and Water

#### F. Fei\*1; X. Song1

1. University of Iowa, USA

Ceramic processing through the combined use of pressure and water offers a promising approach to achieve accelerated mass transport between ceramic particles at reduced temperatures, providing a sustainable and low-temperature method for ceramic synthesis and three-dimensional (3D) printing. While previous studies have explored the roles of pressure and water in the fusion and densification of ceramic particles, the underlying mechanisms, especially for micro-sized ceramic particles, are still debated. This research aims to investigate a potential mechanism for the fusion and densification of micro-sized ceramic particles under the effect of pressure and water. Using a multi-phase level-set simulation model, our results suggest that stress-assisted fracture and dissolution of interparticle contact points can be key factors driving densification of micro-sized ceramic particles in the presence of pressure and water.

## (ICACC-PA080-2025) Synthesis of $\mathrm{B_4C}$ Powder via Sol-gel Approaches

O. Yucel\*1; M. Simmons4; N. Middleton2; C. Roberson5; R. Binner3

- 1. University of Birmingham, Metallurgy and Materials, United Kingdom
- 2. DSTL, United Kingdom
- 3. University of Birmingham, Ceramic Science and Engineering, United Kingdom
- 4. University of Birmingham, School of Chemical Engineering, United Kingdom
- 5. Novamat, United Kingdom

The pursuit of more advanced technologies is inspiring researchers to explore lighter, stronger, and more durable materials. Boron carbide (B4C) stands out as one of the hardest and lowest-density materials, with a high melting point, chemical inertness, and high neutron absorption cross-section. Thanks to these characteristics, it is widely used in the aerospace and defence industries. Carbothermal reduction synthesis is the prevailing method for the industrial production of B4C powder. Despite the affordability and abundance of precursor materials, the need for grinding the final product escalates energy consumption, and costs, whilst diminishing powder quality through the introduction of impurities. As an alternative to the conventional route, sol-gel approaches seem promising to pursue a high-quality powder goal with energy efficiency and future scalability. Choosing the right polymeric precursor is important to obtain the required properties from final powders. This work produced B4C powders without excess carbon and with different morphologies by changing the acid used. Three kinds of acids were chosen with different molecular weights; acetic acid (C2H4O2), tartaric acid (C4H6O6) and citric acid (C6H8O6) with maltodextrin used as the main polymer precursor. It is observed that the use of citric acid creates belt-like morphologies, whilst lower molecular weight acids produce equiaxed particles when used in equimolar amounts.

### Wednesday, January 29, 2025

### FS4 Ceramic/Carbon Reinforced Polymers

### FS 4: Ceramic/Carbon Reinforced Polymers I

Room: Coquina G Session Chair: Masahito Ueda, Nihon University

#### 8:30 AM

#### (ICACC-FS4001-2025) Classification of damage mode of CFRP by AE technique with considering response function of AE sensor (Invited)

T. Sakai<sup>\*1</sup>; T. Shiraishi<sup>2</sup>

- 1. Saitama University, Japan
- 2. Saitama-ken Sangyo Gijutsu Sogo Center, Japan

The damage modes of Carbon Fiber Reinforced Plastics (CFRP) include matrix cracking, interfacial debonding, delamination, and fiber breakage. To elucidate the fracture process of CFRP, it is important to accurately identify each damage mode occurring within the CFRP laminate. Acoustic Emission (AE) technology has used for identifying these damage modes. In this study, we measured the frequency characteristics of AE sensors and examined AE measurement data during tensile tests, considering these characteristics. Furthermore, we performed clustering using k-means++ on the tensile test and AE analysis results of specimens corresponding to each damage mode, correlating the damage modes with the analysis results. We propose a unified damage mode evaluation method that is independent of the sensor's frequency characteristics.

#### 9:00 AM

#### (ICACC-FS4002-2025) Characterization of damage progression in polymer matrix composites using in situ techniques and image processing (Invited)

S. Oshima\*1; S. Kobayashi2

- 1. Tokyo Metropolitan University, Department of Aeronautics and Astronautics, Japan
- 2. Tokyo Metropolitan University, Mechanical Engineering, Japan

Damage in composite materials sequentially or simultaneously occurs at different scales. In order to characterize damage progression in composite materials, various in situ techniques such as optical microscopy, scanning electron microscopy, and X-ray computed tomography have been used in recent years. In addition, quantification of damage progression is performed using image processing on digital images obtained by in situ techniques. In this study, some in situ and image processing techniques are presented to characterize mesoscopic damage progression in polymer matrix composites. We mainly focused on the damage and failure process during crack propagation. Intrinsic damage mechanisms were clarified during crack propagation of composite laminates with different types of specimens (cross-ply laminates, unidirectional laminates, and adhesively bonded joints) under both static and cyclic loading. In addition, the stress state around the fracture process zone was analyzed by numerical simulation and correlated with the experimental results.

#### 9:30 AM

## (ICACC-FS4003-2025) Composite high pressure vessel with ring-shaped axial load members for hydrogen fuel cell vehicle

J. Serizawa\*<sup>2</sup>; T. Ogasawara<sup>2</sup>; T. Yokozeki<sup>1</sup>

- 1. Tokyo Daigaku, Japan
- 2. Tokyo Noko Daigaku Koganei Campus, Japan

A tank module consisting of multiple small-diameter tanks is expected to improve the on-board flexibility of hydrogen storage tanks for fuel cell vehicles. However, simply mounting multiple tanks molded by the conventional filament winding (FW) method is difficult to put into practical use due to its disadvantages in terms of productivity, cost, and weight efficiency. This study proposes a novel tank structure based on the "multi-load path" concept, in which different members individually carry the axial and hoop loads acting on the cylinder portion of the tank. This structure can be designed that almost all fibers reach their failure strain when the tank ruptures, which theoretically reduces the amount of carbon fibers compared to the conventional FW tank and the simple shape of the axial and the cylinder members are superior in terms of productivity and mass production. In this study, two demonstration tanks were designed and fabricated, burst tests were conducted to verify the multi-load path structure concept. The results showed that the burst pressures were respectively 55 MPa and 65 MPa, compared to the design pressure of 100 MPa. Consideration of the failure modes and the strain measured during the burst tests suggested that the burst pressure could be further improved by improving the the assembly accuracy and the detailed design specifications of the axial force members.

#### 9:50 AM

#### (ICACC-FS4004-2025) Novel Polymer-Coated Ceramic Powders for Making Highly Filled Polymer Composites

- D. Bajaj\*1; E. Wojcicki1; P. Elpers1; J. Janse1
- 1. Saudi Basic Industries Corporation, Specialties, Technology and Innovation, USA

Compounding of highly abrasive, low aspect ratio ceramic particle fillers with polymer resins is generally challenging due to high melt viscosity, excessive friction, and potential degradation of resin etc. These challenges limit the maximum loading level of ceramic particle fillers in compounding operations to below 30-40 v%. Percolation theory suggests that dense packing of inorganic fillers in a continuous polymer matrix can bring interesting properties, such as thermal conductivity, tunable di-electrics, hardness, modulus, specific gravity, while maintaining practical toughness, moldability, colorability etc. In this study, we explore a novel process to make highly filled ceramic polymer composites with polymer-coated ceramic powders in core-shell morphology made via Thermally Induced Phase Seperation (TIPS) process. These powders combine a very high loading (50-80 v%) of low aspect ratio ceramic particles with small amounts of polymer resins. These novel coatedceramic powders can be molded into densely packed continuous polymer-matrix ceramic composites in 2D and 2.5D shapes via hot pressing at polymer processing temperatures. Characterization of material properties on molded parts demonstrates desirable features, such as: 1. High specific gravity 2. Ceramic-like aesthetics 3. High strength and stiffness 4. Hardness and scratch resistance 5. Toughness promoted by polymer deformation mechanisms

#### FS 4: Ceramic/Carbon reinforced Polymers II

Room: Coquina G

Session Chair: Takenobu Sakai, Saitama University

#### 10:30 AM

(ICACC-FS4005-2025) On enhancement of axial compressive strength of carbon fiber reinforced plastic by matrix modification (Invited)

M. Ueda\*1

1. Nihon University, Japan

The axial compressive strength of a high-strength unidirectional carbon fiber reinforced plastic is about half of the tensile strength. The reason for the low compressive strength is the matrix since the matrix properties determine the axial compressive strength. The fiber waviness is inherent in the carbon fiber reinforced plastic because of the small diameter of the carbon fibers. Axial compressive loading to the unidirectional carbon fiber reinforced plastic causes the matrix shear deformation due to the fiber waviness. The matrix loses its fiber-supporting capability with increases in the axial compressive load, resulting in compressive failure. The matrix property plays an essential role in determining the axial compressive strength. The enhancement of the axial compressive strength was discussed focused on the matrix. Some examples to improve the matrix properties are presented. The improvement of the compressive strength of unidirectional carbon fiber reinforced plastics by the enhanced matrix properties is quantitatively discussed.

#### 11:00 AM

#### (ICACC-FS4006-2025) In-situ Shear Exfoliation and Post Processing of Hexagonal Boron Nitride Based Polymer Nanocomposite Coating

A. Ridoy\*1; A. Kumar1; A. Ashraf1

1. University of South Florida, Mechanical Engineering, USA

Two dimensional(2D) Hexagonal Boron Nitride(hBN) Nanofiller based coatings have found wide applicability in thermal management and high temperature applications. In this presentation, hBN polymer nanocomposite coating prepared using innovative in-situ shear exfoliation (ISE) technique will be discussed. The ISE technique has the advantage of utilizing low-cost bulk materials to generate 2D nanomaterial by mechanical shear exfoliation in a contaminant and solvent-free, one step process. Additionally, post processing techniques such as heat pressing and direct ink writing and their impact on nanocomposite structure and thermal performance of the nanocomposite will be explored. Structure property relationship will be presented based on microscopic, spectroscopic, rheological and thermographic techniques. This unique hBN nanocomposite has the potential to be used as efficient flame -resistant coating, microelectronic packaging, radiation shield, and coating for mechanical components used for tribological applications. Furthermore, this talk will shed light on ongoing research effort to produce 2D heterostructure (graphene and hBN) based nanocomposites for for emerging technology applications.

### FS6 Innovative material processing for diverse resource circulation loops

# FS6- Innovative material processing for diverse resource circulation loops III

#### Room: Ballroom 5

Session Chairs: Isabella Lancellotti, University of Modena and Reggio Emilia; Masamoto Tafu, Toyama Koto Senmon Gakko

#### 8:30 AM

# (ICACC-FS6024-2025) Holistic material utilization – glass and glass ceramics as the key towards efficient resource circulation loops (Invited)

M. Wahab\*<sup>1</sup>; S. Fuhrmann<sup>1</sup>; S. A. Sander<sup>1</sup>; S. Hossain<sup>1</sup>; J. Grottendieck<sup>1</sup>; M. Milek<sup>1</sup>

1. Technische Universitat Bergakademie Freiberg, Institute of Glass Science and Technology, Germany

The talk will present and summarize the potential of admixing different waste streams for glass manufacturing and for the recovery of critical raw materials via the glass-ceramic route. Exemplarily, it will show a reuse scenario for glass fiber reinforced plastics and will discus design for recycling possibilities. With this, the presentation aims to start the discussion on holistic material use for the design of efficient resource circulation loops.

#### 9:00 AM

#### (ICACC-FS6025-2025) Heavy metal concentration reduction for fertilizer application of sewage sludge incineration ash using Coanda effect-based air classifier (Invited)

M. Ito\*1; K. Zhou2; M. Córdova2; K. Fujimori1; Y. Iwai1; E. Tamura1;

- K. Oyama<sup>2</sup>; H. Kamiya<sup>2</sup>; C. Tokoro<sup>2</sup>
- 1. Sanki Engineering Co Ltd, Japan
- 2. Waseda University, Japan

Sewage sludge incineration ash (SSIA) is rich in Phosphorus (P), considered as a promising source of fertilizer. However, it also contains minute amounts of heavy metals such as As, Cd, Pb which may cause of harmful to human health. For utilizing SSIA as fertilizer, heavy metals concentration must be kept to a level significantly lower than the standard regulation value for fertilizer. In this study, we focused on the air classification based on the Coanda effect to reduce the heavy metal content in SSIA. SSIA particles inside a fluid jet stay attached to a curved surface based on their inertia moment. Hence, three fractions of separated SSIA with different particle size were obtained after the treatment, including fine, medium and coarse fraction, whose sizes were adjustable. The fine fraction tended to include high As, Cd, Pb concentration compared with the medium and coarse fraction. P was also present in slightly higher concentration in the fine, however, the difference was smaller than that of heavy metals. These trends suggest that heavy metal content in the SSIA can be reduced with keeping P content as much as possible, finding the properly fraction size between fine and medium. The results showed that the air classifier can reduce heavy metal content in the SSIA and be a promising method for utilization of it as fertilizer.

### 9:30 AM

### (ICACC-FS6026-2025) Designing electrodialysis with bipolar membrane condition to recover terephthalic acid from depolymerized PET solution (Invited)

H. Iwai\*²; T. Naruse¹; Y. Taniguchi¹; S. Sampei¹; T. Sasaki¹; M. Miwa¹; T. Sasaki¹; C. Tokoro²

1. Kirin Holdings Company, Ltd, Kirin Central Research Institute, Japan

2. Waseda University, Japan

The global demand for polyethylene terephthalate (PET) is rising, and PET recycling is an issue for resource circulation. Chemical recycling of PET by alkaline depolymerization is promising way; however, a substantial amount of acid reagent to recover terephthalic acid (TPA) from its salt are needed. Bipolar membrane electrodialysis (BMED), which performs desalt and supplies protons without additional acid reagents, has the potential to be applied as a novel TPA recovery technique. The present study conducted BMED with a configuration of bipolar membrane (BPM)-cation exchange membrane (CEM) -CEM for water-insoluble TPA recovery, instead of that of BPM-anion exchange membrane-CEM conventionally used for water-soluble organic acid recovery. Terephthalate anions were confined between two CEMs and precipitated here as crystalline TPA solids without clogging the membranes. The ion exchange performance was strongly prevented in the pH buffer range of TPA, at 5 - 6, taking a considerably long time to complete TPA crystallization. Adding a small amount of Na2SO4 as a conductor agent in the sample solution resolved the problem, and the agent assisted in reducing pH below 2 and accelerating TPA crystallization. The designed BMED condition achieved full recovery of TPA, even from a high-concentration solution of TPA-Na<sub>2</sub> (0.4 - 0.6 M).

#### 10:00 AM

### (ICACC-FS6027-2025) Reuse of landfill waste as stabilized inorganic glass fertilizers

A. Tamayo<sup>\*1</sup>; F. Rubio<sup>1</sup>; J. Rubio<sup>1</sup>

1. Institute of Ceramics and Glass, CSIC, Spain

Circular economy is a key plan to achieve the objective to minimize the generation of residues caused by any type of human or animal activity. Nowadays, there is extensive research in reevaluation and reuse of waste by vitrification and synthesis of new materials with an appropriately designed composition to decisively contribute to the zero-waste approach. In this work, there have been used drinking water treatment plant waste and shard glass non suitable for conventional recycling to produce new inorganic materials to be used as slow-release fertilizers in soils of different types of crops. The glasses have been designed to incorporate the most hazardous elements such as Cr, Co, Mo, Cu or Ni into the non-soluble phases to prevent the crop contamination. The leaching rate of the prepared glass materials has been modified by varying the SiO2, Al2O3 and CaO concentration and there have been also determined the elements contained in the crystalline phases and in the glassy matrix as well. The optimized glass composition has been also tested in greenhouse cultivation thus demonstrating the feasibility of making the most of two types of waste materials to produce sustainable fertilizers with high added-value.

## FS6- Circular economy perspectives for inorganic waste/wastewater valorisation/stabilization II

Room: Ballroom 5 Session Chair: Hisanori Iwai, Waseda University

### 10:30 AM

### (ICACC-FS6028-2025) Circular economy perspectives for inorganic waste/wastewater valorisation/stabilization: case studies (Invited)

I. Lancellotti\*1

1. University of Modena and Reggio Emilia, Engineering Enzo Ferrari, Italy

Case studies on the production of materials obtained by ceramic process or geopolymerization for inertization of hazardous waste are presented. Several natural (metakaolin) or secondary aluminosilicate materials (pumice and lapillus from volcanic quarry) are exploited as precursor for valorization and stabilization of liquid and solid wastes. Volcanic materials are used to obtain naturally colored ceramic tiles to limit the use of artificial dyes and natural fluxes. A comparative analysis of the life cycle was carried out to assess the environmental footprint of the final products, the environmental impact can be reduced between a minimum of about 8 % (Freshwater Aquatic Ecotoxicity category) to a maximum of 48 % (Acidification category). Metakaolin is used to inertise tannery wastewaters which are in the form of liquor containing almost 40% of chromium, combined with other pollutants, both anionic and cationic and organic macromolecules of surfactants. 20wt% of wastewater was added with sodium hydroxide and silicate as activating solutions. We focused on the release of chromium cation and soluble anions  $Cl^{-}$  and  $SO_{4}^{2-}$  in water which were proved to be below law limit for reuse or disposal in landfill as non-hazardous material. Results show an increased efficiency in Cr and anions entrapment in the amorphous aluminosilicate network.

### 11:00 AM

# (ICACC-FS6029-2025) Cementitious pastes with partial substitution of BOF steel slag produced with $CO_2$ injection in fresh mixture (Invited)

G. Ferrara\*<sup>1</sup>; P. Humbert<sup>2</sup>; M. Nispel<sup>3</sup>; D. Garufi<sup>2</sup>; P. Palmero<sup>1</sup>

- 1. Politecnico di Torino, Applied Science and Technology, Italy
- 2. CRH Innovation Centre for Sustainable Construction, Netherlands
- 3. Fels Vertriebs und Service GmbH & Co. KG, Germany

Commonly investigated Carbon Capture and Utilisation technologies involve the valorisation of industrial wastes via accelerated mineralisation processes to produce either powders to be adopted in cementitious blends, or carbonated pre-formed manufacts. Direct injection of CO<sub>2</sub> in fresh cement mixtures is emerging as an innovative technique to induce accelerated carbonation and produce sustainable concrete. In this framework, the present study investigates the efficiency of CO<sub>2</sub> injection in fresh mixture including Basic Oxygen Furnace steel slag (SS) as partial substitute of cement. The aim is to prove the efficiency of the process to valorise a waste inducing carbon capture while producing a building material with reduced clinker content. Paste samples, including 70% in weight of cement of type 52.5 N and 30% of SS, were produced with 0.5 water-to-binder ratio and by mixing for 20 m (C-SS-ref). A constant CO<sub>2</sub> flow rate of 250 l/h was adopted to create carbonated samples (C-SS-carb) and samples produced after a pre-carbonation of SS and by using dispersant additive (C-SS-carb+). The experimental outcomes show a CO<sub>2</sub> uptake of the end-product up to 5.7%, and enhanced mechanical properties compared to C-SS-ref samples. The promising results pave the way for further analysis aimed at improving the process and assessing its efficiency to produce mortar elements.

### 11:30 AM

### (ICACC-FS6030-2025) Recovery of carbon-free limes from unused alkaline from cleaning drainage using calcium wastes (Invited)

M. Tafu\*1; K. Ishigane1; T. Tobe2; N. Tobe3

- 1. National Institute of Technology, Toyama College, Japan
- 2. Ecoma Inc, Japan
- 3. Tobe-Shoji Co., Ltd, Japan

Calcium resources depend on the calcination of limestone collected from the eco-sphere and calcination with vast amounts of CO<sub>2</sub> release. Many kinds of research have focused on the production of limes from limestone at lower temperatures without the emission of CO<sub>2</sub>. Some research has pointed out that lime is obtained from calcium sulfate (Gypsum). However, this process is accompanied by the release of sulfate ions in wastewater. We focused on releasing cleaning drainage containing a small amount of alkaline, such as sodium hydroxide (NaOH), from cleaning returnable glass bottles and waste polyethylene terephthalate (PET) chips. The drainage was neutralized for effluent by the addition of hydrosulphic acid. From these backgrounds, we constructed a combination of recovery of unused alkaline from cleaning drainage using gypsum powder collected from waste from the demolition process. Calcium hydroxide was successfully collected from simulated wastewater containing 1 % NaOH with the addition of gypsum powder. The gypsum was transformed into calcium hydroxide by repeated treatment with the alkaline solution. Using this process, the pH of the effluent was acceptable to environmental standards for the effluent. Obtained lime has an extremely small carbon footprint because this process did not use limestone and calcination processes.

### <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

## **S1-** Novel Computational Approaches to Enhance Performance and Characterization

Room: Coquina E

Session Chairs: Gerard Vignoles, University Bordeaux; Walter Krenkel, University of Bayreuth

### 8:30 AM

# (ICACC-S1-029-2025) Numerical evaluation of allowable surface crack size in ceramics based on strength scatter due to internal defects

- S. Ozaki\*1; T. Maeda2; T. Osada3
- 1. Yokohama National University, Japan
- 2. Yokohama National University, Graduate School of Engineering Science, Japan
- 3. Busshitsu Zairyo Kenkyu Kiko, Japan

The ceramic components inherently show a wide range of strength and low reliability. Therefore, understanding the effect of defect size on the strength of ceramics, i.e., the allowable crack size in the components, is the key to ensure the reliability of ceramic components. Under these circumstances, we have proposed finite element analysis (FEA) methodology to predict the scatter of fracture strength based on the stochastic distribution of internal defects. In this study, we aimed to predict the apparent nonlinear relationship between the fracture strength and surface crack size in pressureless sintered alumina specimens with single-edge notched beams using the proposed FEA methodology. Specifically, the effects of both the surface crack and internal defects were considered, and the competitive relationship between the strength caused by the stochastic distribution of internal defects and the strength originating from prescribed surface cracks was simulated. By reproducing the apparent nonlinearity, and within the framework of linear-elastic fracture mechanics, the effectiveness of the FEA methodology for the evaluation of the allowable crack size in ceramics was demonstrated.

### 8:50 AM

### (ICACC-S1-030-2025) Modeling martensitic transformation temperatures in Zirconia-Ceria solid solutions using machine learning interatomic potentials

O. T. Rettenmaier\*1; J. Gabriel2; S. Patala1

- 1. Northwestern University, McCormick School of Engineering, USA
- 2. Canadian Nuclear Laboratories, Canada

Shape memory ceramics (SMCs), despite exhibiting high strength and recoverable strain, tend to shatter under load. Recent developments in SMCs have shown significant promise in enhancing the reversibility of the shape memory phase transformation by tuning the lattice parameters and transformation temperatures through alloying. While first-principles methods such as Density Functional Theory (DFT) can predict the lattice parameters and enthalpy at zero Kelvin, extending these to high temperatures, and calculating phase boundaries using these methods is impractical. In this work, we develop a model to predict transformation temperatures and lattice parameters for Zirconia-Ceria alloys. We construct a Machine Learning Interatomic Potential by iteratively expanding an initial dataset of DFT simulations using active learning. This potential is then employed to calculate the phase boundary as a function of composition, and from that lattice parameters at transformation temperature. We show excellent agreement between the computed transformation temperatures and experimental data across the compositional range. Finally, we compare other relevant design parameters (e.g., transformation volume change) to demonstrate the applicability of MLIAPs in designing shape memory ceramics.

### 9:10 AM

### (ICACC-S1-031-2025) Fracture Simulation of Iron Nitride Polycrystals in Nitrided Steel by Reactive Molecular Dynamics Method

M. Yokoi<sup>\*1</sup>; M. Kawaura<sup>1</sup>; Y. Su<sup>2</sup>; S. Fukushima<sup>1</sup>; Y. Ootani<sup>1</sup>; N. Ozawa<sup>2</sup>; M. Kubo<sup>1</sup>

- 1. Tohoku Daigaku, Institute for Materials Research, Japan
- 2. Tohoku University, New Industry Creation Hatchery Center, Japan

The surface hardness of metallic materials is a critical factor influencing destructive phenomena such as wear and fatigue. Nitriding treatment is widely used to enhance wear resistance and corrosion resistance by forming a nitride ceramic layer composed of iron nitride polycrystals on the steel surface. Depending on the treatment conditions, various crystalline structures and voids form within the layers. These factors can significantly impact their mechanical properties. In this study, we focused on the effects of voids within the iron nitride layer and conducted tensile simulations based on reactive molecular dynamics method. Since the chemical reactions of iron nitride surfaces in various environments are considered, reactive molecular dynamics simulations are useful for analyzing chemical reactions and degradation processes. The simulations were performed for Fe<sub>4</sub>N polycrystal model with intentionally introduced voids and the model without void. The simulations revealed that, in the absence of voids, a phase transition occurs before intergranular cracking. Conversely, when voids are present, cracks are generated at the grain boundaries as multiple voids come together, preventing the phase transition. The effects of microstructures such as crystalline structures and grain size on the degradation process will also be the focus of the presentation in the conference.

### 9:30 AM

### (ICACC-S1-033-2025) Structural characterization and thermomechanical analysis of heat tiles on the SpaceX starship

Z. C. Cordero\*1

1. Massachusetts Institute of Technology, Aeronautics and Astronautics, USA

The SpaceX starship uses radiatively cooled ceramic tiles for thermal protection during re-entry. This talk will describe the structure and properties of these tiles as well as their expected behavior during re-entry.

### 10:10 AM

### (ICACC-S1-034-2025) Thermomechanical behavior of $C_{\rm f}/C$ composites – experiments and image-based modeling (Invited)

G. Couégnat<sup>2</sup>; O. Caty<sup>1</sup>; M. Charron<sup>1</sup>; A. Raude<sup>1</sup>; C. Billard<sup>1</sup>; A. P. Gillard<sup>1</sup>; A. Portal<sup>1</sup>; G. L. Vignoles<sup>\*1</sup>

- 1. Universite de Bordeaux, LCTS Lab. for ThermoStructural Composites, France
- 2. Centre National de la Recherche Scientifique, LCTS Lab. for ThermoStructural Composites, France

One of the most important features of Cf/C composites is their very low heat expansion coefficient. Combined to their outstanding high-temperature capabilities, this property turns them into very desirable materials for solid rocket motor nozzle and divergent, extreme thermal protection systems and for high-energy braking systems. From the design point of view, it is highly desirable to control the relationship between the material's structure and its behavior. This is why LCTS has developed a coupled experimental/ modeling approach featuring image processing and image-based computations, including Digital Volume Correlation applied to in-situ high-temperature tests carried out in a CT scanning facility. The developed tools and the main results obtained with them will be presented and discussed in this talk.

### 10:40 AM

### (ICACC-S1-036-2025) A domain map for the tensile behaviors of unidirectional fiber-reinforced composites

M. McAllister\*1; F. W. Zok2; E. B. Callaway1

- 1. Pratt & Whitney, USA
- 2. University of California, USA

The tensile response of unidirectional fiber-reinforced ceramic composites is critically dependent on constituent properties. Despite a large parameter space of constituent properties, models have been rigorously developed for two behavioral domains: 1) fiber fragmentation around a single initially bridged crack (SBC) present and 2) fiber fragmentation around infinite bridged cracks (IBC). Both are extreme limitations of composite behavior and are unlikely to be realistic. While the range in constituent properties of real composites indicates that SBC and IBC behavior can be obtained, real composite behavior largely falls in an intermediate behavioral domain, where fiber fragmentation occurs around multiple bridged cracks (MBC). Monte Carlo simulations were performed to assess trends in composite performance metrics, strength and failure strain, as behavior transitions between domains. The results show that composite strength is relatively insensitive to behavioral transitions while failure strain can vary greatly from domain to domain.

### 11:00 AM

## (ICACC-S1-037-2025) Finite element analysis of crack growth and crack-healing of oxidation-induced self-healing ceramics

T. Maeda\*4; M. Rahman1; T. Osada2; S. Ozaki3

- 1. Chittagong University of Engineering and Technology, Depertment of Mechanical Engineering, Bangladesh
- 2. Busshitsu Zairyo Kenkyu Kiko Kozo Zairyo Kenkyu Kyoten, Research Center for Structural Materials, Japan
- 3. Yokohama Kokuritsu Daigaku, Faculty of Engineering, Japan
- 4. Yokohama Kokuritsu Daigaku, Graduate School of Engineering Science, Japan

As brittle materials, ceramic materials are highly defect-sensitive, and even small cracks can cause significant fractures. Oxidationinduced self-healing ceramics, which automatically fill surface cracks and recover strength by oxidation reaction under high temperature conditions, are expected to be one possible solution to these challenges. Unlike conventional materials, however, the evaluation of self-healing ceramics requires the development of a novel numerical simulation method that can evaluate both the damage and the healing process. In this study, repeated damage-healing analyses of self-healing ceramics were performed using the damage-healing constitutive model based on oxidation kinetics within the framework of the continuum damage mechanics. Specifically, the sequential analyses consisting of loading, crack-healing, and reloading in a three-point bending test for chevron-notched specimens were conducted. The results showed that the slow crack growth behavior of the chevron-notched specimens can be reproduced due to their geometrical properties. It was also confirmed that it is possible to predict time- temperature-, oxygen partial pressure, and crack width-dependent healing behavior and resulting strength recovery.

### S1- Ceramic Matrix Composites (CMCs) Processing-Microstructure-Mechanical Properties Correlation

### Room: Coquina E

Session Chairs: Walter Krenkel, University of Bayreuth; Gerard Vignoles, University Bordeaux

### 11:20 AM

# (ICACC-S1-077-2025) A Parametric Study to Investigate the Effects of Modifier Oxides on A Baseline EBC $(Si/Yb_2Si_2O_7)$ on Reducing the TGO Growth Rate

A. Sbdul-Aziz\*1; K. Lee<sup>2</sup>

- 1. Kent State University, Aerospace Engineering, USA
- 2. NASA Glenn Research, USA

Spallation of environmental barrier coatings (EBC) is primarily caused by the formation of a thermally grown oxide (TGO) layer, which is induced by steam oxidation. This phenomenon is recognized as a significant failure mode for EBCs. A study was conducted to determine if the growth rates of TGO could be effectively reduced through the addition of modifier oxides. The hypothesis underlying this research suggested that these modifier oxides would dissolve within the SiO2 matrix of TGO, thereby altering its structure and reducing its permeability to oxidants. A modified version of a baseline EBC formulation (Si/Yb2Si2O7) is used to generate a layer by incorporating Al2O3 or Al2O3-containing oxide compounds, such as mullite and YAG (Y3Al5O12). This reduction was tested under conditions of 90% H2O and 10% O2 at a temperature of 1316°C during thermal cycling. To confirm the effect of the modifier oxides on reducing TGO growth rates, an analytical approach is being exercised to examine and investigate how both uniformly and non-uniformly grown oxide layers influence the driving forces that lead to EBC spallation.

### 11:40 AM

# (ICACC-S1-047-2025) Development of novel oxide based ceramic matrix composites with high thermal stability and high mechanical properties

Y. Nawata\*1; I. Ohta1; I. Yamashita1

1. Tosoh Corporation, Japan

Oxide-based CMCs (Ox/Ox CMCs) have lower cost and better stability against corrosive and oxidative environments than SiC-based CMCs. Therefore, Ox/Ox CMCs are promising candidates for thermally resistant materials as alternative to conventional nickel super alloys. The thermal stability and high-temperature properties of Ox/Ox CMCs are important factors for their practical applications. We have developed uniform doping method (UDM) which is a novel method of doping oxide fibers with specific elements to improve the thermal stability and high temperature mechanical properties of oxide fibers. Developed Ox/Ox CMCs which is fabricated by UDM treated mullite fiber (TCM-02) exhibits no reduction in tensile strength after thermal exposure at 1200 °C for 1000 h, and has better thermal stability than the conventional Ox/Ox CMCs. Additionally, creep lifetime of TCM-02 at 1200 °C is superior to those of either a single-crystal nickel-based super alloy or a conventional Ox/Ox CMCs. These results are due to the suppression of grain growth of oxide fibers during thermal exposure, and the suppression of grain boundary sliding or diffusion of oxide fibers during creep loading at high temperature by UDM treatment. The effect of UDM on creep life time will be discussed.

### 12:00 PM

## (ICACC-S1-046-2025) Low Residual Si Reaction Bonded SiC and Diamond Composites

J. Wang\*1; M. Aghajanian1; S. Salamone1

1. Coherent Corp, USA

Silicon reaction bonding, a.k.a. liquid silicon infiltration (LSI), is processed by the infiltration of molten Si into preforms of ceramic particles with carbon additive. Molten Si reacts with carbon additive, forming SiC and leaving some residual Si in the matrix. With a relative low processing temperature of ~1500°C and near zero process shrinkage, the reaction bonding process allows the cost-effective fabrication of large and complex-shape SiC ceramic composites from preforms fabricated by traditional methods or additive manufacturing. The issue with Si reaction bonding for some applications is the presence of a residual Si phase, typically > 20 vol%, that will deteriorate the mechanical, wear and high temperature capability of the materials. In this study, we evaluated the effects of the addition of high-density carbon source (diamond) into the preform materials. By optimizing the diamond particle size, ratio and content, reaction bonded SiC (RBSC) with less than 5 vol% residual Si (> 95 vol% SiC) was fabricated with enhanced mechanical and thermal properties. For reaction bonded diamond composites, optimization of diamond particle sizes, ratio and packing density leads to residual Si < 0.5 vol% with high thermal conductivity (>700 W/m-k). This work presents a study that relates the residual Si content to the microstructure, mechanical and thermal properties of the reaction bonded composites.

### <u>S2 Advanced Ceramic Coatings for</u> <u>Structural/Environmental & Functional</u> <u>Applications</u>

## S2- New testing simulation and material concepts for T/EBC I

Room: Coquina C

Session Chair: Bryan Harder, NASA Glenn Research Center

### 8:30 AM

## (ICACC-S2-027-2025) Ductile phase-toughened oxide coatings for reusable rocket engine turbomachinery

Z. C. Cordero\*1

1. Massachusetts Institute of Technology, Aeronautics and Astronautics, USA

Delamination of protective thermal or environmental barrier coatings is a critical challenge in the development of next-generation high-temperature systems for emerging aerospace and energy platforms. Such coatings are typically made from brittle ceramics that easily fracture and delaminate from thermal stresses under steadystate or transient operating conditions. To overcome this limitation, we have been investigating a novel ductile phase-toughened environmental barrier coating designed specifically to resist delamination. The coating comprises a borate-based glass-ceramic matrix reinforced with Ni, which sinters to the substrate and percolates through the brittle glass-ceramic when its volume fraction exceeds 0.3. Critically our past work suggested that when the coating forms an interpenetrating structure, the Ni topology guarantees extrinsic toughening via crack bridging, imparting sufficient toughness to resist delamination under even the most aggressive operating conditions. In the present work we test this hypothesis, subjecting coated test articles to cyclic thermal shock. We find that the composite coatings develop through-thickness channel cracks but resist delamination because of crack-bridging by the ductile reinforcement. We then use these insights to design coatings with higher operating temperatures, in line with the requirements of deep-throttling reusable rocket engines.

### 8:50 AM

### (ICACC-S2-028-2025) Thermal Stress Analysis of Two Different Thermal Cycling Tests of Thermal Barrier Coatings

X. Liu\*1; L. Zhao1; P. Hsu1

1. Florida Institute of Technology, USA

Thermal cycling testing is commonly used to evaluate the durability of yttrium-stabilized zirconia-based thermal barrier coatings (TBC). The temperature distribution of the topcoat plays a key role in the stress distribution of the TBC sample. Two different temperature distributions on the topcoat surface were imposed using a high heat flux, temperature gradient CO<sub>2</sub> laser rig. By carefully controlling the laser energy delivery, a flat temperature distribution and a Gaussian temperature distribution were achieved during the heating phase of the thermal cycling test. The finite element method is used to determine the transient stress and strain distributions using the temperature data obtained from the experiment. Results show that the Gaussian temperature on the topcoat surface has a stronger stress concentration than that of the flat temperature distribution. The numerical simulations demonstrate the faster and earlier failure of the thermal cycling test with imposed Gaussian temperature distribution on the topcoat surface. The numerical simulation is in agreement with the thermal cycling test results. A follow-up study will consider detailed fracture mechanics failures under two thermal cycling test conditions. Furthermore, the combined experimental and numerical study will have implications for improving the existing international thermal cycling test standard of ceramics coatings.

### 9:10 AM

## (ICACC-S2-029-2025) Effect of water vapor atmosphere changes on TBC characteristics

### J. Pyeon\*1; J. Lee1; S. Baek1; B. Yang2; S. Yang1; Y. Jung1

- 1. Changwon National University, Republic of Korea
- 2. Changwon National University College of Mechatronics, Mechatronics Research Center, Republic of Korea

As a result of environmental factors such as greenhouse gases and fine dust, the need for the expansion of renewable energy in the power market has emerged. As a result, countries around the world are trying to expand clean energy production by utilizing carbonfree fuels such as hydrogen for power generation. Accordingly, research is underway to replace natural gas, the main fuel used in conventional gas turbines, with hydrogen, which produces fewer pollutants. Hydrogen forms active radicals during combustion, ultimately generating water vapor, which may affect the thermal barrier coatings (TBC) applied to protect components inside the gas turbine in high-temperature environments. In this study, to investigate the effect of water vapor on TBC coating, test specimens top coated with 8YSZ were heat treated by passing nitrogen gas containing water vapor at a specific temperature. After the test, SEM and XRD analyses were conducted to observe microstructural changes and phase transitions based on temperature and heat treatment duration. Through this, the impact of hydrogen on thermal barrier coatings in actual gas turbine operating conditions was analyzed, and the development direction for thermal barrier coatings for hydrogen gas turbines was established.

### 9:30 AM

### (ICACC-S2-030-2025) A Dynamic Testing Approach for Particulate Erosion – Corrosion of Gas Turbine Coatings (Invited)

- J. L. Stokes\*1; M. J. Presby1
- 1. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA

Particle interactions in engines can be complex phenomena leading to degradation of thermal (TBCs) and environmental barrier coatings (EBCs). Ingestion of particles into the engine can lead to recession of coatings due to particle erosion. Similarly, these particles can become molten, adhere to coatings and result in thermochemical corrosion. Erosion testing is often carried out where particles are injected into a gas stream, accelerated within a nozzle, and impinge on samples. Conversely, most molten particle corrosion testing is often done in static furnaces, which does not capture the dynamic nature of deposition. These damage mechanisms are often tested separately, and no standard exists to test both erosive/corrosive particle interactions with coating materials under relevant turbine conditions. Understanding the synergies of particle interactions is crucial in determining lifetimes of potential coating materials. Such considerations emphasize the need for realistic approaches in standardizing particle testing in combustion environments. This study outlines efforts at NASA Glenn's Erosion Burner Rig Facility in improving dynamic erosion/corrosion testing methods by assessing the durability of state-of-the-art (SOA) TBC 7 wt.% yttria stabilized zirconia (7YSZ) as a function of particle deposition rate, burner temperature, and particle size.

## S2- New test, simulation, and material concepts for T/EBC II

Room: Coquina C

Session Chair: Ravisankar Naraparaju, DLR - German Aerospace Center

### 10:20 AM

## (ICACC-S2-032-2025) Steam Stability of Xenotime-Inspired Rare Earth Phosphates as Environmental Barrier Coatings

I. Hawthorne\*1; E. Opila1

1. University of Virginia, USA

Multicomponent rare earth disilicates (REDS) have demonstrated promise for use as environmental barrier coatings (EBC) for SiC-based composites. This requires separating and recombining RE elements, creating a cost-prohibitive concept. High-temperature steam exposure of REDS results in the formation of RE monosilicates leading to shorter lifespan due to cracking on cooling. Following a desire to reduce costs, we can look to geological minerals for inspiration. Xenotime-based RE phosphates (REPO<sub>4</sub>), RE = (Y,Gd,Dy,Er,Yb), are a promising material class due to demonstrated improvements to several EBC requirements compared to REDS. Preliminary study of REPO<sub>4</sub> indicates a reduction in parabolic rate of steam reaction through the production of highly stable RE<sub>2</sub>O<sub>3</sub>. Here we present reactivity of REPO<sub>4</sub> in 1400°C high-velocity steam for exposures up to 10 days for individual Y, Gd, Dy, Er, Yb phosphates and multicomponent REPO<sub>4</sub>.

### 10:40 AM

# (ICACC-S2-033-2025) Investigating temperature-dependent optical properties and phononic scattering processes in rare earth multi-cation oxides

W. Riffe\*<sup>1</sup>; S. Zare<sup>2</sup>; H. B. Schonfeld<sup>2</sup>; K. D. Ardrey<sup>1</sup>; P. Balachandran<sup>1</sup>; E. J. Opila<sup>1</sup>; D. Clarke<sup>3</sup>; P. E. Hopkins<sup>2</sup>

- 1. University of Virginia, Department of Materials Science and Engineering, USA
- 2. University of Virginia, Mechanical and Aerospace Engineering, USA
- 3. Harvard University, USA

Multi-cation oxides, such as many mineral compounds and high entropy oxides (HEOs) possess properties such as toughness and chemical/thermal stability which are necessitated for protective barrier systems in extreme environments and catalytic reactions. In these phononically dominated materials, the spectrum of vibrational carriers influences optical properties, phonon scattering processes and thermal transport and the addition of more cations adds to the complexity of materials properties. By extending to high temperature, the fundamental evolution of these properties can be understood. In this work, we experimentally and computationally investigate the thermal and optical properties via laser radiometry, spectroscopic ellipsometry, and Density Functional Theory (DFT) to elucidate optical properties and scattering mechanisms in multication oxides. With a novel laser-based metrology, emissivities of ceramics over 2000 °C can be measured in the visible and nearinfrared (NIR) spectral range. By coupling a heating stage to an infrared spectroscopic ellipsometer, dielectric properties up to 1000 °C can be studied. Investigating these ranges grants insight into both electronic and optical phonon dynamics with respect to temperature. By evaluating pertinent properties, we deconvolute key design considerations for next generation barrier coatings.

### 11:00 AM

### (ICACC-S2-034-2025) Machine Learning Prediction of Entropy Formation Ability of Rare Earth Phosphates

- J. O. Kazeem<sup>\*1</sup>; L. Huang<sup>2</sup>; B. P. Majee<sup>3</sup>; J. Lian<sup>4</sup>; K. Bryce<sup>3</sup>
- 1. Rensselaer Polytechnic Institute, Chemical and Biological engineering, USA
- 2. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
- Rensselaer Polytechnic Institute, Department Of Mechanical, Aerospace, And Nuclear Engineering and Department of Materials Science and Engineering, USA
- 4. Rensselaer Polytechnic Institute, USA

Rare earth phosphates (REPO4) have emerged as promising candidates for environmental barrier coatings (EBCs), providing protection to SiC-based ceramic matrix composites (CMCs) in extreme environments. While calculating the thermo-mechanical properties of REPO4 using high throughput density functional theory (DFT) calculations is relatively straightforward, predicting their ability to form the desired phase remains a significant challenge, complicating the discovery of new materials for EBC applications. Traditional trial-and-error approaches through experimental synthesis are time-consuming and sometimes inefficient. To address this issue, we developed a machine learning (ML) model that leverages chemical attributes of elements to predict the entropy formation ability (EFA) of multi-component REPO4, a key factor in determining their synthesizability in the xenotime phase. Our ML model's accuracy is demonstrated by comparing its predictions with DFT-calculated values and experimental results, particularly for quaternary and quinary REPO4 compositions excluded from training. For these systems, the numerous configurations required even for equal ratio RE compositions make direct EFA calculations via DFT computationally expensive. Our ML accelerates the identification of high entropy REPO4 compositions that are synthesizable in the xenotime phase to meet the stringent requirements of EBCs for CMCs.

### 11:20 AM

### (ICACC-S2-035-2025) Ultrathick Thermal Barrier Coatings Enabled by Featured Additively Manufactured Substrates

S. Sampath<sup>1</sup>; J. Saputo<sup>\*1</sup>; A. Donnelly<sup>1</sup>; R. Subramanian<sup>2</sup>

1. Stony Brook University, Center for Thermal Spray Research, USA

2. Siemen Energy, USA

In high temperature and high heat flux applications the use of passive thermal insulation is often desired. Such strategies have been widely utilized for the insulation of metallic components in gas turbines, where Air Plasma Spray processing is often used to deposit refractory oxide coatings ranging in thicknesses from 100 to 1000 µm. However, the thickness of such overlay coating is often limited by thermal stresses generated within the overlay. Such thickness limitations prohibit the introduction of such coatings into more demanding thermal protection systems. This work explores the use of additive manufacturing and cellular honeycomb structures to enable the production of ultra-thick thermal barrier coatings. The ability to use additive manufacturing to produce novel strain tolerant microstructural features is described along with high heat flux performance test comparisons between coated traditional cast alloys and coated featured additive manufactured parts.

### S3 22th Intl Symp on Solid Oxide Cells Materials Science & Technology

### **S3- Pressurized Operation**

Room: Ballroom 4

Session Chair: Katherine Develos-Bagarinao, National Institute of Advanced Industrial Science and Technology (AIST)

### 8:30 AM

## (ICACC-S3-024-2025) Extreme Pressure Testing of Solid Oxide Electrolyzers including Co-Electrolysis (Invited)

D. McLarty\*1

1. Alternative Energy Materials, USA

Pressurized operation of solid oxide electrolyzer cells, SOEC, offers a unique opportunity to integrate high temperature water splitting with exothermic synthesis reactions for syngas, methane, methanol, and ammonia. We present new results for high pressure steam electrolysis and co-electrolysis with exhaust gas composition measurements. Pumping liquid water and electrolyzing steam at the desired hydrogen pressure eliminates costly and energy intensive hydrogen compressors responsible for 10-15% of the total green hydrogen plant energy consumption. Co-electrolysis of both steam and CO2 at low pressure forms syngas (H2 + CO) and at high pressure can form methane which lowers the OCV and increases current density while creating a fuel that can be transported in existing pipelines without the 10-15% volumetric limits of green hydrogen. With this approach, CO2 emissions can be actively recycled into a fuel, creating an artificial closed carbon loop. Combining steam electrolysis with a boiling water plug reactor for the Haber Bosch process allows for capture of the exothermic ammonia synthesis reaction heat to produce the high pressure steam and reduce energy consumption for green ammonia production by as much as 20%. We give an update on the design and operation of high throughput button cell and single cell test equipment for SOFC and SOEC operation and for pressurized system testing up to 300 bar.

### 9:00 AM

## (ICACC-S3-025-2025) Pressurized testing of solid oxide single cells

C. Grosselindemann\*<sup>1</sup>; A. Weber<sup>1</sup>

1. Karlsruher Institut fur Technologie, Institute for Applied Materials -Electrochemical Technologies, Germany

Pressurized operation of SOCs reached a lot of interest as it improves the SOFC performance, enables a coupling with a gas turbine and reduces efforts to pressurize hydrogen or syngas produced in a SOEC. Well-known facilities for pressurized operation of SOCs are based on pressure vessels enclosing the cell or stack to be tested. In this contribution, experiments were performed in a newly developed test bench without pressure vessel. In the single cell test bench fuel and air side are pressurized by a concept that rules out any differential pressure over the cell. The cell housing is based on welded metallic components and is sealed towards the cell by a glass-ceramic sealant. This sealant could be successfully exposed to a pressure of up to 11 bar<sub>a</sub> during testing and was able to withstand a full thermal cycle. The cell is contacted with metallic flow fields similar to a stack. We will show that in the pressurized mode the increase in open-circuit voltage is in good agreement with the theoretical predictions according to the Nernst-equation. IV-characteristics and impedance spectra measured at elevated pressures of up to 11 bar<sub>a</sub> will be shown. The impact of pressurized operation on loss mechanisms will be discussed with the distribution of relaxation times. The cell performance in SOFC- and SOEC-mode will be presented and compared with predictions from our 0D electrochemical model.

### 9:20 AM

### (ICACC-S3-026-2025) Modeling the Conditions for Stable Operation of Pressurized Solid Oxide Electrolysis Cells

R. M. Tagawa\*1; S. Barnett1

1. Northwestern University, USA

Solid oxide electrolysis cells (SOECs) are often envisioned to operate under pressurized conditions, but little is known about how pressurization affects degradation mechanisms. Here we model how pressurization affects the oxygen potential distribution across the electrolyte. A key question is whether pressurization increases the oxygen potential enough to cause fracture near the oxygen electrode. Using an electrolyte charge carrier and diffuse interface model for a thin bilayer electrolyte consisting of yttria-stabilized zirconia (YSZ) and a gadolinia-doped ceria (GDC) barrier layer, the oxygen potential across the electrolyte is quantified. The results show that the higher oxygen potential due to pressurization is mitigated by reduced oxygen electrode overpotential, depending on how much the polarization resistance R<sub>p</sub> decreases with increasing electrode oxygen partial pressure P<sub>02</sub>. The maximum electrolysis current density J that avoids electrode delamination is determined for different electrode materials and P<sub>O2</sub> values. Electrodes that improve with pressurization slower than  $R_{p} \sim P_{O2}^{-0.25}$  (e.g., LSCF) will fracture at lower J, whereas electrodes that faster than this power law (e.g., nickelate electrodes) will actually allow higher J with pressurization. The findings give insight into the operating conditions and design of electrodes to be used in pressurized SOECs.

### 9:40 AM

## (ICACC-S3-027-2025) Innovative strategies for high-pressure resistant interfaces and coatings for reversible solid oxide cells

F. Smeacetto\*3; M. Salvo1; S. Anelli2; F. Gallo1; F. Puleo3; F. D'Isanto3;

- L. Bernadet<sup>4</sup>; M. Torrell<sup>4</sup>; A. Sabato<sup>4</sup>; A. Tarancón<sup>4</sup>
- 1. Politecnico di Torino, Italy
- 2. Politecnico di Torino, DISAT, Italy
- 3. Politecnico di Torino, Department of Applied Science and Technology, Italy
- 4. Catalonia Institute for Energy Research, Advanced Materials for Energy Applications, Spain

This presentation will discuss the latest results achieved in the framework of two EU projects, HyP3D, and 24/7 ZEN, related to joining and integration approaches. New strategies for surface engineering approaches, to achieve high-pressure resistant joints, thus improving the overall joining reliability, will be presented. 3D-printed corrugated cells with embedded functionality will be joined to a laser treatment surface-modified interconnect, obtaining a mechanical interlocking effect. The shear strength results of the improved joined interfaces will be discussed, showing the positive effects of optimal surface processing on the joining strength and reliability. Innovative manufacturing technologies in reversible solid oxide cell systems, i.e. electrophoretic deposition of ceramic coatings further processed with rapid thermal annealing, will be presented. The results will show the electrophoretic deposition technique as a possible strategy to obtain multilayered protective coatings, with high reliability and scalability, whilst improving their microstructures, electrical properties and the Cr retention capability in a reversible solid oxide mode

### **S3- Simulation & Modeling**

Room: Ballroom 4

Session Chair: Henrik Frandsen, Technical University of Denmark

### 10:20 AM

## (ICACC-S3-028-2025) Using simulation to analyze solid oxide cell degradation

H. W. Abernathy\*1; W. K. Epting2; Y. Lei3

- 1. National Energy Technology Laboratory, Thermal Sciences, USA
- 2. National Energy Technology Laboratory, USA
- 3. US DOE National Energy Technology, USA

Through the US Department of Energy's Reversible Solid Oxide Fuel Cell (R-SOFC) and H2NEW program, the National Energy Technology Laboratory (NETL) has developed a comprehensive solid oxide cell (SOC) multiphysics performance degradation modeling framework. The framework uses microstructurally resolved information about an SOC to simulate lifetime performance under different operating conditions (i.e., fuel cell, electrolysis, reversible operation) while subjected to selected degradation modes (e.g., coarsening, secondary phase formation, cation interdiffusion, cracking/delamination). Having exact control of the microstructural and kinetic parameters of a cell provides insight about the relative importance of different electrode features and different degradation modes. Knowing which features and degradation modes to focus on provides practical research guidance for developing fuel cells and electrolyzers that can meet commercialization metrics such as cost of electricity and levelized cost of hydrogen. The talk will review the current capabilities of NETL's modeling framework and will present case studies to improve SOC electrode design and operation.

### 10:40 AM

# (ICACC-S3-029-2025) 3D Multiphysics model for protonic ceramic cells: impact of structural and operational parameters on hydrogen production and structural integrity

A. Moranti<sup>\*1</sup>; F. Da Prato<sup>1</sup>; S. Anelli<sup>2</sup>; D. Ferrero<sup>1</sup>; M. Santarelli<sup>1</sup>; F. Smeacetto<sup>2</sup>

- 1. Politecnico di Torino, Energy Department (DENERG), Italy
- 2. Politecnico di Torino, Department of Applied Science and Technology (DISAT), Italy

In this work, a comprehensive model for a protonic ceramic electrolysis cell (PCEC), emerging as an alternative to traditional solid oxide cells, is presented. A 3D numerical model has been developed for planar single repeating units (SRUs). This model integrates thermal-fluid-dynamics, electrochemical processes and structural analysis, accounting for the transport of protons, electrons holes and oxygen vacancies through the membrane, typical for barium-based zirconate perovskites, commonly employed in this technology and considered in this model. A key objective of this study is to quantify the impact of several parameters on hydrogen production, establishing the negative effect of electronic leakage on the transference number. Additionally, structural effects on the SRU components resulting from operational conditions, especially temperature gradient induced thermal stresses, are examined for their impact on structural integrity and durability. The analysis explored structural parameters and operational parameters, such as interconnectors' configuration, operating temperature and stream compositions and flow rate. The parameters that most impact performance and structural integrity are identified and quantified providing insights into configurations that could improve hydrogen production and durability of the PCECs.

### 11:00 AM

# (ICACC-S3-030-2025) Investigation of Oxygen Reduction Reaction on Pt and Ag over $BaZrO_3$ via Density Functional Theory

W. Li\*1; V. Drozd1; M. Sozal1; M. Li2; Z. Cheng3

- 1. Florida International University, Mechanical & Materials Engineering, USA
- 2. Idaho National Laboratory, USA
- 3. Colorado State University, Mechanical Engineering, USA

The oxygen reduction reaction (ORR) significant influence the performance of proton conducting solid oxide fuel cells (PC-SOFCs). Despite its importance, the ORR for PC-SOFCs in dry air is still not well understood. In this study, the ORR on metal (Pt or Ag) cathode over BaZrO<sub>3</sub> (BZO) electrolyte is investigated using density functional theory (DFT) based method. The oxygen vacancy formation energy is calculated for both BZO electrolyte and metal cluster over BZO substrate system, which is associated with charge redistribution at the metal/BZO interface. The energy profiles for various elemental steps along two different ORR pathways (metal cluster pathway and triple-phase boundary (TPB) adsorption pathway) were calculated using slab models of a metal (Pt or Ag) cluster over the BZO substrate containing one oxygen vacancy. The results of the calculations are presents and the theoretical implication are discussed.

### 11:20 AM

### (ICACC-S3-031-2025) Defect Thermodynamics Modeling of Proton Conducting Perovskite Electrode and Electrolyte Materials Evaluated Based on Density Functional Theory

Y. Lee<sup>\*1</sup>; Y. Duan<sup>1</sup>; D. Sorescu<sup>1</sup>; W. Saidi<sup>1</sup>; D. Morgan<sup>2</sup>; W. K. Epting<sup>1</sup>; G. Hackett<sup>3</sup>; H. W. Abernathy<sup>3</sup>

- 1. National Energy Technology Laboratory, USA
- 2. University of Wisconsin-Madison, Dept. of Materials Science and Engineering, USA
- 3. National Energy Technology Laboratory Morgantown, USA

Both electron-rich and electron-poor perovskite oxides have been used in solid oxide cell (SOC) applications as electrode and electrolyte materials. Herein, density functional theory-based thermodynamic modeling was carried out to describe the defect chemistry and transport properties of the proton-conducting electrolyte  $BaZr_{1-x}Y_{x}O_{3-\delta}$  (x<0.1) and of the triple-conducting perovskite  $(La,Ba)(Fe,M)O_{3-\delta}$  (M=Y and Zr) for intermediate temperature SOCs (500~750 °C). The defect thermodynamics of intrinsic point defects and the hydrogen-related defect reactions were solved in integrated defect models to predict the Brouwer diagram and the transport properties relevant for their SOC applications. For the electron-poor electrolyte  $BaZr_{0.9}Y_{0.1}O_{3-\delta}$ , in addition to the description on the experimental transport properties, the roles played by the acceptor-bound holes and the intrinsic and hydrogen point defects upon the conductivities of holes, protons, and oxygen vacancies under various gas pressure at various humidity levels were demonstrated. For the triple-conducting perovskite (La,Ba)(Fe,M)O<sub>3-6</sub> (M=Y and Zr), a defect modeling tool was developed to examine the impact of magnetic and electronic structures on the defect reaction energies and entropies, and to elucidate the role played by hydride defect species in reduced conditions.

### 11:40 AM

### (ICACC-S3-032-2025) Design of tubular and planar cells and short-stack based on co-ionic conductor electrolyte layer for cathodic synthesis of light olefins (Invited)

M. Santarelli\*1; D. Ferrero1; A. Moranti1

1. Politecnico di Torino, Italy

In this work, the modeling and design of cells (both planar and tubular) and short-stack composed of triple-conducting oxides (TCOs) that conduct electrons, oxygen ions, and protons, developed in the framework of the EU project ECOLEFINS, is introduced and

discussed. In the TCO solution,  $H^+$  ions, produced in water splitting, migrate from anode to cathode and are available there in ionic form for the reduction reaction of CO<sub>2</sub>, while the O<sup>2-</sup> ions deriving from the cathodic reduction of CO<sub>2</sub> are removed from the cathode by migration towards the anode. In this context, the cathode electrode is designed to develop CO<sub>2</sub> reduction mechanisms via H<sup>+</sup> protons for the direct production of totally deoxygenated hydrocarbons (light olefins). The paper discusses the modeling activities of the cells/ short-stack, with both planar and tubular geometry, devoted to the design of the cathode electrode and the co-ionic conductive electrolyte layer, the design and layout of the complete cell, and the design of the SRU and the consequent short-stack. Preliminary results are presented and discussed.

### 12:10 PM

## (ICACC-S3-033-2025) Characterizing the uncertainty of residual stresses in a solid oxide cell

A. Moncy<sup>\*1</sup>; A. Farshidi<sup>1</sup>; H. L. Frandsen<sup>2</sup>

- 1. Topsoe A/S, Denmark
- 2. Technical University of Denmark, Department of Energy Conversion and Storage, Denmark

The accurate knowledge of residual stresses in the layers of a solid oxide cell (e.g., after sintering process), is crucial towards determining the available structural capacity of the cell for mechanical loads applied during various other production steps and operation. To know these residual stresses, it is important to accurately measure the material properties and thicknesses of the individual layers. Unfortunately, due to the low thicknesses required for the various layers in a solid oxide cell for ensuring high electrochemical performance, it is challenging to acquire such information with great accuracy. An uncertainty in the materials properties and/or thicknesses of layers, implies that there may be an uncertainty in the estimated buildup of residual stresses. This study characterizes the uncertainty in the residual stresses of a solid oxide cell using Monte Carlo simulation. The residual stresses are determined analytically as well as numerically using ANSYS for a bi-layer system through a routine developed using Python. The radius of curvature is found to be a key enabler in characterizing the uncertainty in the residual stresses. The study identifies a minimum number of key parameters, if accurately know, reduces the uncertainty in the residual stresses.

### <u>S5 Next-Generation Bioceramics and</u> <u>Biocomposites</u>

### S5- Bioceramics and composites for tissue

**engineering I** Room: Ponce de Leon

Session Chair: Katalin Balazsi, Centre for Energy Research HAS

### 8:30 AM

## (ICACC-S5-001-2025) Bouncy Bioglass for bone and cartilage regeneration (Invited)

F. Tallia\*1

1. Imperial College London, Materials, United Kingdom

Osteochondral defects involve damage to both articular cartilage and subchondral bone. In this work we designed an osteochondral implant made of a new patented silica/polytetrahydrofuran/ polycaprolactone sol-gel hybrid, named "Bouncy Bioglass". This material, consisting of an interpenetrating co-network of organic and inorganic components, was proven to be 3D printable into 3D porous scaffolds with controlled porosity and tuneable mechanical properties, with great potential to stimulate articular cartilage regeneration. The addition of calcium ions in the inorganic component made it tough and bioactive, with the ability to stimulate the apatite deposition in vitro. The final aim is to 3D print a chondral device, with a bulk articular surface bonded to a 3D printed scaffold both made of Bouncy Bioglass, joined to a bone scaffold, made of the Ca-containing Bouncy Bioglass. Challenges are: 1) achieving a successful bond of the three components; 2) having the lowest possible friction coefficient against living cartilage; 3) guidance of stem cells to produce high quality articular cartilage or bone in the corresponding part of the device. The talk will explore the research from the invention of the material to the translation into a device, including: the mechanical characterisation of the cartilage and the bone components; the tribological properties of the bearing surface; the biological response in vitro and in vivo in sheep.

### 9:00 AM

### (ICACC-S5-002-2025) Bioceramics-based hybrid materials for bone regeneration (Invited)

A. Zima\*1; P. Pantak1; A. Belcarz2; K. Kowalska1; J. P. Czechowska3

- 1. Akademia Gorniczo-Hutnicza im Stanisława Staszica w Krakowie, Department of Ceramics and Refractories, Poland
- 2. Uniwersytet Medyczny w Lublinie, Chair and Department of Biochemistry and Biotechnology, Poland
- 3. Akademia Gorniczo-Hutnicza im Stanisława Staszica w Krakowie, Department of Ceramics and Refractories Employees, Poland

Recent advances in bone implants have led to innovative solutions, particularly hybrid biomaterials, antimicrobial biomicroconcretes, and 3D-printed scaffolds. In our study, biomicroconcretes were created using  $\alpha$ -tricalcium phosphate powder (60 wt.%) combined with hybrid hydroxyapatite/chitosan granules (40 wt.%). Non-modified and gold-modified hydroxyapatite/chitosan granules, produced via a modified wet chemical method, were used to enhance microcrack retention and antibacterial properties. X-ray diffraction and Fourier-transform infrared spectroscopy confirmed the presence of  $\alpha$ -tricalcium phosphate, hydroxyapatite, and chitosan. Mercury intrusion porosimetry showed open porosity between 45-55 vol%. The compressive strength, below 10 MPa, was adequate for non-load-bearing applications. In vitro studies showed bioactivity in simulated body fluid and antibacterial action. In vivo tests on New Zealand White Rabbits revealed bone tissue reconstruction without inflammation. The addition of silane coupling agents allowed for the robocasting of these materials into scaffolds. These hybrid biomaterials show promise for bone tissue engineering but require further clinical validation. Supported by programme "Excellence initiative - research university" for the AGH University of Science and Technology, as well as Faculty of Materials Science and Ceramics AGH University of Science and Technology, Poland (No. 16.16.160.557).

### 9:30 AM

## (ICACC-S5-003-2025) Thermo-physical and biological properties of $Si_3N_4\mbox{-substituted}$ 45S5 bioactive glass (Invited)

- C. Bagci\*1; F. E. Bastan2; A. R. Boccaccini3
- 1. Hitit University, Department of Metallurgical and Materials Engineering, Turkey
- Sakarya Universitesi, Thermal Spray R&D Lab., Department of Metallurgical and Materials Engineering, Turkey
- 3. University of Erlangen-Nuremberg, Institute of Biomaterials, Department of Material Science and Engineering, Germany

Silicon nitride  $(Si_3N_4)$  is increasingly being used as a dense, porous bioceramic or substitution for a bioglass due to its good mechanical and biological benefits. In this study, the effect of 10-30 wt.%  $Si_3N_4$  powder incorporation on thermo-physical and subsequent biological properties of 45S5 Bioglass<sup>®</sup> was assessed. First, varying  $Si_3N_4$ -substituted 45S5 Bioglass<sup>®</sup> composite pellets were subjected to a heat treatment at 1000 °C for 1h in an open-air furnace. It was seen that a strong interaction occurred between the bioglass and  $Si_3N_4$  and hence, the sintering temperature decreased by up to 150 °C. Thus, a balance was achieved between the decomposition of  $Si_3N_4$  and densification in the composites. XRD results showed that with increasing

 $\rm Si_3N_4$  fraction in the samples, the amorphous content of the samples increased and the amount of crystallized phases decreased. In-vitro bioactivity tests of pure and 30 wt.% Si\_3N\_4-added Bioglass were then carried out and characterized by FTIR, XRD and SEM. Si\_3N\_4 addition partially inhibited the formation of hydroxyapatite but also diminished the crystallization. Moreover, cell biology and antibacterial studies of pure and 30 wt.% Si\_3N\_4 added Bioglass were performed. Results showed that Si\_3N\_4 substitution in the Bioglass caused an increment in cell viability and antibacterial activity.

## S5- Bioceramics and composites for tissue engineering II

### Room: Ponce de Leon

Session Chair: Hui-Suk Yun, Korea Institute of Materials Science

### 10:20 AM

### (ICACC-S5-004-2025) Designing multifunctional constructs for tissue regeneration using nanostructured ceramic biomaterials and advanced fabrication techniques (Invited)

G. Montalbano<sup>\*1</sup>; S. Fiorilli<sup>1</sup>; J. Barberi<sup>1</sup>; A. Benedetto Mas<sup>1</sup>; L. Coviello<sup>1</sup>; F. Fiore<sup>1</sup>; C. Vitale-Brovarone<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology (DISAT), Italy

Today, medical devices and engineered constructs must go beyond serving as mere biocompatible supports for tissue regeneration. They are required to actively interact with the host tissue to promote rapid and functional healing. The crucial role of bioactive and stimuli-responsive ceramics in regenerating soft and hard tissues is well established. Their potential can be greatly enhanced when combined with organic phases and processed using advanced (bio) fabrication techniques, enabling the creation of biomimetic and multifunctional systems. This contribution aims to present recent studies conducted in the frame of collaborative European projects concerning the development of multifunctional constructs containing different nanostructured ceramic biomaterials, including bioactive glasses and mesoporous silica nanoparticles able to release therapeutic ions and drugs, engineered nanohydroxyapatites and superparamagnetic iron oxide nanoparticles. The presented studies highlight the importance of optimising hybrid formulations that combine inorganic and organic phases to enhance their suitability for specific applications in advanced fabrication technologies. Furthermore, the functionalities of the developed constructs have been assessed through a comprehensive physicochemical characterization and in vitro/in vivo assessment.

### 10:50 AM

## (ICACC-S5-005-2025) Preparation and in vitro biocompatibility of titania hollow fibers (Invited)

- S. Chen<sup>2</sup>; A. Osaka<sup>\*1</sup>
- 1. Okayama University, Faculty of Engineering, Japan
- 2. Taiyuan University of Technology, College of Biomedical Engineering, China

Hollow fibers are of special interest in developing various bioreactors because of their large surface-to-volume ratio and fibrous feature. In this study, we synthesized titania hollow fibers via a sol-gel process, using gelatin fibers as sacrificial templates. We then incubated osteoblastic MC3T3-E1 cells with the hollow fibers to evaluate their In vitro cytotoxicity. We found that the titania hollow fibers were biocompatible and they favored cell adhesion and proliferation on their surface. We hence concluded that they have potential as biocompatible cell-supporting matrices.

### S6 Advanced Materials and Technologies for Rechargeable Energy Storage

## S6- Electrode and Electrolyte Materials for Lithium-ion Batteries I

### Room: Coquina B

Session Chairs: Donald Dornbusch, NASA Glenn Research Center

### 8:30 AM

### (ICACC-S6-022-2025) Novel Silicon Oxycarbide (SiOC) Polymer-Derived Ceramic Anodes for Next-Generation Lithium-Ion Batteries (Invited)

### K. Marcus<sup>\*1</sup>

1. Semplastics EHC LLC, X-BATT, USA

The growing demand for high-performance energy storage systems has sparked intense research into advanced anode materials for lithium-ion batteries (LiBs). This presentation introduces silicon oxycarbide (SiOC) polymer-derived ceramic (PDC) technology as a promising anode active material, offering superior electrochem-ical performance and scalability compared to traditional graphite anodes. Our proprietary SiOC PDC synthesis method utilizes low-cost precursors and a controlled pyrolysis process to create a unique nanostructured material with tailored composition of silicon, oxygen, and carbon. SiOC PDCs offer several key advan-tages as anode materials for LiBs, including high specific capacities that can reach above 1,000 mAh/g, far exceeding graphite's theo-retical capacity of 372 mAh/g. The PDC route enables tailoring of the amorphous, micro-mesoporous structure to better accommo-date strains during cycling, resulting in mild volume expansion. Additionally, SiOC materials can be synthesized using relatively simple and low-cost methods, making them attractive for large-scale production. While SiOC anodes still face challenges, their unique combination of high capacity, structural stability, and tailorable properties make them a promising next-generation anode material for lithium-ion batteries and other electrochemical applications.

### 9:00 AM

# (ICACC-S6-023-2025) Highly active-material-concentrated cathodes of nickel and cobalt-free cation-disordered rock-salts for Li-ion batteries

D. Seo\*1

1. Korea Advanced Institute of Science and Engineering (KAIST), Republic of Korea

The shift towards electric vehicles and large-scale energy storage systems necessitates cost-effective and abundant alternatives for the commonly used Co/Ni-based cathodes (like LiNi0.6Mn0.2Co0.2O2) in Li-ion batteries (LIBs). Manganese-based disordered rock-salts (Mn-DRXs) have shown a potential to exceed the performance of traditional cathodes at a reduced cost, achieving more than 900 Wh/kg-AM (active material), but this has only been proven in cell designs that are not commercially viable. These designs use diluted electrode films (about 70 wt% AM) with excess carbon and binder. In this work, we reveal that the failures of Mn-DRXs in AM-concentrated electrodes stem from their low electrical conductivity and the collapse of their electrical network with volume change during charge and discharge.[1] We overcome these challenges through the engineering of electrical percolation, showcasing highly concentrated electrode films of Mn-DRX cathodes (approximately 96 wt% AM) and achieving the highest reported energy density at the electrode level (around 1050 Wh/kg-cathode). This research also emphasizes the balancing effect of manganese content on the electrical conductivity and volume change of Mn-DRXs, pushing forward the development of Co/Ni-free LIB technology. Reference 1. E. Lee et al., Energy Environ. Sci., 17, 3753 (2024).

### 9:20 AM

# (ICACC-S6-024-2025) $Ca_2V_2O_7$ as an anode-active material for lithium-ion batteries: Effect of conductive additive and mass loading on electrochemical performance

- L. Trezecik Silvano\*3; J. Sandherr3; M. Valadares Folgueras2;
- E. Ferreira de Souza<sup>1</sup>; P. Kaya<sup>3</sup>; V. Knoblauch<sup>3</sup>
- 1. Universidade Estadual de Ponta Grossa, Chemistry, Brazil
- 2. Universidade do Estado de Santa Catarina Centro de Ciencias
- Tecnologicas, Mechanical Engineer, Brazil
- 3. Hochschule Aalen, Institute for Materials Research IMFAA, Germany

Vanadium oxides were already studied as anodes in lithium-ion batteries (LIBs) for several reasons. Despite interest in vanadates, only a few considered Ca<sub>2</sub>V<sub>2</sub>O<sub>7</sub> (CVO) as an active material for LIB. Therefore, this study aimed to investigate the effects of the conductive additive fraction and active material loading on the electrochemical performance of CVO as anode material. The electrodes were manufactured using the slurry methodology, replacing graphite by synthesized CVO powder by varying amounts of C65. The results reveal an increase in specific capacity by up to 30 % using 10 wt % C65. Such electrodes showed 235 mAh/g<sub>AM</sub> at C/10 and, when cycled at 1 C, completed 300 cycles with a retained capacity of 39 %. During the cycle, a capacity drop after the initial cycles and a recovery behavior were observed. The former was attributed to the irreversible formation of solid electrolyte interphase together with irreversible phase transitions, while the latter was attributed to the reactivation of the CVO particles via crack formation due to a volume change. Finally, this work demonstrates the potential of CVO as cost-effective and environmentally friendly anode material for LiBs, offering promising electrochemical properties, particularly when coupled with an optimized electrode composition.

### 9:40 AM

## (ICACC-S6-025-2025) Water Processed Ultra Low-Cost Solid-State Li-Ion Batteries

S. Yasui\*1

1. Tokyo Institute of Technology, Japan

We have developed a series of oxide-based solid electrolytes with superior ionic conductivity in the order of several mS/cm and handling properties into the air to realize environmentally benign and formable solid-state lithium-ion batteries. Although "water-prohibition" is common in the battery world, we dared to use water processing to consider environmental harmonization and cost performance. As long as water is used, control of electrolysis of water is important, but this can be cleared by precise control. Our prepared battery showed great charge-discharge properties, with over 1000 cycleability at 3C operation and no discharge capacity reduction compared to the first cycle. We will detail the characteristics of solid-state batteries.

## S6- Electrode and Electrolyte Materials for Lithium-ion Batteries II

Room: Coquina B

Session Chairs: Valerie Pralong, CNRS ENSICAEN; Lorenzo Stievano, Universite de Montpellier

### 10:20 AM

### (ICACC-S6-026-2025) Tailoring the fueling capability of Halide Solid Catholyte through composition (Invited)

J. Gaubicher\*1; P. Moreau1; B. Stamenkovic1; E. Quarez1; I. Profatilova2;

- V. Tarnopolskiy<sup>2</sup>; N. Dupre<sup>3</sup>
- 1. Institut des Materiaux Jean Rouxel, Chemistry, France
- 2. Commissariat a l'energie atomique et aux energies alternatives Siege
- administratif, Energy storage, France 3. CNRS-IMN, ST2E, France

This talk relates to the use of the high potential redox electroactivity (4V) of a wide range of  $\text{Li}_x\text{ZrCl}_{4+x}$  compositions used for All-Solid-State Batteries. We show that the direct oxidation of these catholytes above 4V can be used as secondary redox-active centers in conjunction with a primary electroactive material in the cathode. This discovery leads to a remarkable increase in the overall cell-specific capacity by several tens of percent (>4mAh/cm<sup>2</sup>) while enabling large sacrificial capacity for in-situ prelithiation of Si or healing of anode less configurations. Based on several operando characterizations the underlying redox mechanism and the role of the catholyte composition on structural and electrochemical properties will be described.

### 10:45 AM

### (ICACC-S6-027-2025) Direct STEM probing of short-range order in cation-disordered oxide cathode for rechargeable batteries (Invited)

C. Wang\*1

1. Pacific Northwest National Lab, USA

A random occupancy of multi-species atoms at the same equivalent lattice site results in a crystalline solid solution that is chemically fully disordered. Often, when the atomic occupancy at neighboring lattice sites is correlated within only a short distance, a chemical short-range order (SRO) emerges, which has been noticed to dictate the mechanical, magnetic, thermoelectric, and electrochemical properties of crystalline solid solutions. Existence of a chemical SRO in a bulk lattice seemingly can be routinely visualized through diffraction techniques based on X-ray, neutron, or electron, where a diffused scattering intensity that is associated with the chemical SRO is often noticed to be superimposed on the sharply defined Bragg diffraction spots in the reciprocal space. However, derivation of the local atomic configuration associated with SRO is hardly achievable. Here, we develop a new technique based on aberration-corrected scanning transmission electron microscopy (STEM) imaging and simulations of STEM imaging and electron diffraction to directly solve the mystery of SRO and the correlation between SRO and Li transport properties in the recently discovered high-capacity Li-excess cation-disordered rocksalt (DRX) cathode.

### 11:10 AM

## (ICACC-S6-028-2025) Lithium Dendrite-Suppressing Polymer Fiber Frameworks for Anodeless Batteries (Invited)

J. Kim\*1

1. Stevens Institute of Technology, Chemical Engineering & Materials Science, USA

We have developed electrospinning-based manufacturing processing applicable for battery systems that involve metallic lithium. Electrospinning is a widely used to create nano- and micro-porous layers of functional fibers. However, its manufacturing capability is limited at producing randomly-oriented fibers. Topology and tortuosity of the electrospun fibers are poorly controlled, making it difficult to probe structure-property relationships for electrochemical systems. In this talk, we will demonstrate how to obtain threedimensional control of fiber construction. Produced fibrous structures will be used to construct the anode current collectors of an anodeless battery, one of the most promising energy-dense batteries beyond the Li-ion. While incorporating Li metal has proven difficult due to uncontrolled dendrite growth, we found that the anode current collector reinforced by the three-dimensional fiber structure enhances Li storage efficiency over the extended number of cycles, compared to the planar current collector. We will discuss the effect of fiber compositions and controlled geometrical configurations on stabilizing Li plating and stripping morphologies to suppress Li dendrite growth. Significantly, we consider that battery manufacturing advanced by this work will offer a systematic strategy to develop next-generation energy storage systems for a sustainable energy future.

### 11:35 AM

## (ICACC-S6-029-2025) Microstructural Design of Li-Na Alloy Anode for the Lithium-Ion Batteries

C. Li<sup>1</sup>; P. Huang<sup>1</sup>; C. Lee<sup>2</sup>; P. Wei<sup>3</sup>; Y. Luo<sup>3</sup>; Y. Chang<sup>3</sup>; S. Lin<sup>\*1</sup>

- 1. National Cheng Kung University, Materials Science and Engineering, Taiwan
- 2. National Cheng Kung University, Academy of Innovative Semiconductor and Sustainable Manufacturing, Taiwan
- 3. Delta Electronics Inc, Taiwan

Lithium metal and lithium alloys are promising anode materials for lithium-ion batteries (LIB) due to their extremely high energy density. However, the volume change and dendrite formation at the Li or Li-alloy anodes during cycling, which lead to capacity fading and safety concerns, have been significant issues a practical applications. To avoid detrimental volume change in demonstrated in the literature. However, either expensive constituent elements, such as Ag, or complex processes are normally required. In this work, porous Li-Na alloy anores with various chemical compositions and microstructures use e designed based on phase diagram and fabricated with a single electrochemical process. The Li-Na binary system exhibits the monotectic characteristics, which leads to Li-rich and Na-rich phase separation from the two immiscible liquid phases. A meso-scale porous structure was created by selectively extracting the Li-rich phase through electrochemical dealloying. The parameters for forming suitable microstructures were examined, and the cycling performance of the porous Li-Na alloy was also obtained. This work demonstrates a method of microstructure design. The designed porous microstructure was proven to be beneficial for improving the cyclic stability of Li-Na alloy anode in LIB.

### 11:55 AM

## (ICACC-S6-030-2025) Formation of an inorganic-organic bilayer on Li metal for high energy density Li metal batteries

J. Kim<sup>\*1</sup>; S. Myeong<sup>1</sup>; S. Lee<sup>1</sup>; H. Lee<sup>1</sup>; S. Choi<sup>1</sup>; M. Ryu<sup>1</sup>; J. Kim<sup>1</sup>; J. Park<sup>1</sup>;

- I. Hwang<sup>1</sup>; M. Kim<sup>1</sup>; M. Woo<sup>1</sup>; K. Kim<sup>2</sup>; J. Yeo<sup>4</sup>; Y. Jung<sup>3</sup>; T. Song<sup>1</sup>; U. Paik<sup>1</sup>
- 1. Hanyang University, Energy Engineering, Republic of Korea
- 2. Pusan National University, School of Materials Science and Engineering, Republic of Korea
- 3. Changwon National University College of Mechatronics, Republic of Korea
- 4. Korea Institute of Energy Research, Republic of Korea

Lithium (Li) metal is a promising anode material for high energy density batteries due to its exceptional capacity (~3,860 mAh g<sup>-1</sup>) and low redox potential (~3.04 V vs. SHE). However, the practical implementation of Li metal anodes is hindered by challenges such as Li dendrite growth, which leads to low coulombic efficiency and safety concerns. These issues can be mitigated by engineering the interface between Li metal and electrolytes to enhance Li-ion kinetics and interface stability. In this study, we developed an

inorganic/organic bilayer protection layer on Li metal. This bilayer consists of a 200 nm thick inorganic inner layer (LiF, Li<sub>3</sub>N, Li<sub>2</sub>S) adjacent to the Li metal and an outer porous PTFE polymer layer facing the electrolyte. The robust inorganic layer suppresses the formation and growth of Li dendrites, while the flexible and porous polymer layer maintains the integrity of the protection layer. In symmetric cell tests, the Li metal anode with the bilayer protection demonstrated stable cycling for over 600 hours at a current density of 1 mA cm<sup>-2</sup> with a capacity of 5 mAh cm<sup>-2</sup>. In full cell cycling tests, a 20  $\mu$ m thick Li metal anode with the bilayer protection, paired with a high-nickel content NCM811 cathode (5 mAh cm<sup>-2</sup> capacity), exhibited stable cycling performance over 200 cycles, achieving an average coulombic efficiency of 99.6%.

### <u>S7 19th Intl Symp on Functional</u> <u>Nanomaterials & Thin Films for Sustainable</u> <u>Energy Harvesting</u>

## S7- Synthesis, functionalization and assembly of inorganic and hybrid nanostructures

Room: Flagler C

Session Chair: Sedat Ballikaya, Istanbul University

### 8:30 AM

### (ICACC-S7-026-2025) Interfacially coupled magnetic nanocomposites: magnetic materials for sustainability (Invited) T. Sarkar<sup>\*1</sup>

1. Uppsala Universitet, Department of Materials Science and Engineering, Sweden

A promising route towards next generation functional materials are nanocomposites, where, by combining two or more phases, physical properties can be customized beyond single-phase bulk materials. A very important aspect while designing magnetic nanocomposites is the interface that controls the coupling between the two phases so that they can co-operate and interact with each other to produce desirable results. It is necessary then to push beyond the boundaries of conventional and established process technologies to design nanocomposites with controlled interfacial coupling between the two phases. In this talk, I will give examples from our ongoing work on different kinds of magnetic and functional nanocomposites illustrating how simple innovations can lead to the discovery of new fabrication methods in the quest of designing materials with novel functionalities. We will then discuss the use of these nanocomposites for a range of applications that we target - (a) next-generation sustainable magnets, crucial for the transition from fossil to a renewable energy society, (b) environmental remediation via: (i) wastewater treatment and water remediation, critical for survival of humanity and (ii) mitigating electromagnetic wave pollution, often regarded as the fourth category of pollution (after air, water, and soil pollution), and (c) functional thin films for memristors in neuromorphic circuits.

### 9:00 AM

### (ICACC-S7-027-2025) Nanomaterials and Patterning Approaches for Improved Surface-Enhanced Raman Spectroscopy Performance (Invited)

A. Sarakovskis\*1; C. F. Tipaldi1; K. Vitols1; L. Ignatane1

1. Institute of Solid State Physics, University of Latvia, Latvia

Surface-Enhanced Raman Spectroscopy (SERS) is a powerful analytical technique for molecular detection, offering ultra-sensitive identification of chemical species. Central to the success of SERS is the design and development of advanced materials that enhance Raman scattering through localized surface plasmon resonance (LSPR). In this presentation, a review on recent advancements in composite nanomaterials for SERS, focusing on noble metal nanoparticles, plasmonic nanostructures, and hybrid materials that enable higher sensitivity, reproducibility, and tunability will be given. Applications in environmental sensing, medical diagnostics, and chemical analysis will be examined to demonstrate the realworld impact of these material innovations. Recent results obtained in our group on advanced nanopatterning techniques, including both bottom-up and top-down approaches like laser-induced photoreduction of metallic nanoparticles and focused ion beam milling will be presented. These techniques offer precise control over nanoparticle size, shape, and arrangement, optimizing plasmonic hotspots for enhanced sensitivity and reproducibility.

### 9:30 AM

### (ICACC-S7-028-2025) Stöber Method to Amorphous Metal Organic Frameworks Coatings and Colloids (Invited)

#### N. Pinna\*1; W. Zhang1

1. Humboldt-Universität zu Berlin, Department of Chemistry, Germany

The Stöber method is a widely-used sol-gel route for synthesizing amorphous SiO<sub>2</sub> colloids and conformal coatings. Herein, we have extended the Stöber Method to metal organic frameworks (MOFs), a category of organic-inorganic hybrid materials with exceptionally customizable composition and properties. Twenty-two different amorphous MOF colloids were successfully synthesized by selecting 11 metal ions and 17 organic ligands. Moreover, by introducing pre-formed core-nanoparticles (NPs), a conformal and homogeneous amorphous MOFs coating with controllable thickness can be grown on core-NPs to form core-shell colloids. The versatility of this amorphous coating technology was demonstrated by synthesizing over 100 new core-shell composites from 19 amorphous MOF shells and over 30 different core-NPs. Besides, various multifunctional nanostructures, such as conformal yolk-amorphous MOF shell, core@metal oxides, and core@carbon, can be obtained through one-step transformation of the core@amorphous MOFs. This work significantly enriches the Stöber method and introduces a platform, enabling the systematic design of colloids exhibiting different level of functionality and complexity.

## S7- Functional coatings and innovative thin film techniques, e.g., ALD, PECVD- I

Room: Flagler C

Session Chair: Sedat Ballikaya, Istanbul University

### 10:20 AM

## (ICACC-S7-029-2025) Co-sputtered antipathogen composite coatings for air filtration (Invited)

C. Balagna\*3; A. Luceri1; S. Perero1; M. Donalisio2; D. Lembo2; M. Ferraris3

- 1. Politecnico di Torino, DISAT, Italy
- 2. Universita degli Studi di Torino, Italy
- 3. Politecnico di Torino, Department of Applied Science and Technology, Italy

Functional nanomaterials with tailored properties are crucial for sustainable solutions in energy, environment, and health. This work focuses on antiviral and antimicrobial composite coatings for air filtration systems, aligning with energy-efficient and healthfocused materials. The global health crisis has highlighted the need for preventing virus transmission. The European NANOBLOC project aims to provide reliable antimicrobial, antifungal, and antiviral coatings using environmentally friendly technologies. These coatings, designed for air filters, emphasize durability and effectiveness. POLITO, leading the project, has developed composite coatings of glass/ceramic matrices with embedded silver nanoclusters, using the co-sputtering technique. These thin (<200 nanometers) coatings release silver ions slowly, inhibiting bacteria and reducing virus vitality, including coronavirus and influenza. The co-sputtering technique is scalable and green, currently being up-scaled for large-scale production. This technology significantly improves public health

by reducing pathogen transmission, aligning with the symposium's focus on novel synthesis approaches, surface functionalization, and energy-efficient materials for health applications. These nanostructured coatings represent a significant advancement in functional nanomaterials, promoting sustainable global health protection.

### 10:50 AM

### (ICACC-S7-030-2025) External Fields in Chemical Vapor **Deposition Processing of Functional Materials (Invited)**

T. Karimpour<sup>1</sup>; B. Singh<sup>1</sup>; T. Fischer<sup>\*1</sup>

1. Universitat zu Koln Mathematisch-Naturwissenschaftliche Fakultat, Institute of Inorganic and Materials Chemistry, Germany

Chemical vapor deposition (CVD) has emerged as a versatile technique for fabrication of thin films and coatings with a wide range of mechanical, electrochemical, electrical, tribological and optical properties. In CVD, the parameters such as precursor/substrate characteristics, flow rate, temperature, and pressure have been conventional process-control parameters, influencing the deposition characteristics. Over the years, however, the advent of novel functional materials for bespoke applications have necessitated the researchers devising new ways to modulate the CVD process, independent of the conventional process-control parameters. In this regard, external fields (electric, magnetic and electromagnetic) create new frontiers beyond the conventional CVD processing. Only operando characterization and simulation of the CVD process provides a holistic view of the atomistic and microscopic effects of external fields on the gas phase and on-surface reactions, surface reconstruction and ordering phenomena. This talk will provide an overview of different external field assisted CVD methods and provide examples on the alternate process parameter space for functional thin-films.

### 11:20 AM

### (ICACC-S7-031-2025) Oxides thin films for chalcogenide photovoltaics (PV) by chemical bath deposition (CBD)

C. Rossi\*<sup>1</sup>; D. Garzon<sup>2</sup>; I. Gushchina<sup>1</sup>; M. Grotti<sup>1</sup>; F. Soggia<sup>1</sup>; E. Puzo<sup>1</sup>; S. Sadewasser2; D. Colombara1

- 1. Universita degli Studi di Genova, Chemistry and Industrial Chemistry, Italy
- 2. International Iberian Nanotechnology Laboratory, Portugal

Recently, Cu(In,Ga)Se2 PV reached an outstanding 23.6% efficiency record. However, this device exploits a CdS layer prepared with CBD whose toxicity obstacles its commercialization and whose light absorption limits the efficiency. Since CBD is among the best techniques to maximize device efficiency, following other authors, we exploited it to prepare Zn(1-x)MgxO buffer from a reported CBD of ZnO. However, thermodynamics limits the solubility of MgO into ZnO posing a synthetic challenge. Consequently, the role of different complexing agents, Mg sources and concentrations were investigated. Citric acid (CA) improved the MMZ ([Mg]/([Mg]+[Zn]) above all when MgSO4 was used as Mg source instead of MgAc2\*4H2O. Similarly to other works, CA affects also the morphology, transparency and thickness of the films. The reaction mechanism is investigated through potentiometric titrations, speciations and dynamic light scattering to understand what limits the MMZ in the film at ~ 2% preventing the ideal MMZ range 10-25%. Interestingly, the surface contains up to 24% MMZ, suggesting a remarkable depth compositional gradient. In conclusion, a novel strategy to prepare CBD ZnMgO is proposed: Mg is mainly at the surface, providing insights about the reaction mechanism and synthetic improvements. CBD ZnMgO might positively affect not only chalcogenide PV but also other fields of optoelectronics and catalysis.

### <u>S8 19th Intl Symp on APMT for Structural &</u> **Multifunctional Materials & Systems**

### S8- Advanced powder synthesis and processing Room: Flagler A

Session Chairs: Tohru Suzuki, National Institute for Materials Science; Young-Wook Kim, WORLDEX Industry & Trading Co., Ltd.

### 8:30 AM

### (ICACC-S8-026-2025) Spray freeze granulation drying using aqueous slurries of graphene-coated aluminum nitride powder with high water resistance (Invited)

J. Tatami\*1; R. Yamazaki1; M. Iijima1

1. Yokohama National University, Japan

In order to give water resistance to aluminum nitride particles for preparation of ceramics using aqueous slurry, graphene coating by mechanical treatment on the particles was investigated. Graphene coating was observed on the surface of the fine aluminum nitride particles which was obtained by mechanical treatment of mixed powder of graphene and aluminum nitride in a compression and shear field. The graphene-coated aluminum nitride particles showed excellent water resistance, since the pH value of the aqueous suspension did not change and aluminum hydroxide was not detected even after stirring for long time. The relative density of the aluminum nitride ceramics obtained with the composite particles was high, and their secondary phase was also found to be yttrium aluminate having less oxygen than those prepared without graphene coating, due to suppressed hydrolysis.

### 9:00 AM

### (ICACC-S8-027-2025) Chemical synthesis of Magnesium Aluminate Spinel (MAS) powders by self-combustion method

H. Balmori\*1; A. Mauro Nolasco1; J. Ortiz-Landeros1; L. Tellez-Jurado2;

- A. M. Paniagua-Mercado<sup>2</sup>
- 1. Instituto Politecnico Nacional, Metallurgical and Materials Engineering, Mexico
- 2. Instituto Politecnico Nacional, Materials science, Mexico

The effect of soft chemistry route in the purity, crystallinity, surface area and particle size of MAS powders synthesized at low temperatures was evaluated. MAS powders were produced by self-combustion method using organic salts Mg(NO<sub>3</sub>)<sub>2</sub>, Al(NO<sub>3</sub>)<sub>3</sub> as cation sources and urea as fuel to obtain a deep eutectic solvent (DES) that was fired from 400°C to 1100°C for 5h. Samples were characterized by Scanning Electron Microscopy, specific surface BET and X-ray diffraction to evaluate phase evolution and morphology. Well-defined peaks of spinel phase were observed in samples fired at 600°C, becoming highly crystalline at 800°C, the calculated lattice parameter is 8.08067 Å with a crystallite size of 19.40 nm on (311) and a specific surface area of 14.5  $m^2/g$  for the sub-micron powders. Self-combustion route presented a simple and time-saving experimental setup which significantly reduced the crystallization temperature and produced non-porous (close to stoichiometric) spinel powders.

### 9:20 AM

### (ICACC-S8-028-2025) Anisotropic Grain Boundary Mobility and **Microstructural Evolution of Alumina**

I. Naamne<sup>1</sup>; R. Marder<sup>1</sup>; W. D. Kaplan<sup>\*1</sup>

1. Technion - Israel Institute of Technology, Dept. of Materials Science and Engineering, Israel

Grain growth occurs together with densification during sintering of polycrystalline ceramics. The size and shape of grains can influence the properties of a material, and thus it is important to understand the reasons behind morphological changes. Previous studies have

clearly demonstrated that doping alumina with Ca below the solubility limit results in accelerated and anisotropic grain growth, and as a result changes the crystal shape, where elongated plate-like alumina grains form. It is not clear if the elongated shape is due to the system approaching equilibrium, i.e. the equilibrium crystal shape (ECS) due to anisotropic adsorbed Ca, or if this is a kinetic shape where Ca results in anisotropic grain boundary mobility. In this work, the rate of motion of the interface of oriented single crystals of sapphire into Ca-doped polycrystalline alumina was used to derive the anisotropic grain boundary mobility, showing that while Ca increases the mean mobility, it significantly increases the mobility of boundaries parallel to the rhombohedral plane, resulting in elongated grains. This indicates that the elongated shape is due to kinetic reasons rather than grain boundary energy. These results will be compared to similar effects due to external fields.

### 9:40 AM

# (ICACC-S8-029-2025) Microstructural control of nano phase-separated features of CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub>/Cr<sub>2</sub>O<sub>3</sub> produced by a redox-driven eutectoid decomposition reaction

R. Maier<sup>\*1</sup>; A. Johnston-Peck<sup>1</sup>

1. National Institute of Standards and Technology, MML, USA

Lamellar, phase-separated microstructures with controlled size domains of CeO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> are synthesized using a novel redox driven eutectoid processing route. Synthesis of nano-sized  $CeO_2/\alpha$ -Al<sub>2</sub>O<sub>3</sub> features is achieved by first making phase-pure perovskite CeAlO<sub>3</sub>. CeAlO<sub>3</sub> is synthesized by a calcination step under highly reducing conditions that stabilizes the Ce<sup>3+</sup> valence. This material, however, is unstable in oxidizing conditions, and at high temperatures, decomposes into its constituent CeO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> phases. Microstructural control of this system has been established by studying the decomposition kinetics, resultant microstructure, and phase composition of the CeAlO<sub>3</sub> +  $1/4O_2 \rightarrow CeO_2 + 1/2Al_2O_3$ reaction using thermogravimetric analysis, X-ray diffraction, and electron microscopy. Electron microscopy results reveal a cooperative (lamellar-forming) growth mechanism. When Cr is substituted in place of Al on the perovskite B-site, the CeCrO3 material also undergoes a high temperature eutectoid decomposition; however, the resultant microstructure exhibits no indications of cooperative growth. The relationship between the crystal chemistry of Ce-based perovskites and the nature of the eutectoid reaction will be discussed further, and new results related to functional properties of these materials will be presented.

### 10:20 AM

## (ICACC-S8-030-2025) Hot atoms in neutron irradiated $\beta\text{-MoO}_3$ for medical radioactive isotope production

H. Suematsu<sup>\*1</sup>; Y. Yang<sup>1</sup>; M. Ngo<sup>2</sup>; T. Kitagawa<sup>1</sup>; Y. Fujita<sup>3</sup>; Y. Takahashi<sup>1</sup>; T. Suzuki<sup>1</sup>; T. Nakayama<sup>1</sup>; T. Do<sup>1</sup>; K. Niihara<sup>4</sup>

- Nagaoka University of Technology, Japan
- National Institute of Advanced Industrial Science and Technology (AIST), Multi-material Research Institute, Japan
- Nihon Genshiryoku Kenkyu Kaihatsu Kiko, Department of Japan Materials Testing Reactor, Japan
- 4. Nagaoka Sutoku Daigaku, Japan

Mo-99 is a parent nuclide of Tc-99m which has been used for various nuclear medicines. Most of Mo-99 is produced as a fission product in highly enriched uranium fuel, which is currently difficult to be utilized because of the nuclear security reasons. Instead, nuclear reaction methods by irradiating neutrons on various Mo-98 compounds including MoO<sub>3</sub> have been attempted. Among them,  $\beta$ -MoO<sub>3</sub> draws interests of researchers because of its high extraction rate to water. This phenomenon was explained by hot atoms of Mo-99 with a high kinetic energy produced by the nuclear reaction to assist the release from the  $\beta$ -MoO<sub>3</sub> target. In this study, temperature and time dependence of extraction rate of Mo-99 in water was measured. The measured extraction rate reached 66% at 60 °C for 5.5 h. From the measured activation energies, possible extraction process is discussed.

### 10:40 AM

## (ICACC-S8-031-2025) Molecule Intercalation into $MoO_{3\cdot\delta}\text{-II}$ under high oxygen partial pressure

J. Zhao\*1; D. Terasawa1; T. Do1; T. Nakayama1; H. Suematsu1

1. Nagaoka Gijutsu Kagaku Daigaku, Extreme Energy-Density Research Institute, Japan

High temperature and high pressure (HTHP) treatment, as a prime example of extreme energy manufacturing processes, offers a unique method to obtain phases that are impossible to synthesize under normal conditions. Molybdenum trioxide, as a two-dimensional layered metallic oxide linked by van der Waals force, has certain research value in superconductivity. The transition from  $\alpha$ -MoO<sub>3</sub> to high-pressure phase MoO<sub>3</sub>-II was known to take place at 700°C and 6 GPa. This study aims to investigate the effects of oxygen doping and element intercalation in MoO<sub>3</sub>-II. In the experiments,  $\alpha$ -MoO<sub>3, $\delta$ </sub> and Ag<sub>2</sub>O powders were loaded into gold capsules and heat-treated in a cubic anvil-type high-pressure apparatus. One of the capsules was pressurized at 5.5GPa and then heated to 500~800°C for 1 h. Then the capsule was quenched to room temperature and unloaded to atmospheric pressure. Additional samples were prepared by incorporating SrO<sub>2</sub> powder into the raw materials, and pressurized at 5.5GPa and 700°C. The lattice parameters and surface oxygen content were measured by X-ray diffraction and photoelectron spectroscopy, respectively. Stable high-pressure phase of molybdenum trioxide was successfully synthesized. The unit cell volume showed a decrease trend with increasing temperature, while the oxygen content increased gradually. More detailed analytical results will be shown in presentation.

### 11:00 AM

### (ICACC-S8-032-2025) Challenges of 21<sup>st</sup> Centuries and modification of Dual Solid State electrolytes for next generation Lithium Metal batteries (LMB)

S. H. Siyal\*1

1. Dawood University of Engineering and Technology, Metallurgy and Materials Engineering, Pakistan

All-solid-state lithium-ion batteries (ASSLB) demonstrate significant advancements in energy density and safety comparing the traditional lithium-ion batteries, which using solid state electrolyte. Smart lithium-metal batteries (LMBs) offer high capacity and low electrochemical potential, but face challenges such as imbalanced electrolyte-electrode interfaces and high risk. This study introduces a novel nanoceramic-based electrolyte fillers integrated with polyethylene oxide to form a flexible, free-standing film. This film improves battery safety and stability, showing excellent ionic conductivity, high transference number, and a wide electrochemical stability window at room temperature. The Enhanced ionic conductivity in LATP/LLTO nano fillers help build a stable solid electrolyte interphase (SEI) and prevent dendrite growth, enabling reliable performance at different current densities of without short-circuiting. The resulting battery demonstrates superior cyclic stability and high coulombic efficiency, highlighting the potential of this electrolyte design for high-performance applications.

### <u>S13 Development & Applications of Adv</u> <u>Ceramics & Composites for Nuclear Fission/</u> <u>Fusion Energy Sys</u>

## S13- SiC material technologies for core structures of light water reactors and advanced reactors I

Room: Coquina D

Session Chair: Wen Jiang, NC State University

### 8:30 AM

## (ICACC-S13-001-2025) Physics Informed Non-Destructive Evaluation of $SiC_{f}/SiC_{m}$ Cladding (Invited)

G. Subhash\*1; M. P. MacIsaac1; A. Beck2; C. Tran3; W. Eum3; J. Harley3

- 1. University of Florida, Mechanical and Aerospace Engineering, USA
- 2. University of Florida, Department of Physics, USA
- 3. University of Florida, Department of Electrical and Computer Engineering, USA

The current NDE approach to monitoring defects in SiC<sub>f</sub>/SiC<sub>m</sub> cladding is limited to x-ray computer tomography (XCT) which is expensive and time consuming. To alleviate this problem, a generalized framework for on-line defect monitoring in materials and composite structures is being developed by employing physics-informed machine learning (PIML) and guided wave propagation principles. The approach involves extraction of ultrasonic spatial-spectral anisotropic and heterogeneous relationships within a structural system. The proposed PIML framework extracts knowledge of structural features in terms of wave number plots directly from experimental data without an underlying analytical basis and learns material characteristics from only the wave equation. Thus, the framework can adapt to many complex scenarios. The feasibility of this approach will be illustrated with several examples of materials and composite structures with and without defects. The challenges to applying this method for the detection of manufacturing defects in highly heterogeneous SiC<sub>f</sub>/SiC<sub>m</sub> woven ceramic composite tubes for nuclear fuel cladding will be discussed.

### 9:00 AM

### (ICACC-S13-002-2025) Damage Progression and Failure of SiC/SiC Composite Tubes under Hard-Contact Radial Expansion

E. Cakmak\*1; N. Cinbiz1; J. D. Arregui-Mena3; T. Koyanagi2

- 1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
- 2. Oak Ridge National Laboratory, USA
- 3. Oak Ridge National Lab, Nuclear Materials Science & Technology Group, USA

Silicon carbide matrix silicon carbide fiber (SiC/SiC) ceramic composites are promising candidates for accident tolerant fuel cladding material. The SiC/SiC tube is expected to be deformed by the nuclear fuel where fuel tube gap is closed at the end of life, depending on the initial fuel-to-cladding gap. Therefore, the mechanical response of the SiC/SiC tube under strain-driven loading conditions must be investigated to improve or tailor the LWR fuel design. The mechanical behavior of the SiC/SiC that mimics the strain-driven conditions have been investigated using soft plug expansion tests. However, no mechanical tests to mimic hard contact conditions relevant to nuclear fuel has been performed to understand the microscopic characteristics of the SiC/SiC composites. In this work, we report the microscopic failure characteristics of short segments of the SiC/SiC tubes that were subjected to strain-driven deformation via low speed hard-plug expansion using a surrogate ceramic. Mechanical tests were performed under X-ray computed tomography (XCT) to monitor the evolution of the initial SiC/SiC microstructure. Deep learning aided segmentation and systematic

data analysis revealed that the presence of inhomogeneous deformation applied by the hard-contact which was exaggerated by the presence of inner surface imperfections left behind from the matrix densification process.

### 9:20 AM

### (ICACC-S13-003-2025) CMC Tubular Components in High-Temperature Reactor (HTR) Nuclear Applications: ASTM Draft Standard for Compressive Strength of Axially-Loaded Tubes

M. G. Jenkins<sup>\*1</sup>; J. E. Gallego<sup>1</sup>

1. Bothell Engineering and Science Technologies, USA

US DOE is supporting the use of advanced materials for the core and the reactor unit components in various advanced, high-temperature reactor concepts. SiC-SiC ceramic matrix composites (CMCs) could greatly expand the design window for various components in terms of operating temperatures, applicable stresses, and service lives, compared to heat-resistant metallic alloys, while significantly improving accident tolerance and safety margins. Examples of CMC tubular components include fuel rods, control rod sleeves, and control rod joints. Possible failure modes for these components include axial and hoop tension, axial flexure, axial and diametral compression, and axial shear. A draft ASTM standard test method has been developed and submitted for full-consensus ballot to determine the longitudinal compressive strength of ceramic matrix composite tubes subjected to axial compression. Modeling and empirical tests of composite tubes provided validation of the parameters specified in the test method. The draft standard addresses the following experimental issues -- test specimen geometries/preparation, test fixtures, test equipment, interferences, testing modes/procedures, data collection, calculations, reporting requirements, precision/bias.

### 9:40 AM

## (ICACC-S13-004-2025) Compatibility of SiC/SiC composite ATF cladding materials with high-temperature steam

M. K. Grosse<sup>\*1</sup>; M. Steinbrück<sup>1</sup>; S. Huang<sup>2</sup>; J. Vleugels<sup>2</sup>; C. Sauder<sup>3</sup>; K. Lambrinou<sup>4</sup>

- 1. Karlsruhe Institute of Technology, Institute for Applied Materials, Germany
- 2. KU Leuven, Materials engineering, Belgium
- 3. CEA, DRMP, France
- 4. University of Huddersfield, School of Computing and Engineering, United Kingdom

The aim of accident-tolerant fuel (ATF) cladding material development after the Fukushima event is to enhance nuclear energy safety. SiC/SiC composites are a 'revolutionary' ATF cladding material concept that combines refractoriness and pseudo-ductility with a lack of accelerated oxidation during a loss-of-coolant scenario. Despite the SiC potential in addressing the ATF requirements, all material variants exhibit inadequate compatibility with water & steam, and an early (<2 dpa) saturation of radiation swelling during nominal operation. In this work, the accident tolerance of SiC/SiC composite claddings was assessed by means of high-temperature (1473-2100 K) steam oxidation tests. These tests showed excellent material performance up to the melting of the silica (SiO<sub>2</sub>) scale that forms on the surface of SiC/SiC composites in steam; at higher temperatures, material degradation proceeds at an acceptable rate until the outer monolithic CVD SiC layer is consumed and steam penetrates into the fiber-reinforced area, leading to fast material deterioration and release of gaseous species. This work also presents results of transient steam oxidation tests (heating rate: 4 K/min) in the 773-1873 K range on different grain boundary (GB) engineered SiC ceramics. These tests, done in the SCORPION project, revealed differences in material performance, depending on the compounds used for GB decoration.

## S13- SiC material technologies for core structures of light water reactors and advanced reactors II

Room: Coquina D

Session Chair: Tatsuya Hinoki, Kyoto University

### 10:20 AM

### (ICACC-S13-005-2025) Horizon scorpion: Improving the Performance of SiC/SiC Composites for LWRs (Invited)

T. Fey\*<sup>1</sup>; K. Lambrinou<sup>5</sup>; C. Sauder<sup>4</sup>; M. K. Grosse<sup>3</sup>; M. Steinbrück<sup>3</sup>; S. Huang<sup>2</sup>; J. Vleugels<sup>2</sup>

- 1. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany
- 2. KU Leuven, Materials engineering, Belgium
- 3. Karlsruhe Institute of Technology, Institute for Applied Materials, Germany
- 4. CEA, DRMP, France
- 5. University of Huddersfield, School of Computing and Engineering, United Kingdom

The Fukushima Daiichi incident in 2011 showed the need for improved nuclear energy safety, driving global investments in accident-tolerant fuels (ATFs). SiC/SiC composites are an ATF cladding material concept characterised by refractoriness, pseudo-ductility and a lack of accelerated oxidation during a LOCA. Unfortunately, all state-of-the-art SiC/SiC composites are characterized by inadequate coolant compatibility and early saturation of radiation swelling during nominal operation. The SCORPION project attempts to improve the coolant compatibility and radiation stability of SiC through material tailoring on different scales, e.g., via grain boundary engineering on the nanoscale or the development of protective coatings on the macroscale. This work reports results of autoclave tests (360°C, 28 days, PWR water) and steam oxidation tests (1600°C, 1 h) on candidate coating materials, whilst two of them (i.e., Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> & Yb<sub>2</sub>SiO<sub>5</sub>) were subjected to synergistic proton irradiation/aqueous corrosion tests (5.4 MeV p<sup>+</sup>, 320°C, 48 h, PWR water with 3 ppm H<sub>2</sub>). Moreover, SCORPION considers using porous SiC layers (pores filled with a weak & conductive material) to improve the impact resistance of SiC/SiC composites. In this work, porous biomorphic SiC ceramics with good mechanical strength were made from paper-derived C fibers, phenolic resin and Si; some contained sacrificial polymer lattices to form macrochannels.

### 10:50 AM

### (ICACC-S13-006-2025) Progressive Irradiation Approach Is Advancing SiGA\* Cladding Towards Lead Test Rods

S. Gonderman\*1; L. Borowski1; D. Frazer1; C. Deck1

1. General Atomics, NTM, USA

General Atomics Electromagnetics (GA-EMS) is developing SiGA\* composite technology, an engineered silicon carbide fiber reinforced, silicon carbide matrix (SiC-SiC) composite, for light water reactor applications to deliver improved operational performance and enhanced safety. Progress will be reported on fabrication scaling and irradiation testing of SiGA® cladding conducted to support lead test rods (LTRs) by the late 2020s. Specifically, advances have been made towards demonstrating fabrication of full-length SiGA® cladding rods. Advances in fabrication have enabled successful unfueled irradiations at both INL Advanced Test Reactor (ATR) and MIT's research reactor (MITR). Rods from both of these tests maintained integrity providing a pathway for fueled testing in ATR in the spring of 2025. Additional cladding samples have been prepared for irradiation in the Limerick BWR commercial nuclear power plant to capture commercial reactor relevant performance data on SiGA\* cladding. Finally, irradiations at the high flux isotope reactor (HFIR)

at ORNL are underway on GA-EMS nuclear grade SiC fiber and SiGA\* composite samples with modified processing to validate a domestic, cost competitive path for nuclear grade SiC-SiC structures. Pre-irradiation and post-irradiation test data will be presented in the context of how this work is closing the gap to commercialization of SiGA\* cladding.

### 11:10 AM

## (ICACC-S13-007-2025) Bowing of SiC/SiC composite materials under fast neutron flux gradients

C. Petrie\*1; P. Doyle1; D. Chandler1; T. Koyanagi2

- 1. Oak Ridge National Laboratory, Nuclear Energy and Fuel Cycle Division, USA
- 2. Oak Ridge National Laboratory, USA

Silicon carbide (SiC) fiber-reinforced, SiC ceramic matrix composites (SiC/SiC composites) are being considered for various in-core applications in light water reactors, including as fuel cladding and channel boxes in boiling water reactors. A common concern for both applications is the lateral bowing that can result from differential radiation-induced swelling. Although significant efforts have been dedicated to developing multiphysics models to predict the extent of bowing, to date there are no data to validate these models. This work summarizes post-irradiation examinations of tube specimens that were irradiated in the High Flux Isotope Reactor under intentional fast neutron flux gradients with varying magnitudes. The measurements are compared with both analytical and 3D finite element models. Some specimens exhibited bowing that matched well with the models whereas others showed discrepancies that may have been influenced by some combination of residual stresses in the as-fabricated specimens, anisotropic swelling, creep, and unintended neutron flux gradients resulting from adjacent experiments. The implications of these phenomena on light water reactor deployment will be discussed.

### 11:30 AM

### (ICACC-S13-008-2025) Development of CVI/CVD-SiC/SiC Composite for Accident-Tolerant Fuels of LWR Applications

S. Suyama\*1; M. Ukai1; T. Nishimura1; S. Kuboya1; M. Akimoto1;

F. Kawahara<sup>1</sup>; T. Takada<sup>1</sup>; F. Sawa<sup>1</sup>

1. Toshiba Energy Systems & Solutions Corporation, Japan

CVI-SiC/SiC composites have been investigated for use in nuclear reactor cores because of its inherent low activation, low neutron absorption cross-section, and stability under irradiation due to its high purity and crystalline SiC matrix. After the nuclear power plant accident in Fukushima in March 2011, it started to be developed in many research programs as a component of accident-tolerant fuels (ATFs). Toshiba Energy Systems Corporation has been developing process technologies for thin-walled and long tubes and boxes made of CVI/CVD-SiC/SiC since 2012. This CVI-SiC/SiC is expected to be resistant to water vapor environments above 1200°C during accidents. In addition, resistance to hydrothermal corrosion for the operating duration under normal LWR conditions is required. This study gives an account of progress in the development of process technology for thin-walled and elongated CVI/CVD-SiC/SiC-based tubes and boxes. It explores the use of coatings of CVD-SiCs on the surface layer of CVI-SiC/SiC to improve the hydrothermal corrosion resistance under LWR conditions. In particular, the hydrothermal corrosion resistance properties of CVD-SiC, measures to improve these properties and the progress of irradiation tests under BWR conditions will be presented.

### 11:50 AM

### (ICACC-S13-009-2025) Accelerated Development of Silicon Carbide Cladding through Multiscale Modeling

G. Jacobsen\*<sup>1</sup>; H. Shatoff<sup>1</sup>; J. Kosmata<sup>1</sup>; C. Ellis<sup>1</sup>; J. Rizk<sup>1</sup>; K. Spilker<sup>2</sup>; G. Singh<sup>3</sup>; K. Gamble<sup>3</sup>

- 1. General Atomics, Nuclear Technologies and Materials, USA
- 2. Los Alamos National Laboratory, USA
- 3. Idaho National Laboratory, USA

The accelerated fuel qualification (AFQ) methodology brings together physics-based modeling with experimentally obtained data to increase the speed of development of new nuclear materials and shorter the licensing/qualification time of said materials, while still maintaining high standards for safety. Through using this framework, General Atomics Electromagnetic Systems has begun development of a physics informed modeling tool of SiGA® Silicon Carbide based cladding. Current efforts are focused on the development of several individual models at different length scales. These models include a homogenized fiber tow model, a Fast Fourier Transform based weave model, a finite element based weave model, and a BISON fuel performance model. Initial comparison of these models to experimental separate effects tests will be presented showing models overall match well to mechanical test data. The short-term development benefits being reaped by these models and how they are being used to support irradiation testing as part of the greater SiGA® cladding development program will be discussed.

### <u>S15 9th International Symposium on</u> <u>Additive Manufacturing and 3-D Printing</u> <u>Technologies</u>

## S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies- Laser Lithography

Room: Coquina A

Session Chairs: Soshu Kirihara, Osaka University; Paolo Colombo, University of Padova

### 8:30 AM

### (ICACC-S15-001-2025) Powder bed fusion of polymeric preforms and their conversion into a ceramic: properties and applications after their densification by PIP, RMI, CVI (Invited)

A. Ortona\*1

1. Scuola Universitaria Professionale della Svizzera Italiana, DTI, Switzerland

In this work, we propose a novel hybrid additive manufacturing technique, which combines powder bed fusion (PBF) of polyamide powders and subsequent preceramic polymer infiltration and pyrolysis (PIP) to manufacture ceramic preforms with precise complex architectures. This presentation explores three key methods for further densifing these preforms: PIP, reactive melt infiltration (RMI) and chemical vapor infiltration (CVI). The final step, improves densification, enhancing the mechanical properties and thermal stability of the final ceramic product for high-performance applications. Some applications are finally proposed

#### 9:00 AM

#### (ICACC-S15-002-2025) Elucidating laser processing-property relationship in aluminum nitride towards laser powder bed fusion

R. McNamara<sup>\*1</sup>; J. Ma<sup>1</sup>

1. University of Virginia, Materials Science and Engineering, USA

Aluminum nitride (AlN) is a piezoelectric wide band-gap semiconductor with excellent thermal properties, making it a promising high-temperature structural material. AlN parts are usually sintered, but laser powder bed fusion can enable microstructural engineering, improving performance and broadening applications. The implementation of additive manufacturing can enable enhanced defect control and has potential to decrease the production cost of functional semiconducting materials compared to traditional methods. Under ambient conditions, AlN will decompose into diatomic nitrogen gas and aluminum gas instead of melting, though this decomposition can be suppressed by reducing the partial pressure of nitrogen gas in the system. Laser powder bed fusion (LPBF) allows control over the gas environment, allowing melting of AlN. This project seeks to establish the processing conditions that result in consistent melting of AlN, characterize structural, microstructural, and compositional changes of laser processing, and investigate the viability of LPBF of AlN.

### 9:20 AM

#### (ICACC-S15-003-2025) Fabrication of Micro-embossed Lithium Lanthanum Zirconate sheets by ceramic stereolithography for solid electrolyte applications

F. Spirrett\*1; S. Kirihara1

1. Osaka University, Joining and Welding Research Institute, Japan

Lithium-ion batteries have revolutionised portable electronics but pose safety risks due to flammable organic solvents and lithium dendrite formation. Solid-state batteries, which use solid electrolytes, offer a safer and more efficient alternative with higher energy and power densities. In this research the fabrication of solid electrolytes by ceramic stereolithography was investigated, specifically targeting lithium lanthanum zirconate (LLZ) for its high ionic conductivity, chemical stability, and potential to enhance battery performance. A photosensitive paste of 40-43 vol% LLZ was developed, and suitable parameters of 100 mW laser power, 1000 mm/s scan speed, and a 50 µm laser spot size were identified, allowing effective material curing and interlayer lamination. Thin embossed LLZ sheets were designed to improve ion exchange pathways, reduce internal resistance, and enhance overall electrochemical performance. The effect of cold isostatic pressing on the sintered microstructure was investigated, demonstrating its role in promoting solid-phase diffusion and achieving dense ceramic microstructures. These findings demonstrate the feasibility of ceramic stereolithography for the fabrication of solid electrolytes with optimised geometries, laying the foundation for safer and more efficient next generation mobile and telecommunications devices.

#### 9:40 AM

## (ICACC-S15-004-2025) Ceramic Stereolithography for Multi-Dimensional Geometries

S. Kirihara\*1; F. Spirrett1; N. Tsuruta1

1. Osaka University, Joining and Welding Research Institute, Japan

In stereolithographic additive manufacturing (STL-AM), 2-D cross sections were created through photo polymerization by UV laser drawing on spread resin paste including nanoparticles, and 3-D models were sterically printed by layer lamination. The lithography system has been developed to obtain bulky ceramic components with functional geometries. As the row material of the 3-D printing, nanometer sized metal and ceramic particles were dispersed into acrylic liquid resins. These materials were mixed and deformed to obtain thixotropic slurry. The resin paste was spread on a glass substrate with 50 µm in layer thickness by a mechanically moved knife edge. An ultraviolet laser beam of 355 nm in wavelength was adjusted to 50 µm in variable diameter and scanned on the spread resin surface. Irradiation power was automatically changed for an adequate solidification depth for layer bonding. The composite precursors including nanoparticles were dewaxed and sintered in the air atmosphere. In recent investigations, ultraviolet laser lithographic additive manufacturing (UVL-AM) was newly developed as a direct forming process of fine metal or ceramic components. As an additive manufacturing technique, 2-D cross sections were created through dewaxing and sintering by UV laser drawing, and 3-D components were sterically printed by layer laminations with interlayer joining.

### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies-Vat Photopolymerization 1

Room: Coquina A

Session Chairs: Fiona Spirrett, Osaka University; Alberto Ortona, SUPSI

### 10:20 AM

## (ICACC-S15-005-2025) Volumetric additive manufacturing of SiOC by xolography

K. Huang<sup>1</sup>; G. Franchin<sup>1</sup>; P. Colombo<sup>\*1</sup>

1. University of Padova, Industrial Engineering, Italy

Additive manufacturing (AM) of ceramics suffers from defects induced by the layer-by-layer approach on which traditional AM techniques are based. This study presents volumetric AM of a SiOC ceramic from a preceramic polymer using xolography, a linear volumetric AM process that allows to avoid the staircase effect. Besides optimizing the trade-off between preceramic polymer content and transmittance, a pore generator was introduced to create transient channels for gas release before decomposition of the organic constituents and moieties, resulting in crack-free solid ceramic structures even at low ceramic yield. The viscosity of the resin formulation was optimized without compromising transmittance, alleviating sinking of printed parts during printing and preventing shape distortion. With the optimization of printing parameters, including UV irradiance and moving speed, solid and porous ceramic structures with a smooth surface and sharp features were fabricated. This work provides a new method for the AM of ceramics at µm/mm scale with high surface quality and large geometry variety in an efficient way, opening the possibility for applications in fields such as micromechanical systems and microelectronic components.

### 10:40 AM

### (ICACC-S15-006-2025) Laser-induced slip casting for Silicon Carbide: Enhancing Printability Through Rheological Optimization

J. Feldbauer\*<sup>1</sup>; C. L. Cramer<sup>1</sup>; B. L. Armstrong<sup>2</sup>; D. Gilmer<sup>5</sup>;

M. Schwentenwein3; M. Mohammadi3; S. M. Allan4

- 1. Oak Ridge National Lab, Manufacturing Science Division, USA
- 2. Oak Ridge National Lab, Material Science & Technology, USA
- 3. Lithoz GmbH, Austria
- 4. Lithoz America, LLC, USA
- 5. The University of Tennessee Knoxville Tickle College of Engineering, USA

Silicon carbide (SiC) remains the material of choice for many industrial and energy applications at high temperatures. However, SiC can be difficult to shape and process to high density, especially by additive manufacturing. For materials with high refractive indexes, vat photopolymerization techniques remain difficult. Thus, methods that utilize aqueous colloid SiC suspensions and drying are under development. Here, laser-induced slip casting (LIS) uses a low viscosity slurry that can be dried in-situ with the laser to build up layers for a 3D printed part. The slurries for this process are still under development, so by optimizing chemical interactions, specifically between dispersants and SiC particles, the rheological properties of the slurry can be manipulated to enable successful printing. These dispersant interactions can alter the slurry's flowability and stability, depending on the volume percent, molecular weight, and chemical structure of the dispersants. Therefore, optimizing these rheological properties is crucial to maintaining slurry stability and printability during the LIS process, ensuring the production of high-density, geometrically complex SiC components for advanced applications.

### 11:00 AM

## (ICACC-S15-007-2025) Strength Dependence on Print Orientation and Strength-Size Scaling in Additively-Manufactured Alumina

### J. Nance\*1; K. T. Strong1

1. Sandia National Laboratories, Materials Mechanics and Tribology, USA

Lithography-based ceramic manufacturing (LCM) is a technique that enables the creation of dense ceramic parts with complex geometries unattainable through conventional ceramic processing methods. A 94 wt.% alumina ink was used for LCM printing. To investigate how different printing orientations affect the strength of standard parts, specimens were printed in three orientations, each aligned with an orthogonal coordinate axis relative to the build platform. Additionally, the study aimed to determine whether additively manufactured parts exhibit the same size-scaling effects as traditional ceramics. Four-point flexural strength was performed on ASTM standard specimens of sizes A and B, as well as ring-on-ring specimens, to evaluate impact on strength variation with respect to effective area. Characteristic strength and Weibull modulus are reported, as well as fractography was used to identify the defect origins for each type of specimen. The results indicated that both print orientation and the specific printer used for printing significantly influence the strength of the printed materials. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

### 11:20 AM

# (ICACC-S15-008-2025) Structural characterization of joined ceramic components manufactured via digital light polymerization

- C. Albunio<sup>2</sup>; R. Fordham<sup>1</sup>; S. M. Allan<sup>\*1</sup>; S. Sobhani<sup>2</sup>
- 1. Lithoz America, LLC, USA
- 2. Cornell University, USA

The ability to join 3D printed parts allows for the creation of larger, more complex structures while reducing print time and potential print errors. Moreover, joining parts extends the print volume capability, enabling fabrication of larger objects that surpass the size constraints of the build plate. This represents a major step toward increasing the relevance of ceramic additive manufacturing beyond current applications. In this work, several joint designs (Flat, Notch, Mouse Door, T-Slot), ceramic materials (Alumina, Cordierite, and Zirconia), and print orientations are examined. Preliminary probing of the effect of surface roughness at the joining interface is also performed. Joining is done in the green state using the same photosensitive slurry that is used during printing. The parts are sintered in an unpressurized environment to allow for more complex parts in future iterations. Flexural strength of the parts before and after thermal cycling are characterized. Bonding interfaces are characterized before and after breaking via SEM analysis.

### 11:40 AM

### (ICACC-S15-009-2025) Wear Response of Al<sub>2</sub>O<sub>3</sub> Ceramics Produced Using Digital Light Processing Additive Manufacturing

- A. David<sup>\*1</sup>; K. P. Plucknett<sup>1</sup>
- 1. Dalhousie University, Mechanical Engineering, Canada

Digital light processing (DLP) is a 'layer-by-layer' additive manufacturing (AM) technology based on a vat polymerisation approach. In the current study, DLP has been used to print alumina (Al<sub>2</sub>O<sub>3</sub>) based ceramics for assessment of their reciprocating wear response. The effects of both the printed layer thickness (from 10 to 75  $\mu$ m) and the build angle (from 0 to 90°, varied in 15° increments) have been investigated for sintered Al<sub>2</sub>O<sub>3</sub> formed using DLP. In addition, several surface micro-patterns were also developed and assessed, such that the surface modification aids in lubrication retention when used. After pre-conditioning and burnout steps, the Al<sub>2</sub>O<sub>3</sub> samples were sintered in air (typically 1650 °C for 2 h). Wear rates were measured against a  $\beta$ -Si<sub>3</sub>N<sub>4</sub> counter face sphere, with reciprocating

wear tests conducted at a frequency of 5 Hz, for a maximum duration of up to 60 minutes. The tests were performed at room temperature  $(22 \pm 2 \,^{\circ}C)$ , with loads of up to 80 N, applied normal to the wear surface being evaluated. The presented material will outline the effects of the printed part design on the measured coefficients of friction, specific wear rates, and microstructural damage. These studies highlight the important design criteria that need to be considered when utilising AM technologies for the manufacturing of advanced ceramic wear components.

### **<u>S16 Geopolymers Inorganic Polymers and</u>** <u>Sustainable Construction Materials</u>

## S16-Synthesis, processing, microstructure of geopolymers I

Room: Ballroom 1-2 Session Chair: Waltraud Kriven, University of Illinois at Urbana-Champaign

### 8:30 AM

### (ICACC-S16-001-2025) Ammonium hydroxide activation of metakaolin and engineered additives enabling direct ink writing of mullite ceramics (Invited)

P. Scanferla<sup>2</sup>; A. Ourgessa<sup>2</sup>; H. Elsayed<sup>1</sup>; J. Kraxner<sup>2</sup>; D. Galusek<sup>2</sup>; E. Bernardo<sup>\*1</sup>

- 1. University of Padova, Department of Industrial Engineering, Italy
- 2. Trencianska Univerzita Alexandra Dubceka v Trencine Centre for Functional and Surface Functionalized Glass, Slovakia

Aqueous suspensions of fine silicate and alumino-silicate powders undergo gelation even in the absence of alkaline activators. 'Non-alkaline' hydroxides, such as ammonium hydroxide ( $NH_4^+OH^-$ ), used in low concentrations (3-5 M), still supply OH ions. These ions determine the cleavage of Si-O-Si and Si-O-Al bonds at the surface of powders, with the formation of hydrated layers. Si-OH and Al-OH groups at the surface of one particle may react with similar groups of another adjacent particle, with the regeneration of Si-O-Si and Si-O-Al bonds, by condensation. The progression of condensation reactions, before complete drying, turns slurries into pseudoplastic pastes, used in the manufacturing of reticulated constructs, by direct ink writing. The absence of alkali is useful for the transformation of activated metakaolin, added with reactive alumina (y-Al<sub>2</sub>O<sub>3</sub>), into phase pure mullite (3Al<sub>2</sub>O<sub>3</sub>•2SiO<sub>2</sub>) ceramics, by firing at 1300-1400 °C. Mullite scaffolds, as final products, can be widely explored as catalytic supports. Boro-alumino-silicate glass powders, from dismantled pharmaceutical containers, used additional supplier of Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>, may offer further opportunities: chemical components not 'absorbed' by mullite crystallization, such as Na2O and B2O3, yield an intergranular glass phase, later dissolved (by acid attack) to achieve extra porosity.

### 9:00 AM

### (ICACC-S16-002-2025) Compositional Effects in Potassium Metakaolin Geopolymers Containing Alumina and Glass Frit (Invited)

- P. F. Keane\*4; R. Jacob1; M. Belusko2; N. Stanford3; F. Bruno4; W. M. Kriven5
- 1. Forschungszentrum Julich GmbH, Institute of Energy Materials and
- Devices, Microstructure and Properties of Materials (IMD-1), Germany 2. Mondial Advisory Pty Ltd, Australia
- 3. University of South Australia, STEM, Australia
- 4. University of South Australia Future Industries Institute, Australia
- 5. University of Illinois at Urbana-Champaign, USA

Geopolymer composites are promising candidates for molten salt containment due to their cost-effectiveness, ease of manufacture, and thermochemical stability. This study investigated the optimization of potassium metakaolin-based geopolymer composites with alumina platelets and glass frit powder for improved molten salt containment at 800°C. Material properties, including viscosity, porosity, density, and glaze formation, were evaluated before and after sintering at 900°C. Results showed that composites with a minimum of 65 vol% geopolymer content exhibited suitable workability for additive manufacturing. The presence of glass frit significantly reduced open porosity and enabled the formation of an impermeable surface glaze when its content exceeded that of alumina. The most promising candidates for molten salt containment were identified as those with KGP:alumina:glass ratios of 50:25:25 and 50:15:35, demonstrating a combination of low porosity, glaze formation, and ease of manufacturing. This study highlights the potential of geopolymer composites as a sustainable and efficient solution for high-temperature molten salt containment applications.

### 9:30 AM

(ICACC-S16-003-2025) Influence of Graphene Nanoplatelets on Physical Properties of Geopolymers (Invited)

N. Buettner<sup>2</sup>; A. Akono<sup>\*1</sup>

- 1. North Carolina State University, USA
- 2. Northwestern University, USA

Graphene nanocomposites are appealing as a means to increase the electrical conductivity along with the stiffness, strength, and toughness. We study the influence of graphene oxide nanoplatelets on the microstructure and mechanical properties of metakaolin-based geopolymers. The nanocomposites are prepared by first dispersing graphene oxide nanoplatelets in deionized water using ultrasonic energy, and later mixing the nanofiller dispersion with potassium hydroxide and fumed silica to form the potassium silicate solution. A source of aluminosilicate is mixed in afterward to yield the nanocomposite in the fresh state. Curing occurs at 50 C for 24 hours under continuous mechanical stirring. The mechanical behavior is characterized using advanced depth-resolved methods such as nanoindentation to probe the indentation modulus and indentation hardness, and scratch test to yield the fracture toughness. Meanwhile, the microstructure is resolved using optical microscopy and by application o inverse micromechanical relationships. In addition, high-resolution imaging is employed to study fracture micromechanisms. Thus, this study yields a fundamental understanding of the impact of graphene nanoplatelets on the behavior of geopolymer nanocomposites.

### S16-Synthesis, processing, microstructure of

**geopolymers II** Room: Ballroom 1-2

Session Chair: Henry Colorado L., Universidad de Antioquia

### 10:20 AM

### (ICACC-S16-004-2025) Effects of Core and Corona Composition on the Properties of Preceramic Polymer Grafted Nanoparticles

J. Ponder\*2; N. D. Posey1; A. Advincula2; T. Pruyn1; M. B. Dickerson1

- 1. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
- 2. UES, A BlueHalo Company / Air Force Research Laboratory, USA

Processable materials suitable for high temperatures are becoming increasingly important for various aerospace applications, ranging from aircraft brakes to atmospheric re-entry shielding, with silicon-based ceramics being a key class of materials for these harsh applications. The functionalization of preceramic polymers (PCPs) onto inorganic cores to yield grafted nanoparticles (GNPs) combines the processability of PCPs with greater tunability and increased mass retention upon pyrolysis from the ceramic cores. Previously, we have reported that grafting of linear polycarbosilanes onto silica (SiO2) cores produces a flowable material that yields polymer-derived ceramics (PDCs) upon thermal treatment (i.e. curing) and pyrolysis. While these initial results have demonstrated the potential of GNP systems, numerous questions remain regarding the grafting chemistry and optimal GNP composition. Recent efforts have explored tuning both corona and core chemistries to allow for control over the rheology, ceramic yield, and final ceramic composition. From these results, GNPs can be better implemented for novel applications (e.g. additive manufacturing) in either their neat form or in formulations.

### 10:40 AM

## (ICACC-S16-005-2025) Mineral coating to waterproof concrete structures

O. Pardessus\*1; A. Gharzouni2; X. Bourbon4; O. Helson4; S. Rossignol3

- 1. Institut de Recherche sur les Ceramiques, 87000, France
- 2. IRCER, France
- 3. Laboratoire SPCTS, France
- 4. Agence nationale pour la gestion des dechets radioactifs, France

In the context of radioactive waste management, minimizing the physical and chemical degradation of surface installations at the Industrial Centre for Geological Disposal and the Aube surface disposal facility is capital. Current industrial waterproofing uses organic compounds that degrade under UV light. This research aims to develop a more durable, mineral-based hydrophobic coating using alkaline silicate solutions. Hydrophobicity was determined by measuring the contact angle to assess coating suitability. To ensure the robustness and durability performance were studied after an accelerated ageing test in accordance with standard NF T30-049. Initial results indicate that the alkali/silica molar ratio and the nature of the alkali cation influence the contact angle. A threshold concentration ([M] < 4mol/L) was identified above which hydrophobicity degrades. Aging tests were conducted on various solutions, including a commercial organic solution, in three environments: controlled (20 °C and 60 % RH), outdoor (-5  $^{\circ}C < T < 30 ^{\circ}C$  and 25 % < RH < 100 %), and accelerated (-20 °C < T < 60 °C and 25 % < RH < 100 %). After 100 days of outdoor exposure and 30 accelerated aging cycles, the contact angle remains stable for the prepared solutions, while the commercial solution loses its hydrophobic properties. Tests are ongoing to optimize the coating application method and further improve its durability.

### 11:00 AM

## (ICACC-S16-006-2025) Investigation of thermo-chemical modification of sepiolite on its geopolymerization (Invited)

C. Bagci\*1; P. Mokhtari2; W. M. Kriven2

- 1. Hitit University, Department of Metallurgical and Materials Engineering, Turkey
- 2. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA

In geopolymer formulation, besides typically using aluminosilicates, magnesium hydrosilicates like sepiolite could be of interest for expanding upcycling of local sources in a circular economy based on a sustainable approach. Sepiolite stone collected from the Türktaciri region in Turkey was crushed, powdered and sieved to a fine particle size. To enhance reactivity of the as-received sepiolite, some of the powder was subjected to chemical treatment with ammonium nitrate (NH<sub>4</sub>NO<sub>3</sub>) for ionic exchange of MgO following thermal treatment at 800 °C for amorphization and subsequently, some mixed with metakaolin at 1:1 molar ratio to modify the Si/Al ratio in the formulation. After characterization of the as-received and modified powders by XRF, XRD and SEM, they were activated under highly alkaline conditions (11 M NaOH). The resins were poured into Delrin molds having sample dimensions according to the relevant ASTM standards for mechanical testing, sealed with a clamp and cured in a humidity-controlled oven at room temperature. After curing for 7 days at room conditions, the resulting solid materials were characterized by flexural and compression tests and followed XRD and SEM analyses. The results showed that the final geopolymers could be tailored depending on the modification conditions of the as-received sepiolite.

### 11:30 AM

### (ICACC-S16-007-2025) Impact of Alumina Platelets, Sand, and Basalt Fiber on Squeeze Flow and Shape Retentive Properties of Geopolymer Paste (Invited)

A. S. Brandvold\*1; A. C. Trindade1; W. M. Kriven2

- 1. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA
- 2. University of Illinois at Urbana-Champaign, USA

Geopolymer (GP) composites show great potential as a replacement for Ordinary Portland Cement (OPC) in construction material, extrusion-based, additive manufacturing. In this study, the basic rheological properties of highly reinforced, geopolymer composites with potential for 3D printing are innovatively investigated with "Squeeze Flow" and "Flow Table" tests commonly used in civil engineering. The impact of two composites were investigated: highly frictional alumina platelets for refractory applications, and a combination of sand and basalt fiber to investigate deformation resistance. Squeeze flow rates of 0.1, 1.0 and 3.0 mm/s were assessed to further understand how deformation rate influences extrusion and phase separation within fresh composite materials. It is shown that the deformation resistance because of particulate jamming increases with increasing solid reinforcement percentages, but that the overall effect of fiber size is somewhat inconclusive. In addition, the effect of squeeze flow rate exhibits an increase in load required to initiate flow at lower squeezing rates, but upon reaching a certain rate of solids to liquid in the matrix, the results become variable. The work to squeeze values are also calculated and discussed.

### **<u>S17 Advanced Ceramic Materials and</u> <u>Processing for Photonics and Energy</u>**

## S17- Advanced Ceramic Materials and Processing for Photonics and Energy III

Room: Coquina H

Session Chairs: Davide Janner, Politecnico di Torino; Oomman Varghese, University of Houston

### 8:30 AM

# (ICACC-S17-015-2025) Microwave-Assisted Routes towards Ln<sup>3+</sup>-Doped Nanomaterials with Controlled Composition and Morphology (Invited)

E. Hemmer<sup>\*1</sup>

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

Lanthanide-based nanoparticles (Ln-NPs) are known for their outstanding optical properties. Yet, challenges remain, including low emission intensity and efficiency of small Ln-NPs, and reliable, fast synthesis routes. As material chemists, we tackle these challenges with new designs of Ln-NPs by chemically controlled synthesis and the establishment of structure-property-relationships. NaGdF<sub>4</sub> being one of the preferred host materials for luminescent Ln-NPs, we developed a fast and reliable microwave-assisted synthesis approach allowing crystalline phase and size control in the sub 20nm realm. Such control is crucial for the understanding of fundamental structure-property relationships and to optimize their optical properties when aiming for the design of multifunctional probes. Gd<sub>2</sub>O<sub>2</sub>S is an alternative host material of interest. However, the synthesis of nanoscale Gd<sub>2</sub>O<sub>2</sub>S remained challenging as, for instance, the size control and uniformity of the particles could not keep up with other upconverting and NIR emitting hosts. Control over precursor chemistry and reaction conditions allowed us to obtain nanoscale Ln-doped Gd<sub>2</sub>O<sub>2</sub>S, exhibiting various morphologies and photoluminescence in the visible and NIR spectral regions. This presentation will highlight recent advances and remaining challenges in the microwave-assisted synthesis of luminescent NaLnF<sub>4</sub> and beyond.

### 9:00 AM

### (ICACC-S17-016-2025) Isostructural Lattice Alloying to Boost Broadband Light Emission from Self-Trapped Excitons for High Performance Lead-Free X-ray Scintillators (Invited)

J. Bao\*1; T. Chen2; D. Mu3; F. Lin2; W. Tang4; X. Li3; S. Ye2; Y. Wang2;

- J. Yang<sup>2</sup>; R. Wang<sup>2</sup>; X. Wen<sup>5</sup>; S. Yue<sup>6</sup>; X. Xu<sup>3</sup>; W. Zhang<sup>2</sup>; H. Chen<sup>4</sup>; C. Wang<sup>2</sup>
- 1. University of Houston, USA
- 2. Yunnan University, China
- 3. Kunming University of Science and Technology, China
- University of Electronic Science and Technology of China, China
   Swinburne University of Technology, Australia
- Swinburne Oniversity of Technology,
   Chinese Academy of Sciences, China

Metal ion doping is a widely adopted method to enhance light emission from self-trapped excitons (STE) in metal halide perovskites; however, identifying suitable metals that enhance STE emission without introducing unwanted impurities remains challenging. Here, we propose a new technique: alloying two perovskites with the same lattice structure but different metal ions to create a high density of lattice distortions. This approach is based on the principles of traditional bandgap engineering and the mechanism of STE emission. To illustrate this concept, we selected one-dimensional (1-D) metal halides CsAg<sub>2</sub>I<sub>3</sub> and CsCu<sub>2</sub>I<sub>3</sub>. CsAg<sub>2</sub>I<sub>3</sub> exhibits no STE light emission at room temperature, while CsCu<sub>2</sub>I<sub>3</sub> shows only modest emission quantum yield. However, single crystals of CsAg<sub>2-x</sub>Cu<sub>x</sub>I<sub>3</sub>, synthesized via a solution method, display broad STE emission centered at 475 nm. The emission can be tuned by varying the Cu concentration, with nearly 100% quantum efficiency achieved when  $x \approx 0.05$ . We subsequently used CsAg<sub>2-x</sub>Cu<sub>x</sub>I<sub>3</sub> as X-ray scintillators by embedding CsAg<sub>2-x</sub>Cu<sub>x</sub>I<sub>3</sub> powders in a PMMA film. A high X-ray-to-light conversion efficiency of 92,000 photons/MeV and a high resolution of 26 lp/mm were achieved, making CsAg<sub>2-x</sub>Cu<sub>x</sub>I<sub>3</sub> an excellent leadfree metal halide for X-ray scintillators.

### 9:30 AM

### (ICACC-S17-017-2025) Giant Auxetic Two-Dimensional Materials and their Photonics and Energy Applications (Invited)

### G. Fanchini\*1

1. University of Western Ontario, Physics and Astronomy, Canada

Materials exhibiting auxeticity, defined as positive strain normal to an applied strain, are receiving tremendous interest in recent years. This highly unusual behavior can quantified in terms of Poisson ratio, defined as the of the response strain over applied strain, where auxetic materials have a negative Poisson ratio. Giant auxetic metals are auxetics in which the density-of-electronic states at the Fermi level increases upon stretching thus leading to an increase in electrical conductivity in both directions. We report on a specially designed dual-zone remote plasma system conceived to grow giant-auxetic carbides out of thermodynamic equilibrium with well-tuned ratios of precursors.[1] For example, 2D tungsten semicarbide (W<sub>2</sub>C) was theoretically predicted to exhibit giant auxeticity, but had yet to be synthesized before the use of our and other out-of-equilibrium techniques, as the full carbide is energetically favored under thermodynamic equilibrium synthesis processes, such as chemical vapor deposition. In the last part of our talk, we focus on potental applications of 2D giant auxetics in photonics and energy, which include the photomodulation of charge collection, for example in electrodes for stretchable solar cells and phototransducers. [1] Stocek et al (Fanchini) Mater Horizons 11 (2024) 3066.

### 10:20 AM

## (ICACC-S17-018-2025) Solution processing of complex semiconductors (Invited)

G. Westin<sup>\*1</sup>

1. Uppsala University, Sweden

Oxide semiconductors such as titania and zinc oxide offer low cost and environmentally benign materials for photocatalytic, solar-cell, electrode and sensing applications. The development for applications in the mentioned areas require optimization of the crystal quality and surface facets and often doping and/or addition of ultra-thin coatings. Solution based routes to thin film, nano-sponge and nano-particle structures will be presented, as well as doping with 3d and 4f elements. The possibility of extending the doping range beyond the thermodynamic stability through the use of alkoxide based precursors will be presented, as well as the surprising molecular-like local structure of Eu-oxide dopants in ZnO. Solution processing of thin- and ultra-thin films with promise to expand the available coatings compared to ALD will be presented for homo and heterometallic systems. The focus will be on synthesis and detailed structure, although properties will be mentioned in relation to the structures.

### 10:50 AM

## (ICACC-S17-019-2025) Design of Optoelectronic Properties in Covalent Organic Frameworks (Invited)

D. Perepichka\*1

1. McGill University, Department of Chemistry, Canada

Covalent Organic Frameworks (COFs) are covalent 2D/3D polymers with a well-ordered structure and precisely controlled porosity. The combination of high accessible surface area (often >1000 m<sup>2</sup>/g) and strong electronic coupling in COFs creates new opportunities for applications in photonics and energy. In this presentation, I will summarize the achievements of the field of the last decade and present our latest work in molecular design of COFs with phosphorescent, semiconducting and magnetic properties. Time permitted, I will share our preliminary results on the use of semiconducting COFs in photovoltaic cells.

### 11:20 AM

# (ICACC-S17-020-2025) Characterization of PMN-0.30PT-Er-Yb ceramic for photoluminescent properties tuned by applied bias electric field

S. Yakubu\*1; J. A. Eiras2; M. H. Lente1

- 1. Universidade Federal de Sao Paulo, Meterial Science and Engineering, Brazil
- 2. Federal University of Sao Carlos, Physics, Brazil

The crystal structure of ferroelectric perovskites can be distorted by temperature, pressure, and magnetic or biased electric fields, affecting the photoluminescence properties of rare-earth doped ferroelectrics (RE-F), potentially enhancing optical applications in photonic displays and medical ultrasonic imaging transducers. This work reports the synthesis of PMN-0.30PT-Er-Yb ceramics and the characterization of their physical properties, mainly the photoluminescent one, aiming at the investigation of the potential applications of such compounds for piezo-photonics and ferro-photonic applications. The room temperature up-conversion photoluminescence spectrum of the as-sintered ceramic bodies revealed two emissions at about 553 nm and 669 nm corresponding to the transition from  ${}^{4}S_{_{3/2}}$ to  ${}^{4}I_{15/2}$  and  ${}^{4}F_{9/2}$  to  ${}^{4}I_{15/2}$  of  $Er^{3+}$  ions, respectively. Then, it was verified that the emission intensity is proportional to the n<sup>th</sup> power of the excitation intensity, as proposed by theoretical models in the literature. The dependence of the behavior on the applied electric BIAS field was investigated and the results discussed were based on the photoluminescent properties driven by changes in the local crystal field around the RE ions.

### 11:40 AM

### (ICACC-S17-021-2025) Highly Ce(III)-Doped Boron-Aluminosilicate-Lanthanum Glass for Advanced Photonic Devices

V. D. Dubrovin<sup>\*1</sup>; X. Zhu<sup>1</sup>; L. Li<sup>1</sup>; J. K. Lee<sup>1</sup>; T. N. ten Broek<sup>1</sup>; R. A. Norwood<sup>1</sup>; N. N. Peyghambarian<sup>1</sup>

1. The University of Arizona James C Wyant College of Optical Sciences, USA

Trivalent cerium (Ce(III))-doped optical materials have attracted significant attention due to their wide-ranging applications in high-energy radiation detection, medical imaging, radiation-resistant components, lighting, and magneto-optic devices. Among available glass materials, silicate glasses are typically preferred for their favorable mechanical and chemical properties. However, the concentration of Ce(III) ions in these glasses is limited to  $\leq 3.7 \times 10^{20}$  ions/cm<sup>3</sup>, primarily due to the tendency of Ce(III) to oxidize to Ce(IV) during the glass melting process. In this study, we developed a novel solution for producing highly Ce(III)-doped silicate glass, addressing a longstanding challenge in the field. By utilizing unconventional precursor materials and precisely controlling the oxidation-reduction conditions, we developed a stable boron-aluminosilicate-lanthanum (BASL) system with a record Ce(III) concentration of 9.4×10<sup>21</sup> ions/cm<sup>3</sup>, far surpassing previously established limits. Analysis of the resulting BASL glass demonstrated the absence of concentration quenching or Ce(III) oxidation, along with a strong magneto-optical response. This breakthrough paves the way for the development of advanced photonic devices using highly Ce(III)-doped robust BASL glass. This material is based upon work supported by the National Science Foundation under Award No. DMR-2310284.

### **S18 Ultra-High Temperature Ceramics**

### **S18- Advanced Characterizations and Simulations** Room: Coquina F

Session Chair: Gregory Thompson, University of Alabama

### 8:30 AM

### (ICACC-S18-026-2025) Connecting Microscale-to-Macroscale Fracture Toughness from Single Grain Transition Metal Carbide Testing (Invited)

A. Stubbers<sup>2</sup>; S. Hossain<sup>3</sup>; J. P. Santiago<sup>6</sup>; O. A. Graeve<sup>5</sup>; C. R. Weinberger<sup>4</sup>; G. Thompson<sup>\*1</sup>

- 1. University of Alabama, Metallurgical & Materials Engineering and the Alabama Materials Institute, USA
- 2. University of Alabama, Alabama Materials Institute, USA
- 3. Colorado State University, School of Advanced Materials Discovery, USA
- 4. Colorado State University, Department of Mechanical Engineering and the School of Advanced Materials Discovery, USA
- University of California, San Diego, Mechanical and Aerospace Engineering and the Program in Materials Science and Engineering, USA
- 6. University of California San Diego, Department of Mechanical and Aerospace Engineering, USA

We report a distinct methodology to test the conditional fracture toughness of transition metal carbides as a function of a pseudo-single crystal preparation method. By using a single crystal, a specific crystal orientation evaluation that is absent of microstructure contributions can be assessed. By coupling electron backscattered diffraction, the grain sizes and crystallite orientations are mapped onto a polycrystalline microstructure. Using a site-specific focus ion beam milling process, a series of pentagonal cross-sectioned shaped micro-cantilever beams are produced at various beam lengths and tested for their conditional fracture toughness. The experimental values are then compared to atomistic computational predictions. Specifically, we characterized TaC and HfC cubic structures as well as the Ta<sub>2</sub>C trigonal structure. The former monocarbides exhibit different dislocation densities upon mechanical loading, with TaC nominally nucleating more dislocations. While Ta<sub>2</sub>C has a lower crystal symmetry, it readily exhibits a high dislocation density facilitated by its anisotropic metal-to-metal bonding within its unit cell. As the size of these beams was reduced, the plasticity mechanisms became more prevalent in contributing to a size effect of the fracture response.

### 9:00 AM

## (ICACC-S18-027-2025) Phase exploration of TM-X-C (X = Al, Si) thin film materials:Correlation between theory and experiments

S. Richter\*1; C. Gutschka1; R. Hahn1; T. Wojcik1; E. Ntemou2;

- D. Primetzhofer<sup>2</sup>; S. Kolozsvári<sup>3</sup>; P. Polcik<sup>3</sup>; C. Jerg<sup>4</sup>; J. Ramm<sup>4</sup>; H. Riedl<sup>5</sup>
- 1. Christian Doppler Laboratory for Surface Engineering of highperformance Components, TU Wien, Austria, Austria
- 2. Uppsala universitet Institutionen for fysik och astronomi, Sweden
- 3. Plansee Composite Materials GmbH, Germany
- 4. OC Oerlikon Balzers AG, Liechtenstein
- 5. TU Wien, Institute of Materials Science and Technology, Austria

Transition metal carbides (TMCs) are known for their remarkable thermal stability, with melting points of up to 4000 °C, and their excellent mechanical properties, including exceptional hardness. These properties make TMCs indispensable materials for demanding applications in the aerospace or tooling industries. However, their limited oxidation resistance inspires the alloying of strong oxide formers such as Al and Si to improve their performance. To explore the phase space of TM-X-C (TM = Ti, Zr, Hf, Ta, W) thin film materials, density functional theory (DFT) calculations have been employed to screen initially the phase formation of single-phase structured fcc TM-X-C solid solutions, using the energy of formation and lattice constants as benchmark parameters. In a second step, these theoretical findings are correlated with an experimental approach in which over 260 different compositions within these ten material systems are grown by combinatorial magnetron sputtering. Phase formation, mechanical properties, and oxidation resistance are subsequently analyzed by X-ray diffraction, nanoindentation (CSM method), and TEM for selected states. The comprehensive analysis of structure-property relationships of these ternary TMCs provides crucial insights into the so-far relatively unexplored phase space and opens up opportunities for advanced applications.

### 9:20 AM

### (ICACC-S18-028-2025) Effect of Valence Electron Concentration on Slip Behavior in Sub-Stoichiometric Rocksalt Carbides and Nitrides

B. Watkins\*1; C. H. Blacksher2; G. Thompson2; C. R. Weinberger1

- 1. Colorado State University, Department of Mechanical Engineering, USA
- 2. University of Alabama, Metallurgical & Materials Engineering, USA

The "anomalous" hardness behavior of the tantalum carbides, TaC<sub>x</sub>, has been known since the 1960s. While the IVB transition-metal carbides (TMCs)-TiC<sub>x</sub>, ZrC<sub>x</sub> and HfC<sub>x</sub>-all exhibit monotonic declines in hardness with loss of carbon content, TaC<sub>x</sub> initially sees a sizeable increase in hardness with some reduction in the carbon-tometal ratio, x. Though somewhat less discussed, NbC, also displays this counter-intuitive behavior; in fact, the IVB transition-metal nitrides (TMNs) TiN<sub>x</sub> and ZrN<sub>x</sub> have been observed to increase in hardness with some loss of nitrogen content as well. The IVB TMCs are generally seen to slip only on {110}<sub>B1</sub> planes at low temperatures, while the VB TMCs and IVB TMNs prefer {111}<sub>B1</sub> slip. Using a semi-discrete variational Peierls-Nabarro (SVPN) model, we determine that the superficially bizarre hardness behavior of the VB TMCs and IVB TMNs arises primarily as a result of dramatic increases in the Peierls stress-the resolved shear stress required to move dislocations—on the  $\{111\}_{B1}$  planes at lower x. Thus, slip on

 $\{111\}_{B1}$  planes becomes unfavorable as nonmetal atom content is lost, and consequently much greater stresses are required for general plastic deformation. In the IVB TMCs, wherein  $\{111\}_{B1}$  slip is not favored at any x, no anomalous trend is observed.

### **S18- Super-hard UHTCs**

### Room: Coquina F

Session Chair: William Fahrenholtz, Missouri University of Science & Technology

### 10:20 AM

### (ICACC-S18-029-2025) New Superhard Boride Ceramics: An Integrated Computational and Experimental Study (Invited)

W. Fahrenholtz\*1

1. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA

A new super-hard (Hf,Mo,Ti,V,W)B<sub>2</sub> was identified by machine learning, predicted by be stable by thermodynamic simulations, and then synthesized by boro-carbothermal reduction. This composition was produced for the first time as a single-phase ceramic in the present research. The optimized ceramic had a single hexagonal AlB<sub>2</sub>-type crystalline phase with a grain size of 3.8  $\mu$ m and homogeneous distribution of the constituent metals. The Vickers hardness exhibited the indentation size effect, increasing from 27 GPa at a load of 9.8 N to as high as 66 GPa at a load of 0.49 N. This is the highest hardness reported to date for high entropy boride ceramics. The presentation will discuss the integrated approach for identification of new compositions and fabrication of ceramics with superior properties.

### 10:50 AM

## (ICACC-S18-030-2025) Superhard Refractory High-Entropy Ceramics

D. Hossain<sup>\*1</sup>; N. S. McIlwaine<sup>2</sup>; N. O. Marquez Rios<sup>2</sup>; R. Mayanovic<sup>4</sup>;

- E. Zurek<sup>5</sup>; D. Brenner<sup>3</sup>; W. Fahrenholtz<sup>6</sup>; D. E. Wolfe<sup>2</sup>; S. Curtarolo<sup>7</sup>; J. Maria<sup>2</sup>
- 1. The University of Tennessee Knoxville Tickle College of Engineering, Mechanical Aerospace and Biomedical Engineering, USA
- 2. The Pennsylvania State University, Materials Science and Engineering, USA
- 3. NC State University, Materials Science and Engineering, USA
- 4. Missouri State University, Physics Astronomy and Materials Science, USA
- 5. University at Buffalo, Department of Chemistry, USA
- 6. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA
- 7. Duke University, Materials Science, Electrical Engineering and Physics, USA

This study outlines the design and synthesis of super-hard refractory high entropy ceramics. By utilizing density functional theory-based calculations, we illustrate that valence electron concentration (VEC) dictates the bonding characteristics of high-entropy diborides and that by optimizing bonding based on VEC, one can produce super-hard refractory high entropy ceramics. Analysis of electronic structures and elastic constants reveals that optimal electronic filling of the bonding states leads to the highest resistance to shear deformation; thus, hardness is maximized when all bonding states are filled. Representative high entropy diborides are synthesized using high-power impulse magnetron sputtering. All compositions form a single-phase AlB<sub>2</sub>-type hexagonal structure. We establish a self-consistent hardness measurement protocol to correlate Knoop microhardness with VEC. Our experiments indicate that the designed high-entropy diborides are inherently superhard.

### 11:10 AM

## (ICACC-S18-031-2025) Microindentation of Hard Ceramic Thin Films at Low Loads

N. S. McIlwaine\*1; N. O. Marquez Rios1; J. Maria1

1. The Pennsylvania State University, Materials Science and Engineering, USA

Hard ceramics are critical in demanding applications such as advanced armor, cutting and metal-joining tools, and hypersonic thermal protection systems. Thin film coatings fabricated via physical vapor deposition, particularly transition metal borides, present a promising avenue for novel hard material discovery and architectures, primarily in regard to high entropy borides (HEBs) and superlattice structured films, respectively. However, accurate hardness characterization of these thin films is challenging due to measurement artifacts. Critical parameters influencing the precision of such measurements include surface roughness, film thickness, and indenter condition. Furthermore, films with high hardness values, meaning on the order of single crystal silicon carbide, pose additional complexity due to the extremely small residual indent size at low loads. This work addresses the challenges of using microindentation, a widely accessible technique, at low loads for hard ceramics, and demonstrates a reproducible and unambiguous methodology for hardness testing of thin films.

### 11:30 AM

## (ICACC-S18-032-2025) Superlattice of high entropy borides for high hardness alloys

N. O. Marquez Rios\*1; N. S. McIlwaine1; J. Maria1

1. The Pennsylvania State University, Materials Science and Engineering, USA

Transition metal high-entropy boride multilayer thin films are created through physical vapor deposition (PVD) using a co-sputtered RF and bipolar high power impulse magnetron sputtering (HIPIMS). Waveform generators are used to asynchronously modulate two different HIPIMS cathodes with varying multicomponent transition metal compositions. This process leads to a multilayer superlattice of two single phase aluminum diboride (S.G. #191) solid solutions of high entropy borides. Superlattice crystallinity is examined by X-Ray diffraction (XRD) while topography and morphology is examined by atomic force microscopy (AFM) and scanning electron microscopy (SEM), respectively. Finally, hardness was determined using Knoop micro indentation to study the effect of high entropy boride thin film multilayer periodicity on hardness. By controlling the waveform generator, the conditions of the asynchronous modulation and the PVD process changes the multilayer periodicity, morphology and hardness which can result in developing materials that maximize the hardness of high entropy alloys with the goal of creating high hardness boride coatings.

### **<u>S19 Molecular-level Processing and Chemical</u>** <u>Engineering of Functional Materials</u>

### **S19- Precursor-derived ceramics for sustainability I** Room: Ballroom 3

Session Chair: Gurpreet Singh, Kansas State University

### 8:30 AM

### (ICACC-S19-026-2025) Polymer derived ceramics as the source of carbon for the electrocatalytic layer in proton exchange membrane fuel cells (Invited)

A. Tamayo\*1; E. Chinarro1; J. Rubio1

1. Institute of Ceramics and Glass, CSIC, Spain

Among the different options to address the rising energy demands while reducing greenhouse gas emissions, there withstand the proton exchange membrane fuel cells which directly converts chemical energy into electrical energy by electrochemical reaction. The performance of the cell is dependent on the electrochemically active surface area available in the electrodes for reaction and the uninterrupted flow of reactants and products to and from the reaction sites. Carbide derived carbons (CDC) were prepared from commercially available polycarbosilanes and polysiloxanes with silicon alcoxides at different concentrations. The preceramic materials were pyrolyzed and subsequently dry etched to extract the carbon phase have been used to manufacture electrocatalytic membranes for PEMFC. The obtained materials possess a microporous / mesoporous structure, which is dependent on the composition of the preceramic polymer used. The carbon-based catalyst was processed by direct deposition of Pt nanoparticles on the CDC. The catalyst ink was sprayed over a Teflon-coated gas diffusion layer and the H2 production was evaluated through cyclic voltametric analysis. The results show the relevance of tunning the distribution of the carbon phase on the preceramic polymer to achieve the best textural / electrical conductivity balance for the maximum H2 evolution.

### 9:00 AM

# (ICACC-S19-027-2025) Photopolymerization-assisted solidification templating of Ni-modified polysiloxane for $\rm CO_2$ methanation

K. Rauchenwald\*2; K. Föttinger1; T. Konegger2

- 1. Technische Universitat Wien, Institute of Materials Chemistry, Austria
- 2. Technische Universitat Wien, Institute of Chemical Technologies and Analytics, Austria

Polymer-derived ceramics (PDCs) allow structuring and chemical modification of preceramic polymers. PDCs can further be combined with freeze-casting to introduce directional macroporosity. Crosslinking at low temperature is assisted by photopolymerization and the polysiloxane is modified with Ni<sup>2+</sup> to derive monolithic Ni/SiOC catalysts, where in-situ formed Ni nanoparticles provide an alternative to conventional coatings prone to sintering-induced deactivation. Polysiloxane is modified with amine- and acrylatesilane compounds in a co-hydrolysis reaction before Ni(NO<sub>3</sub>)<sub>2</sub> is added, complexing with amine groups bound to the polymer. The complexation shifts the absorption maximum from 408 nm to 390 nm in case of the aqua or amine complex, respectively, enhancing photopolymerization-assisted crosslinking at 405 nm. The modified resin is freeze-cast in cyclohexane and photopolymerized at -20 °C, templating dendritic macroporosity. After drying and pyrolysis at 900 °C, Ni/SiOC monoliths are obtained with 5 wt.% of metallic Ni in amorphous SiOC matrix. The monoliths are evaluated for catalytic performance in CO<sub>2</sub> methanation. The results show a promising approach towards monolithic Ni/SiOC-based CO<sub>2</sub> methanation catalysts as an alternative to catalysts prepared by wet impregnation, which showed severe degradation upon operation of 50 h due to sintering of Ni nanoparticles coating.

### 9:20 AM

# (ICACC-S19-028-2025) Topochemical fluorination and de-fluorination in the context of photocatalysis and tailoring optical properties (Invited)

S. Perween<sup>\*1</sup>

1. University of Stuttgart, Institute for Materials Science, Germany

Topochemical modifications of the anion sublattices in Ruddlesden-Popper-type (RP) oxides,  $A_{n+1}B_nO_{3n+1}$ , and their derived metastable oxyfluorides/de-fluorinated oxides,  $A_{n+1}B_nO_{3n+1-x}F_{2x}$  (0 < x ≤ 2; A = La, Y, Ca, Ba, Sr; B = In, Sb, Ti), significantly impact the crystal and electronic structures of the newly synthesized phases. This lecture focuses on low-temperature topochemical reactions of RP oxides, indates, and titanates, as a novel approach to investigating the structural–optical properties and their impact on the photocatalytic performance of H<sub>2</sub> evolution. Using polymer-based chemicals like PVDF/PTFE, and hydride-based reducing agents (NaH, CaH<sub>2</sub>), at low temperature, enables reversible tuning of these properties. The resulting changes were analyzed through various diffraction and spectroscopic techniques. The materials also demonstrate broad reactivity for topochemical anion sublattice modifications, e.g. for n = 1, LaBaInO<sub>4</sub> to LaBaInO<sub>3</sub>F<sub>2</sub>, via non-oxidative fluorination, show altered structural and optical properties, with both exhibiting photocatalytic activity for H<sub>2</sub> generation. This study highlights the potential of oxyfluorides as a new class of photocatalysts, and its topochemical de-fluorination which is reversibly possible to extract via hydride-based reduction offering insights into designing advanced materials for tailoring the optical properties.

### **S19- Precursor-derived ceramics for sustainability II** Room: Ballroom 3

Session Chairs: Shama Perween, University of Stuttgart; Peter Kroll, University of Texas, Arlington

### 10:10 AM

# (ICACC-S19-029-2025) Wet-chemical assisted synthesis approaches to access MAX phases and antiperovskite phases (Invited)

N. Kubitza\*1

1. Technische Universitat Darmstadt, Eduard-Zintl-Institute, Germany

MAX phases and antiperovskites, two fascinating material classes exhibiting a unique set of different characteristics. While the former are classically defined as ternary transition metal-based carbides and (carbo)nitrides that combine metallic and ceramic properties, the latter are defined as electronically inverted perovskites, showing promising functionalities (e.g. magnetism). Despite the potential of both material classes, their synthesis is still mainly achieved by solely conventional-based solid-state methods showing drawbacks in the energy efficiency, chemical versatility, or morphology. A promising alternative to circumvent these drawbacks is to combine conventional preparation steps with wet-chemical-based methods such as the sol-gel synthesis or the liquid ammonia method. This led to the synthesis of new carbo(nitride) MAX phases, a highly underrepresented group within the family of MAX phases. Additionally, by analyzing the magnetic and transport behavior of these samples, it was shown that the incorporation of nitrogen beneficially influences the materials properties. On the other hand, in the field of APVs, a one-step sol-gel method was applied which led to the successful synthesis of Mn-based carbide antiperovskite phases with the power to specifically influence magnetic properties by only slight adjustments of parameters within the wet chemical-based synthesis procedure.

### 10:40 AM

## (ICACC-S19-030-2025) Voltage Cutoff Techniques to Improve Cycling Stability in WS $_2$ Nanocages for Na $^+$ and K $^+$ Storage

A. Roy\*1; G. Singh1

1. Kansas State University, Mechanical and Nuclear Engineering, USA

The large interlayer spacing in transition-metal dichalcogenide (TMD)-based electrodes enhances the storage of Na and K ions. However, side reactions and volume changes that damage the TMD crystalline structure remain significant challenges for their use in next-generation devices. This study investigates whether the structural distortion leading to poor cycling stability is also present in inorganic fullerene-like (IF) tungsten disulfide (WS<sub>2</sub>) nanocages (WS<sub>2</sub>IF). To mitigate these issues, the study introduces upper and lower voltage cutoff experiments to limit specific reactions in Na<sup>+</sup>/WS2IF and K<sup>+</sup>/WS2IF half-cells. Three-dimensional (3D) differential capacity curves and surface plots reveal that applying a high upper cutoff technique maintains reversible reactions, indirectly indicating restricted structural dissolution. This approach results in better capacity retention, stable performance, and higher Coulombic efficiency, supporting the potential use of TMD-based materials beyond Li-ion storage devices.

### 11:00 AM

## (ICACC-S19-031-2025) PDC $MoS_2$ nanocomposites—preparation and performance as Li-ion battery electrode

A. Roy<sup>1</sup>; G. Singh\*<sup>1</sup>

1. Kansas State University, Mechanical and Nuclear Engineering, USA

Layered transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS<sub>2</sub>), have attracted widespread attention due to their unique microstructure and potential application in electrochemical storage systems. In this study, the MoS<sub>2</sub> nanosheets were chemically modified with polymer-derived ceramics (PDCs), and their electrochemical performances were studied for use in lithium-ion batteries. Three analogous precursors with similar chemical structures and functional groups were analyzed to synthesize the silicon oxycarbide (SiOC) ceramic in the functionalized MoS<sub>2</sub>-SiOC structures. This modification of TMD enables enhanced resistance to dissolution and material degradation while maintaining its lithium storage properties. The polymer-to-ceramic transition of SiOC and the morphological features of MoS<sub>2</sub> were analyzed using electron microscopy and spectroscopic techniques.

### 11:20 AM

## (ICACC-S19-032-2025) Contribution of ceramic-based cathodes for long-term lithium-sulfur batteries

M. M. Amaral\*1; J. Nelson Weker3; H. G. Zanin1; G. Singh2

- 1. Universidade Estadual de Campinas, Electrical and Computer Engineering, Brazil
- 2. Kansas State University, Mechanical and Nuclear Engineering Dept., USA
- 3. SLAC National Accelerator Laboratory, Stanford Synchrotron Radiation Lightsource, USA

Lithium-sulfur batteries' low cyclability, which results from their accelerated degradation due to the shuttle effect, is a well-known issue. Furthermore, the encapsulation of sulfur into porous hosts is an alternative to inhibit the migration of lithium polysulfides to the lithium anode, thereby enabling the design of long-term lithium-sulfur batteries. Porous polymer-derived ceramics (PDCs) have rarely been investigated as sulfur hosts. Among PDCs, silicon oxycarbide (Si<sub>x</sub>O<sub>y</sub>C<sub>z</sub>), which contains Si-O, SiC, and C-phases, can physically confine intermediate lithium-polysulfides in the porous carbon domains and possibly adsorb intermediate lithium-polysulfides in their Si-O domains. Then, we investigated the contribution of SiOC derived from the pyrolysis of a polysiloxane as a sulfur host. The SiOC provided a reversible capacity of 515 mAh gs<sup>-1</sup> after 200 cycles at a gravimetric current of 167.5 mAg<sub>s</sub><sup>-1</sup>. This result indicates that PDCs, particularly SiOC, can efficiently mitigate the shuttle effect and support the design of long-term lithium-sulfur batteries. Acknowledgments: FAPESP (grant numbers: 2021/09387-1; 2023/11416-5).

### 11:40 AM

# (ICACC-S19-033-2025) Enhancing Lithium-Ion Battery Performance with $\rm C_{60}$ -Reinforced Self-Supporting SiOC Composite Electrode

A. Roy\*1; G. Singh1

1. Kansas State University, Mechanical and Nuclear Engineering, USA

Precursor-derived silicon oxycarbide (PDC SiOC) has attracted considerable interest as a promising high-capacity anode material for lithium-ion batteries. The unique polymer processing and pyrolysis method characteristic of PDC enables chemical interactions with various nano-precursors and nanofiller phases, facilitating the creation of low-dimensional composite structures such as fibers and coatings, which are difficult to achieve with traditional sintered ceramics. In this study, buckminsterfullerene ( $C_{60}$ ) was incorporated into a 1,3,5,7-tetramethyl-1,3,5,7-tetravinyl-cyclotetrasiloxane (TTCS) hybrid precursor to produce electrospun fibermats. These fibermats were subsequently subjected to heat treatment at low and then high temperatures to form SiOC ceramic composite fibers reinforced with  $C_{60}$ . The morphology and chemical evolution of the as-spun, stabilized, and ceramicized fibermats were analyzed using electron microscopy and various spectroscopy techniques. When tested as a self-supporting working electrode in a lithium-ion half-cell, the  $C_{60}$ -reinforced fibermats demonstrated superior performance compared to pristine  $C_{60}$ , SiOC, and carbon fiber electrodes in terms of reversible capacity, cycle efficiency, rate capability, and capacity retention at high current densities.

### FS7 Ceramics for global decarbonization

### FS7- Carbon Capture, Utilization, and Storage

Room: Ballroom 5

Session Chairs: Charles Lewinsohn, Colorado State University System; Marta Boaro, Universita degli Studi di Udine

### 1:30 PM

## (ICACC-FS7001-2025) Opportunities for ceramics to decarbonize power generation through fusion (Invited)

Y. Katoh\*1

1. Oak Ridge National Laboratory, USA

Fusion energy holds great promise for generating abundant power with minimal greenhouse gas emission on a global scale. Advanced ceramics and composites are essential enabling technologies for fusion, much like their roles in various modern energy and power systems. Materials in fusion power systems must maintain their functionality and structural integrity throughout their service life that must be sufficiently long to prove economic viability. What makes fusion materials research and development uniquely challenging is their harsh operating environment that combines multiple extremes, typically including high temperature and high heat flux, corrosive media, ionizing radiation, interactions with plasma and fuel hydrogen, and high energy neutrons generating atomic displacement damage and nuclear transmutations simultaneously. Advanced engineering ceramics, structural composites, and special purpose ceramics are considered for a variety of functional and thermostructural components. This presentation provides an overview of applications of ceramics and composite materials in key in-vessel components in proposed fusion system concepts, followed by discussion on the opportunities of materials science and engineering research. This study was partly supported by the US Department Energy (DOE), Office of Fusion Energy Sciences under contact DEAC05-00OR22725 with ORNL, managed by UT Battelle, LLC.

### 2:00 PM

## (ICACC-FS7002-2025) Taking Flight with Direct Air Carbon Capture (Invited)

L. McMillon-Brown\*1; J. Stenlid²; A. Ravichandran²; E. Skountzos²; J. Lawson²

- 1. NASA Glenn Research Center, Photovoltaics and Electrochemical Systems Branch, USA
- 2. NASA Ames Research Center, USA

Human activities have significantly altered the composition of the Earth's atmosphere, leading to a rise in greenhouse gasses including carbon dioxide ( $CO_2$ ) and methane ( $CH_4$ ). These two gases are responsible for the dramatic increase in the Earth's average temperature. In addition to limiting greenhouse gas emissions, there is a need to remove carbon from the atmosphere to preserve the climate and maintain Earth's habitability. The current state of the art for direct air carbon capture (DAC) are large, fixed, ground based systems, limited to where they can installed. Here we present an airborne direct air carbon capture solution that is autonomous, mobile, and versatile. NASA's Sustainably-powered Planetary RejUvenation via Carbon Entrapment (SPRUCE) project, is designing a high throughput, direct air capture system that can be deployed across the planet. SPRUCE will enable sustainable and scalable GHG

sequestration and could be deployed via aircraft to enable airborne DAC. This talk will include a project overview, systems analysis, and identification of technological gaps which the ceramics community could aid to close.

#### 2:30 PM

## (ICACC-FS7003-2025) High temperature electrolysis for decarbonization and syngas production

A. Michaelis<sup>\*1</sup>

1. Fraunhofer IKTS, Germany

Ceramic materials and components play a key role in the production, transport, and application of green hydrogen and syngas. We present new results for ceramic based steam electrolysis systems: SOE (solid oxide electrolysis). SOE offers three essential unique advantages: Co-electrolysis capability, i.e. both water steam and  $CO_2$  can be simultaneously processed to form syngas (H<sub>2</sub> + CO). With this, CO<sub>2</sub> can be actively removed from the environment. The produced syngas can be used for PtX products like e-fuel, higher alcohols, waxes, etc. For this, we present a fully integrated co-electrolysis Fischer Tropsch System. 30 % higher efficiency for power to green hydrogen conversion compared to competing technologies (e.g. alkaline and PEM electrolysis) with the use of waste heat at a heat level of 100 °C. Complete reversibility. SOE systems can be operated in the reverse mode, i.e they can be used as fuel cells using hydrogen or/and syngas or other hydrocarbon fuels as well as ammonia to generate power. Moreover, the combination of SOE with the Haber Bosch process allows for green ammonia NH<sub>3</sub> production. As a hydrogen carrier Ammonia can contribute to the transport challenge in a future hydrogen economy.

#### 2:50 PM

### (ICACC-FS7004-2025) Producing Onsite Hydrogen and Syngas for Manufacturing Feedstocks, Distributed Fuels and Onsite Energy

S. Reinartz\*1; B. Blackburn1

1. Utility Global, Inc., USA

This presentation covers the operational and performance results of a zero-electricity electrolytic reactor installed at a steel mill to produce high-purity hydrogen from blast furnace waste gases. Traditional methods of low carbon intensity hydrogen production often require significant electricity inputs, infrastructure and CAPEX, which are at odds with many operational and business objectives. The tested and demonstrated zero-electricity electrolytic hydrogen reactor offers a solution to this challenge. This presentation covers the science and technology of this novel reactor and the underlying eXERO(TM) technology platform, as well as the results of an extensive operation which took place over the span of nine months and achieved several groundbreaking results. This presentation provides valuable insights into the function of the zero-electricity electrolytic hydrogen reactor and its implications for the ongoing energy transition and industrial transformation. It offers a viable pathway for hard-to-abate industries to transition to cleaner energy sources while maintaining their productivity and competitiveness in a rapidly evolving global market.

### FS7-Energy Efficiency

Room: Ballroom 5

Session Chairs: Charles Lewinsohn, Colorado State University System; Alexander Michaelis, Fraunhofer IKTS

### 3:30 PM

# (ICACC-FS7005-2025) Development of Aurivillius-based photoelectrodes for the photoelectrochemical CO<sub>2</sub> reduction reaction (Invited)

S. Casadio<sup>1</sup>; N. Sangiorgi<sup>1</sup>; A. Sanson<sup>\*1</sup>

1. CNR-ISSMC, Italy

In recent years, bismuth-based photocatalysts have been receiving increasing attention in photocatalysis, due to their appropriate bandgap and tunable surface structure, which make them suitable for several photocatalytic processes. Their performances, however, are still limited by the fast charge-carriers recombination. Recently, the exploitation of piezo/ferro-electric potentials in photo-active semiconductors has been adopted as an effective strategy to modulate the charge transfer properties both in the bulk phase and at the surface of semiconductors (i.e., piezo-phototronic effect). In this work, Aurivillius compound (ie.g, Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> - BiTO,) as photo-electrode material for solar conversion has been studied in detail, targeting the  $CO_2$  reduction reaction ( $CO_2RR$ ). The effect of the ferroelectric potential on the photo-electrochemical performances of the optimized photo-electrodes was therefore accurately studied. Density current increments and enhanced charge transfer ability were registered under the optimal ferroelectric polarization, proving the possibility of adopting ferroelectric polarization coupled with an external bias to effectively control the migration of photo-generated charges in bismuth-based Aurivillius semiconductors for the CO<sub>2</sub>photoelectrochemical reduction.

### 4:00 PM

### (ICACC-FS7006-2025) Sustainable solid sorbents for CO<sub>2</sub> capture – Amine functionalized layered oxides

P. Behr<sup>+1</sup>; M. Pizzoccaro-Zilamy<sup>2</sup>; S. Baumann<sup>1</sup>; O. Guillon<sup>1</sup>; W. Brilman<sup>2</sup>; W. Meulenberg<sup>1</sup>; L. Lefferts<sup>2</sup>

- 1. Forschungszentrum Julich GmbH, IMD-2, Germany
- 2. University Twente, Netherlands

According to the latest IPCC reports utilization of negative emission technologies (NETs) is mandatory to reach our climate goals. Among NETs the direct capture of CO<sub>2</sub> from ambient air (DAC) offers a decentralized and scalable approach. State of the art sorbents show high capacities but lack in terms of sustainability and cost. Naturally abundant layered oxides functionalized with amines could offer sufficient performance at lower cost and higher sustainability. In this context, clay minerals were intercalated with amines via ion-exchange to make the interlayer accessible for air and introduce a strong affinity for CO<sub>2</sub>. Additionally, the layered structure of hydrotalcite was collapsed via heat-treatment and the resulting material functionalized with tetraethylenpentamine and aminomethylphosphonicacid via wet-grafting under reflux. Success of functionalization was investigated via XRD, FT-IR and elemental analysis, CO<sub>2</sub> capacity was evaluated via sorption isotherms. Intercalation of L-Arginine and Guanidium into the interlayer of montmorillonite was successful, leading to an increase in CO<sub>2</sub> capacity, depending on the amount of amine in the interlayer. A comparison between both molecules shows that L-Arginine leads to higher capacity at 1 bar, while Guanidium performs better at low pressure. A MgAl-mixed metal oxide was synthesized from hydrotalcite and functionalized successfully.

### 4:20 PM

### (ICACC-FS7007-2025) Role of catalysis in promoting chemical looping processes and oxygen transport in perovskite-derived oxides

M. Boaro\*1; F. Orsini2; A. Strazzolini1; D. Ferrero2; M. Santarelli2;

- A. Trovarelli<sup>1</sup>
- 1. Universita degli Studi di Udine, Polytechnic Department of Engineering and Architecture, Italy
- 2. Politecnico di Torino, Italy

Chemical looping (CL) processes are currently considered a promising strategy for the efficient use of CO<sub>2</sub> and the synthesis of green H<sub>2</sub>. They consist of performing redox reactions in two separate steps, using a reducible oxide as a mediator for oxygen transfer. Perovskites and parent perovskite oxides have been extensively studied due to their compositional versatility, which offers several ways to tune their redox properties [1], but these structures have limitations in the reversibility of the redox cycle or the kinetics of the two steps. Based on our recent results [2,3], in this work we aim to illustrate several strategies to improve the reactivity and long-term stability of CL processes. The segregation of nickel metal from the double perovskite Sr<sub>2</sub>FeMo<sub>0.6</sub>Ni<sub>0.4</sub>O<sub>6</sub> and the catalytic promotion of Ca<sub>2</sub>Fe<sub>2</sub>O<sub>5</sub> by Ni are the cases presented to illustrate the role of transformation and co-presence of a catalyst in promoting oxygen transport. This allows some guidelines to be drawn for the design and optimisation of highly versatile, low-cost oxygen carriers for technology developments based on thermo/chemical redox cycles that can be integrated with the direct use of renewable energy for greenhouse gas reduction. 1. Y. Kim et.al J. CO<sub>2</sub> Utilizat., 63, 2022, 102139. 2. F. Orsini et al. Chem. Eng. J. 475 (2023) 146083 3. A. Strazzolini et.al Vol. 2 (2023): SolarPACES 2023.

### 4:40 PM

### (ICACC-FS7008-2025) Solar Thermochemical Fuel Production: Multiphysics Modeling of the Ceria Redox Cycle with Non-Uniform Porous Morphologies

F. Orsini<sup>\*1</sup>; D. Ferrero<sup>1</sup>; M. Santarelli<sup>1</sup>

1. Politecnico di Torino, Department of Energy, Italy

In solar-driven thermochemical splitting of H<sub>2</sub>O and/or CO<sub>2</sub>, solid Oxygen Carriers (OCs) are used in the solid-gas oxygen transfer reactions, with the generation of high-energy molecules (H<sub>2</sub>/CO) as the net result. Ceria  $(CeO_2)$  is the state-of-art nonstoichiometric OC thanks to its fast kinetics and good stability upon cycling. The redox cycle is composed of a thermal reduction step, in which oxygen is abstracted from the OC lattice at high temperature (around 1500 C) and low oxygen partial pressure, followed by a re-oxidation step, in which the solid OC reacts with  $H_2O/CO_2$ , thereby replenishing the lattice oxygen and releasing H<sub>2</sub>/CO. This work dives into the multiphysics modeling of a reactor device for solar thermochemical fuel production, addressing the detailed coupling among fluid flow, heat and mass transfer, radiation, and solid-gas chemistry. The ceria redox-active medium is modeled as a dual-scale porosity reticulated porous ceramics, making use of literature correlations for the effective heat and mass transport properties. We present the results in terms of temperature and nonstoichiometry fields considering different non-uniform morphology distributions, giving insights on the optimal configurations. We show how our model can be used to optimize the solar thermochemical fuel production process in terms of geometry and morphology of the redox medium.

### <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

### **S1- Ceramic Matrix Composites (CMCs) Processing-Microstructure-Mechanical Properties Correlation** Room: Coquina E

Session Chairs: Walter Krenkel, University of Bayreuth; Dietmar Koch, University of Augsburg; Tadashi Matsunaga, UBE Corporation

### 1:30 PM

### (ICACC-S1-038-2025) Continuous Silicon Carbide-based Ceramic Fibers (Tyranno Fiber®) Developed by UBE Corporation and their Mini-Composite Performance

T. Matsunaga\*1

1. UBE Corporation, Specialty Products Division, Japan

UBE Corporation has developed several types of silicon carbidebased fibers which is called to "Tyranno Fiber®" for a few decades. The silicon carbide-based fibers are often used as a reinforcement materials for a silicon carbide fiber reinforced silicon carbide ceramic matrix composite (SiC/SiC-CMC). The SiC/SiC-CMC requires high-temperature capability because the SiC/SiC-CMC is expected to be utilized in various harsh environments such as a hot-section of turbine engine, a cladding rod of nuclear reactor, blanket of fusion reactor and so on. Besides since the silicon carbide fiber strongly governs to the SiC/SiC CMC, the higher temperature capability silicon carbide fibers are required accordingly. Thus, the high temperature capability, mechanical properties and so on of silicon carbide fibers has been improved. In the presentation, we would like to explain not only a few grades of Tyranno Fiber\* developed by UBE Corporation but also SiC/SiC minicomposites reinforced by the Tyranno Fiber\*.

### 1:50 PM

# (ICACC-S1-039-2025) Development and mechanical characterization of short fibers ceramic matrix composites through bending tests

- U. Legallois\*1; S. Beaudet-Savignat1; P. Hourquebie1; D. Brandt1; J. Gerard2
- 1. Commissariat a l'energie atomique et aux energies alternatives Direction des applications militaires Le Ripault, Material, France
- 2. Ingenierie des Materiaux Polymeres, France

Oxide Ceramic Matrix Composites (OCMC) combine good mechanical properties with high thermal resistance (in the range of 800 - 1200 °C) even in oxidizing atmosphere. This type of material offers many advantages compared to classically used nickel-based super alloy and appears as a good candidate for high-temperature structural applications. However, the manufacturing process of continuous fibers CMC is difficult to master and generally expensive. Moreover, the composite parts used in aerospace industry often have complex fiber architectures, which can lead to anisotropic mechanical behavior. Using short fibers in the composite material would allow for more consistent properties and easier processing while still reinforcing the material compared to the monolithic ceramic. This study aims to develop a Short Fiber Oxide Ceramic Matrix composite (SF-OCMC). A manufacturing process has been develop to obtain SF-OCMC by a casting method. The samples were characterized by 4 points bending tests to understand the mechanical properties of SF-OCMC and a comparison was made with monolithic ceramics.

### 2:10 PM

# (ICACC-S1-040-2025) Processing - microstructure – mechanical properties relationship of discontinuous SiC fibers reinforced-intermetallic matrix composites

#### E. Daufresne de la Chevalerie\*1; M. Bechelany3; O. Dezellus2; Y. Le Petitcorps1

- 1. Laboratoire des Composites Thermostructuraux, France
- 2. Laboratoire des Multimateriaux et Interfaces, France
- 3. Safran Tech, Safran Ceramics, France

Discontinuous SiC fibers reinforced-intermetallic matrix composites have been prepared by Spark Plasma Sintering (SPS). The multicomponent matrix is composed of the hexagonal (Mo,Ti)Si2 disilicides solid solution as well as SiC particles. Hi-Nicalon chopped SiC fibers were homogeneously dispersed within the matrix material up to 30 vol% and the composite powder was sintered by SPS in a single-step. To avoid the degradation of SiC fiber properties, a low temperature and short time cycle was developed by controlling the composition of the matrix. Room-temperature (RT) flexural strength and Young modulus were measured with 4-point bending tests. Both the effect of the fibers volumic fraction and the sintering cycle on the RT-mechanical behavior were investigated. Additionally, the matrix alone was also characterised in order to further understand the composite's properties. In the investigation range, an optimal SiC fibers amount for good densification of ~ 25 vol% has been found. This study underlines the role of the matrix composition and microstructure as well as the sintering cycle on the composite's RT mechanical properties.

### 2:30 PM

### (ICACC-S1-041-2025) Development of a Novel Oxide Composite for Use as a High-Temperature Solid-State Lubricant

C. Grimley\*<sup>1</sup>; E. Volpe<sup>2</sup>; J. Kweder<sup>2</sup>; A. Kupferberg<sup>1</sup>

- 1. Lucideon Ltd, United Kingdom
- 2. Technetics Group, USA

In the push for de-carbonization in energy production and use, many industrial applications seek to operate at higher and higher temperatures in order to improve efficiency. This effort requires the development of a new suite of materials and coatings which resist mechanical and chemical degradation at high temperatures. One of these material needs is the development of more robust lubricants. While solid-state lubricants are not a new research topic, their compositions usually belong to the MXene family due to their favorable laminar crystal structures. However, these transition metal compositions are usually based on non-oxide anions (C, F, etc.) which possess limited oxidation resistance. This talk focuses instead on the development of a novel Al2O3-based composite for high temperature performance and increased oxidation resistance, specifically for dynamic wear applications. It will walk through the development cycle of this new material from lab-scale pellets to prototype-scale components, addressing both the practical manufacturing considerations and performance optimization. The phase and microstructural characteristics of the composite under different processing conditions and relative compositions will be discussed, and these results will be connected with performance in friction tests.

#### 3:10 PM

### (ICACC-S1-042-2025) Advances in additive manufacturing of carbon and carbide complex architectures: from replica of 3D printed templates to ceramic matrix composites (Invited)

A. Ortona<sup>\*1</sup>

1. SUPSI, MEMTi, Switzerland

Ceramic additive manufacturing (AM) has been successfully employed across various industrial fields to produce components with medium to high dimensional precision. In this presentation, we show the state of the art and the latest advancements in the most promising ceramic AM techniques for carbon and carbide materials: binder jetting and selective laser sintering (SLS) of polymers. These AM techniques produce an intermediate product that undergoes further processing, such as polymer infiltration and pyrolysis (PIP), reactive melt infiltration (RMI), or chemical vapor infiltration (CVI). These technologies offer several advantages, including high maturity, low cost, and improved resolution, driven by the latest AM machines available on the market.

#### 3:40 PM

### (ICACC-S1-043-2025) Understanding gas phase formation of silicon carbide during reactive melt infiltration of carbon substrates (Invited)

M. Prakasan<sup>1</sup>; T. Schneider<sup>2</sup>; D. Koch<sup>\*1</sup>

- 1. Universitat Augsburg, Institute of Materials Resource Management MRM, Germany
- 2. ArianeGroup GmbH, Germany

Carbon-Carbon composites with Silicon Carbide surface (C/C-SiC) are valued for their exceptional thermal and oxidation resistance. Reactive Melt Infiltration (RMI) is used to impart oxidation resistance to the composites by transforming the surface of carbon matrix into silicon carbide (SiC). Prior studies prove that SiC can occur from gas phase reactions before silicon reaches its melting point. This SiC is green, porous in nature and impedes the melt infiltration process by consuming the available silicon. Such unsuccessfully siliconized components with green surface possess lower thermal resistance, inducing high-temperature surface damage during application. Gas phase reactions during RMI also have other inadvertent consequences such as incomplete infiltration, unmolten Si particles and green deposits in the furnace. Hence, a complete understanding of these gas phase reactions is vital to improve the success rate of infiltration process. This study, through experiments in a high temperature graphite analytical furnace, confirms SiC formation via gas phase during RMI and examines the factors influencing it. Corresponding reaction paths are investigated using in-situ Fourier Transform Infrared (FTIR) spectroscopy. Finally, this study also explores microstructural differences in green SiC, proposing a fourstep reaction model for gas-phase reactions in the RMI system.

### 4:10 PM

## (ICACC-S1-044-2025) Ceramic Matrix Composites (CMC) made of newly available SILAFIL\* SiC Fibers (Invited)

- W. Humbs\*1; M. Rothmann1; K. Jaeger1
- 1. BJS Ceramics GmbH, Germany

BJS Ceramics has developed SiC fibers in Germany using locally sourced raw materials. Commercial production has started. An update on the status of our different generations of SILAFIL\* SiC fiber will be presented. Ceramic Matrix Composites (CMCs) have been developed based on a European supply chain with the availability of SILAFIL\* fibers. Due to the material being classed as an export controlled good, a regional supply chain is an essential element to develop CMC components in next generation applications such as aero engines, energy generation (gas turbines, fission and fusion) and space. The CMCs consist of SILAFIL\* SiC fiber reinforced SiC matrix produced via a CVI (Chemical Vapor Infiltration) process resulting in a SiC/SiC composite. We will present highly promising and interesting mechanical performance data, insight into microstructures and compositions, and give an outlook into future applications and fiber quality.

### 4:40 PM

### (ICACC-S1-045-2025) Synthesis and Processing of YSZ/SiBCN Ceramic Matrix Composites for Hydrogen-Fueled Gas Turbine Engines

Y. Wang\*1; F. Faysal1; C. Maitti1; J. Gou1

1. University of Central Florida, Mechanical and Aerospace Engineering, USA

Gas turbine engines for power generation are under transition to hydrogen-based combustion systems to achieve net-zero carbon emissions. However, the materials utilized in combustion engines powered by hydrogen must withstand high temperatures and enhanced chemical corrosivity brought due to the production of water vapor during hydrogen combustion. To meet such rigorous requirements, ceramic matrix composite (CMC) utilizing yttria-stabilized zirconia (YSZ) fiber reinforced SiBCN matrix has been developed in this study. YSZ fibers can withstand temperatures up to 2,200C and are corrosion resistant against oxidizing and reducing atmospheres. SiBCN ceramic was synthesized from liquid polyborosilazane precursor followed by curing and pyrolysis. Presence of Boron in the resin helps for better high-temperature anti-oxidation performance than their counter part. Surface structure and elemental analysis of YSZ/SiBCN composites has been performed by SEM and XRD measurements. Thermal stability, anti-oxidation behavior, and ablation performances were explored using high-temperature TGA (up to 1,350C) and providing heat flux exposure in real time by the Hydrogen Torch Test. Tests involving combustion environment demonstrate that the CMC remains stable making it a promising candidate material for hydrogen-fueled gas turbine engines.

### <u>S2 Advanced Ceramic Coatings for</u> <u>Structural/Environmental & Functional</u> <u>Applications</u>

## S2- New testing simulation and material concepts for T/EBC III

Room: Coquina C Session Chair: Eric Jordan, University of Connecticut

### 1:30 PM

(ICACC-S2-036-2025) Development of a Multi fuel-Multi geometry-Multi atmosphere rig for testing high temperature performance of thermal/environmental barrier coatings (Invited)

R. Naraparaju\*1

1. DLR - German Aerospace Center, Materials Research, Germany

High temperature testing of thermal and environmental coatings under aggressive environments such as high gas/steam velocities, CMAS/VA deposition, application of thermal gradient under cyclic conditions etc. is quite challenging. Completely different experimental set ups were in use in order to simulate each condition. Sometimes, due to the limitations of the setup, a compromise has to be made in terms of sample geometry. However, testing of the engine hard ware such as vanes or blades made of alloys or ceramic composites is very complicated. A novel test set up has been designed and constructed in order to integrate all the aforementioned environments in a single set up for the first time. M<sup>3</sup> test rig mainly contains a burner which can handle hydrogen, methane and their mixtures, inter changeable substrate holder module, a combustion chamber where coated specimen or hardware can be placed and tested under gas velocities up to 45m/s.

### 2:00 PM

# (ICACC-S2-037-2025) Environmental Barrier Coating Surface Temperature Mapping Using a Compatible Er-Doped $\rm Sc_2SiO_5$ Temperature Sensing Layer

J. I. Eldridge\*1; K. Lee1; J. A. Setlock2

- 1. NASA Glenn Research Center, USA
- 2. The University of Toledo, USA

Accurate surface temperature-mapping capabilities in the 1300 to 1500 °C range are needed for SiC/SiC ceramic matrix composites protected by environmental barrier coatings (EBCs) under testing in turbine engine environment facilities. The strong background thermal radiation at these higher temperatures is a challenging issue. Er-doped Y<sub>2</sub>SiO<sub>5</sub> was previously shown to be capable of achieving luminescence lifetime-based temperature mapping up to 1560 °C as a standalone material. However, compatibility issues between an Er-doped Y<sub>2</sub>SiO<sub>5</sub> surface temperature sensing layer and an underlying Sc<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>-based EBC topcoat limited temperature mapping of the EBC surface to a maximum of 1380 °C. Therefore, an Er-doped Sc<sub>2</sub>SiO<sub>5</sub> temperature sensing layer has been subsequently developed with better compatibility with the Sc<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>-based EBC topcoat. Localized spot temperature measurements as well as luminescence lifetime imaging-based temperature mapping were demonstrated up to 1535 °C from a 15 µm thick Er-doped Sc<sub>2</sub>SiO<sub>5</sub> layer at the surface of a Sc<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>-based EBC topcoat, a significant improvement over the Er-doped Y<sub>2</sub>SiO<sub>5</sub> layer 1380 °C temperature sensing limit. No degradation of the Er-doped Sc<sub>2</sub>SiO<sub>5</sub> temperature sensing layer was observed.

### 2:20 PM

### (ICACC-S2-038-2025) Pull Adhesion Testing of HfO<sub>2</sub> Coatings

- A. Vozar<sup>2</sup>; R. Sarrafi-Nour<sup>3</sup>; B. J. Harder<sup>4</sup>; J. Salem<sup>\*1</sup>; M. Slizik<sup>4</sup>; M. J. Presby<sup>4</sup>
- 1. NASA Glenn Research Center, Materials and Structures, USA
- 2. GE Research, Performance Coatings, USA
- 3. GE Aerospace, Research Center, USA
- 4. NASA Glenn Research Center, Environmental Effects and Coatings, USA

The introduction of silicon carbide/silicon carbide (SiC/SiC) ceramic matrix composites (CMCs) into the aviation turbine engine hot section enabled increased inlet temperature and reduced cooling requirements. Environmental barrier coatings (EBCs) are required to achieve the durability needs of CMC aerospace turbine components. Future EBC oxide topcoats will need to provide sufficient thermal capability to support turbine inlet temperatures in excess of 3000°F (1650°C), thermal barrier function and acceptable mechanical properties such as adhesion strength. Hafnium oxide (HfO2) has been evaluated as a prospective oxide topcoat material and can be deposited in a pseudocolumnar structure for increased in-plane compliance to better manage the thermal expansion mismatch stresses with Si-based ceramics, thus, to help adhesion to Si-based ceramics. Coatings were applied using two different processing methods on bulk  $\alpha$ -SiC substrates to compare the properties of the two deposition methods. Samples were exposed to aging heat treatment from 2500-2800°F (1371-1538°C) in air and mechanical pull testing was conducted at room temperature to track the adherence with aging. The pull adhesion test results revealed sensitivities to the strength of the monolithic SiC substrate and potential confounding effects associated with bonding adhesive layer and preparation conditions.

### 2:40 PM

### (ICACC-S2-039-2025) Foreign Object Damage in Environmental Barrier Coatings Deposited on a Ceramic Matrix Composite

- L. C. Hoffman\*1; M. J. Presby2
- 1. HX5, LLC, NASA Glenn Research Center, USA
- 2. NASA Glenn Research Center, Environmental Effects and Coatings Branch, USA

Foreign object damage (FOD) is one of the key damage modes in environmental barrier coatings (EBCs) developed for gas turbine engines. While there has been extensive research on FOD in metals, ceramics, and ceramic matrix composites (CMCs), there has been limited studies on the effects of FOD in EBC systems. Previous work studied FOD in NASA's Ytterbium Disilicate EBC deposited on monothilic Silicon Carbide substrates. The present work will investigate FOD of the same Ytterbium Disilicate EBC deposited on a SiC/SiC CMC substrate. A limiting factor of EBC development is the growth of a SiO<sub>2</sub> thermally grown oxide (TGO) layer which exacerbates spallation. As such, the effects of steam exposure on FOD will also be explored. FOD testing was conducted at room temperature using a 1.59 mm steel ball projectile with particle velocities ranging from 50 - 300 m/s at a normal incidence angle. Samples were impacted in the as deposited state as well as after steam exposure in a 1316 C furnace. The impact damage was characterized by optical profilometry and scanning electron microscopy (SEM) of the cross-sections.

### S2- Advanced ceramic coatings for extreme

### environments

Room: Coquina C Session Chair: Peter Mechnich, DLR - German Aerospace Center

### 3:22 PM

# (ICACC-S2-040-2025) Electrochemical corrosion and long-term oxidation resistance of Ti-Al-C, (Ti, Mo)-Al-C and (Ti, Cr)-Al-C coatings (Invited)

T. Prikhna\*1; V. Podhurska2; V. Shtefan3; O. Ostash2; M. Karpets4;

- V. Sverdun<sup>1</sup>; S. Ponomryov<sup>5</sup>; T. Serbenyuk<sup>1</sup>; A. Kuprin<sup>6</sup>
- 1. Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Ukraine
- Karpenko Physico-Mechanical Institute of the NAS of Ukraine, Department of Hydrogen Technologies and Alternative Energy Materials, Ukraine
- 3. Leibniz Institute for Solid State and Materials Research Dresden, Germany
- 4. National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute", Ukraine
- 5. Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, Ukraine
- 6. National Science Center Kharkov Institute of Physics and Technology, Ukraine

Ti-Al-C, (Ti,Mo)-Al-C and (Ti,Cr)-Al-C coatings 5-11 µm thick were deposited on OT4-1 alloy substrates by the method of hybrid magnetron sputtering and cathode-arc evaporation of a MAX phase target, and in the case of coatings with Mo and Cr, a cathodearc plasma source made of Mo or Cr was used in parallel. X-ray structural analysis showed that all the deposited coatings were near amorphous. The (Ti,Cr)-Al-C coating showed the highest stability against electrochemical corrosion in 3.5 wt.% NaCl aqueous solution at 20 °C: corrosion potential 0.044 V, corrosion current density 2.48×10<sup>-9</sup> A/cm<sup>2</sup>, anodic current density 5.18×10<sup>-9</sup> A/cm<sup>2</sup>. This coating also showed the highest long-term oxidation resistance and after heating in air at 600 °C, 1000 h its electrical conductivity s=  $9.84 \times 10^6$  S/m was slightly higher than before heating  $s = 4.35 \times 10^5$  S/m, the nanohardness and Young's modulus are in the range of 15 GPa and 240 GPa, respectively. Thus, the hybrid deposited (Ti,Cr)-Al-C coatings exhibit high corrosion and oxidation resistance while maintaining electrical conductivity and can be used to protect lightweight titanium alloy interconnects of Molten Carbonate Fuel Cells as substitution of 316L stainless steel. Acknowledgments. The work was supported by the III-7-22 (0785) Project of the NAS of Ukraine, the NATO project SPS G6292, and MES Ukraine project No. 0122U001258.

### 3:52 PM

## (ICACC-S2-041-2025) $\beta$ -SiAlON synthesis and application as a surface coating for Si\_3N\_4 heating elements

T. J. Wineger\*1; W. M. Kriven1; D. do Carmo Silva1

1. University of Illinois Urbana-Champaign, Materials Science and Engineering, USA

In the aviation industries, pursuit of sustainable aviation fuels (SAF), silicon nitride-molybdenum disilicide heating elements are utilized as ignition assistants for low cetane number fuels. Due to longer operating times and higher surface temperatures commercially available silicon nitride glow plugs oxidize, eventually causing them to short or crack. One proposed a solution to this oxidative failure is by applying a coating with increased oxidation resistance to the surface of the ignition assistant. SiAlON was selected for its structural similarity to Si<sub>3</sub>N<sub>4</sub> and similar coefficient of thermal expansion. Due to limitations in commercially available SiAlON,  $\beta$ -SiAlON micropowder was synthesized via carbothermal reduction and nitridization of aluminosilicate geopolymer. Purity of the SiAlON powder was increased by the substitution of NaOH and KOH with guanidinium hydroxide during the geopolymer synthesis. SiAlON coatings were applied to sintered Si<sub>3</sub>N<sub>4</sub> bodies via colloidal-gel-casting, resulting in coating thicknesses varying from <10 µm to 50 µm depending on slurry viscosity and sintering method. Coated parts were sintered with a CO<sub>2</sub> laser to focus heating to the surface and prevent excess heating of the already dense body. Isothermal and non-isothermal oxidation tests were completed to determine effectiveness of the coatings as oxidation resistant barriers.

### 4:12 PM

### (ICACC-S2-042-2025) Heat Management in Anodic Spark Deposition: A Potential Solution with other Challenges

R. Ali\*1; M. Shah2

- 1. University of Kentucky, Department of Electrical and Computer Engineering, USA
- 2. Shaheed Benazir Bhutto University Shaheed Benazirabad, Pakistan

Anodic Spark Deposition (ASD) is a significant technique used for the deposition of various materials, including metals, onto substrates. Despite its advantages, such as the ability to produce coatings with unique properties, ASD faces numerous challenges that impact its efficiency and applicability. This paper examines the current challenges of ASD in 2024, such as uniformity of coating, control of deposition parameters, substrate compatibility, surface preparation, process stability, safety concerns, material properties, post-processing requirements, and environmental impact. By identifying and addressing these challenges, advancements in ASD can be achieved to enhance its performance and expand its applications. Heat management is crucial in ASD processes as it affects the quality of the coating, energy efficiency, and overall process control. ASD involves high-energy discharges that can generate significant heat, potentially leading to substrate damage or undesired coating properties if not properly managed. Common heat management strategies in ASD might include optimizing electrolyte composition and flow, controlling current density and pulse parameters, implementing cooling systems, designing appropriate electrode configurations to name a few. Counting major work from experts in ASD, detailed study till year 2024 will be presented on heat management in ASD process.

### 4:32 PM

### (ICACC-S2-043-2025) Harnessing Energy from Salinity Gradients: Enhanced Asymmetric Capacitive Mixing with MnO<sub>2</sub>-Coated Activated Carbon Electrodes

I. Hwang\*1; J. Kim1; J. Park1; M. Woo1; C. Park1; G. Cha1; S. Han1; J. Sun1;

- S. Hong<sup>1</sup>; Y. Lee<sup>1</sup>; J. Jeong<sup>1</sup>; J. Yeo<sup>2</sup>; Y. Jung<sup>3</sup>; K. Kim<sup>4</sup>; T. Song<sup>1</sup>; U. Paik<sup>1</sup>
- 1. Hanyang University, Department of Energy Engineering, Republic of Korea
- 2. Korea Institute of Energy Research, Republic of Korea
- 3. Changwon National University, Republic of Korea
- 4. Pusan National University, Republic of Korea

The potential of salinity gradient power as a renewable energy source is significant, and capacitive mixing with flow-electrodes (F-CapMix) offers a novel method to exploit this potential. Conventional F-CapMix systems are limited by the charge storage capacity of porous carbon materials, which rely on the electrical double-layer mechanism. This research introduces manganese dioxide-coated activated carbon (MO@AC) as an innovative flow-electrode material for F-CapMix, focusing on an asymmetric flow-electrode configuration. We systematically analyze the electrochemical performance of both activated carbon (AC) and MO@AC flow-electrodes, examining their effectiveness as positive and negative electrodes in both symmetric and asymmetric F-CapMix setups. The findings show that significant performance improvements are unique to the asymmetric F-CapMix system, demonstrating the enhanced efficiency of MO@AC in this design. The asymmetric F-CapMix system with MO@AC electrodes achieves a notable power density of 2.22 W m-2 through reversible redox reactions with Na<sup>+</sup> ions. These results expand the possibilities for application and illustrate the potential for our approach to be adapted to various materials that interact with Na<sup>+</sup> and Cl<sup>-</sup> ions in F-CapMix systems.

### 4:52 PM

# (ICACC-S2-044-2025) Comparative Analysis between alumina $(Al_2O_3)$ , titania $(TiO_2)$ , and zirconia $(TiO_2)$ as ceramic materials for moisture sensors

M. Shah<sup>2</sup>; R. Ali<sup>\*1</sup>

- 1. University of Kentucky, Department of Electrical and Computer Engineering, USA
- 2. Shaheed Benazir Bhutto University Shaheed Benazirabad, Pakistan

Common ceramic materials for moisture sensors include alumina (Al<sub>2</sub>O<sub>3</sub>), titania (TiO<sub>2</sub>), and zirconia (ZrO<sub>2</sub>). The choice of material depends on factors like sensitivity, stability, and operating conditions. TiO<sub>2</sub> generally shows the highest sensitivity to moisture due to its surface chemistry and ability to form hydroxyl groups while Al<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub> have moderate sensitivity, with Al<sub>2</sub>O<sub>3</sub> often being slightly more sensitive than ZrO<sub>2</sub>. TiO<sub>2</sub> typically offers the fastest response to changes in humidity, Al<sub>2</sub>O<sub>3</sub> has a moderate response time, and ZrO2 tends to have slower response times compared to the other two. ZrO<sub>2</sub> exhibits excellent temperature stability, making it suitable for high-temperature applications, Al<sub>2</sub>O<sub>3</sub> also has good temperature stability, and TiO<sub>2</sub> is less stable at higher temperatures compared to the other two. Both Al<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub> offer excellent chemical stability. TiO<sub>2</sub> has good stability but can be reactive under certain conditions, especially under UV light. TiO<sub>2</sub> allows for excellent control over porosity, which is crucial for sensor performance, and also Al<sub>2</sub>O<sub>3</sub> offers good control over porosity, while ZrO<sub>2</sub> can be more challenging to control in terms of porosity. A detailed study will be presented on symposium.

### S3 22th Intl Symp on Solid Oxide Cells Materials Science & Technology

### S3- Fuel electrodes & electrolytes

Room: Ballroom 4

Session Chair: Vincenzo Esposito, Technical University of Denmark

### 1:30 PM

# (ICACC-S3-034-2025) Exsolution mechanisms, phase stability, and redox-behavior of substituted strontium titanate perovskites (Invited)

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- 1. Forschungszentrum Julich GmbH, IMD-2, Germany
- 2. Forschungszentrum Julich GmbH, PGI-7/IMD-2, Germany
- 3. Forschungszentrum Julich GmbH, PGI-7, Germany

Exsolution is defined as the phase separation of a solid solution due to a miscibility gap under specific conditions. In the context of catalysis, exsolution refers to the reduction of metal cations to the metallic state, forming nanosized particles on the surface. At surfaces and interfaces, however, strong electrostatic gradients and space charges typically control the properties of oxides. Here we reveal that the nature of the surface-dopant interaction is the main determining factor for the exsolution kinetics of nickel in strontium titanate thin films. The electrostatic interaction of dopants with surface space charge regions results in strong surface passivation, which manifests in a retarded exsolution response. We furthermore demonstrate the controllability of the exsolution response via engineering of the perovskite surface chemistry. Since the exsolved nanoparticles are not percolated, their function is very different from standard Ni network and the electrode performance will strongly depend on the properties of the oxide backbone. We thus investigated the exsolution behavior and phase stability of bulk Sr<sub>1-x</sub>(Ti<sub>0.3</sub>Fe<sub>0.7-v</sub>Ni<sub>v</sub>)O<sub>3-d</sub> ceramics at various temperatures and atmospheres. Above a given temperature, it partially transforms to a Ruddlesden-Popper phase, while reverting back to the perovskite phase during reoxidation.

### 2:00 PM

# $(ICACC-S3-035-2025) \ SrTi_{1\,x}Fe_xO_{3\,\delta} \ Under \ Solid \ Oxide \ Cell \ Fuel-Electrode \ Conditions: \ Connecting \ Electrochemical \ Degradation \ and \ Phase \ Instability$

### J. M. Reinke\*1; S. Barnett1

1. Northwestern University, Materials Science and Engineering, USA

The search for solid oxide cell fuel electrode materials that showcase long term electrochemical stability and high performance has yielded significant interest in perovskite oxides with nanoparticle exsolution. One example is SrTi<sub>0.3</sub>Fe<sub>0.7</sub>O<sub>3-8</sub> (STF) substituted with Ni or Ru on the B site; exsolution of Ni or Ru rich nanoparticles occurs upon exposure to reducing fuels, resulting in improved electrochemical performance. However, exposure to too-reducing conditions can lead to extensive reduction of Fe and conversion of the perovskite oxide to a Ruddlesden-Popper (R-P) structure. In this study, we explore the stability of the base oxide with varying compositions  $SrTi_{1-x}Fe_xO_{3-\delta}$  (x≥0.5) to determine their stability under highly reducing conditions. Ex situ and in situ x-ray diffraction, complemented by electron microscopy and energy dispersive x-ray spectroscopy imaging, are used to detail the decomposition process, generally observed for  $H_2/H_2O$  ratios  $\ge 10$ . This study not only shows the decomposition of the host perovskite but seeks to link structural decomposition of the fuel electrode material to electrochemical degradation. By examining compositions with differing Fe content, we show that, while higher Fe-content leads to decreased charge transport resistances in the electrode, cell degradation proceeds more rapidly compared to lower Fe-content cells.

### 2:20 PM

### (ICACC-S3-036-2025) Development and characterization of novel fuel electrode supported solid oxide electrolysis cells in the COMPAS project

H. L. Frandsen\*<sup>1</sup>; A. Lopez de Moragas<sup>1</sup>; J. Taubmann<sup>1</sup>; M. P. Klitkou<sup>1</sup>;

M. Yarahmadi<sup>1</sup>; P. Hendriksen<sup>1</sup>; P. Khajavi<sup>1</sup>

1. Technical University of Denmark, Department of Energy Conversion and Storage, Denmark

The COMPAS project targeted fuel electrode supported (FES) solid oxide electrolysis cells enduring -1.25 A/cm<sup>2</sup> with a degradation below 15 mV/kh at 750 C. To achieve this ambitious target, three main cell development tracks with three distinct fuel electrodes were initiated, ranging from replacement of Ni-8YSZ in fuel electrode with Ni-ScYSZ and to more complex structures with LSFNT perovskite electrode and a Ni-CGO active electrode. Common for all tracks is a Ni-3YSZ support, which was sintered at 1200-1250 C to maintain small grains, ensuring mechanical robustness over the lifetime. To obtain a gas-tight electrolyte at the lower sintering temperatures ScYSZ electrolytes were also used in all tracks. CGO infiltrated LSFNT (La<sub>0.4</sub>Sr<sub>0.4</sub>Fe<sub>0.03</sub>Ni<sub>0.03</sub>Ti<sub>0.94</sub>O<sub>3</sub>) have previoulsy showed a strong potential in metal supported cells. Although the integration in the FES structure was succesfully achieved, the performance did not reach those observed in the metal supported cells. ScYSZ showed very promising performance and lower degradation than Ni-8YSZ and we here present our hypothesis for this, which was supported by measurements of model electrodes operating in-situ a Raman microscope. Despite potential worries on the chemically expanding Ni-CGO electrode, the cells turned out to be robust and after many optimizations the desired stable operation.

#### 2:40 PM

#### (ICACC-S3-037-2025) Ni-GDC fuel electrode supported cells: An alternative for extending the lifetime of solid oxide electrolyzers

A. Lopez de Moragas<sup>\*1</sup>; M. Phan Klitkou<sup>1</sup>; M. Yarahmadi<sup>1</sup>; P. Khajavi<sup>1</sup>; H. Lund Frandsen<sup>1</sup>

1. Technical University of Denmark, Department of Energy Conversion and Storage, Denmark

Despite improvements in performance and durability of SOC, the lifetime, when operating at high current densities (-1A/cm<sup>2</sup> or above), is moderate and further cost cuts could be achieved by extending it. Ni-8YSZ FESC typically operate around 700-800°C. These cells degrade consistently at rates between 50 and 300 mV/kh when operated at -1A/cm<sup>2</sup>. Some Ni-GDC ESC offer much lower degradation rates (below 10 mV/kh) at similar current densities. However, their operation temperature must be higher (800-850°C) to achieve similar current densities at the thermoneutral potential. Fuel electrode supported cells with Ni-GDC electrodes are an alternative to both designs. After showing that such cells can be fabricated, tested, and that they sustain extreme conditions (overpotential) without breaking, this work shows how they can maintain very low degradation rates (< 10mV/kh) for thousands of hours while operating at -1 A/cm<sup>2</sup>, 750 °C, 90/10 H<sub>2</sub>O/H<sub>2</sub>, 56 % fuel utilization. However, their high "interface resistance" makes the ASR larger than in Ni-8YSZ alternatives and therefore the voltage to be 300 mV above thermoneutral at these conditions. Current efforts focus on optimizing the fabrication to reduce the interface resistance generated by poor GDC-YSZ contact and excessive GDC-YSZ mixing. The effect of sintering aids, profiles and temperatures will be studied.

#### 3:20 PM

### (ICACC-S3-038-2025) Characterization of a metal-based nickel electrode (Ni-GDC) under steam electrolysis conditions

- L. Balice\*<sup>2</sup>; C. Frantz<sup>1</sup>; K. Lawand<sup>1</sup>; E. Boehm-Courjault<sup>1</sup>; J. Van Herle<sup>1</sup>;
- C. Lenser<sup>2</sup>; N. H. Menzler<sup>2</sup>; O. Guillon<sup>2</sup>; M. Bram<sup>2</sup>
- 1. EPFL Valais Wallis, STI-SCI-JVH Group of Energy Materials (GEM, Switzerland
- 2. Forschungszentrum Jülich GmbH, IMD-2, Germany

In solid oxide electrolysis cells, the hydrogen electrode suffers from long term degradation. In the typical NiO-YSZ cermet reduced during operation, the Ni particles tend to agglomerate and migrate away from the electrolyte interface, decreasing the triple phase boundary area. Here, we investigate the degradation under electrolysis of an alternative electrode made of metallic nickel and gadolinium-doped ceria (Ni-GDC). This concept demonstrated already great performances for fuel cell mode. Under the reducing conditions of the hydrogen electrode, the partial reduction of GDC  $(Ce^{4+} to Ce^{3+})$  makes it a mixed ionic electronic conductor, compensating for the Ni depletion. In addition, as Ni is already metallic and in form of large particles, further coarsening and microstructure changes are retarded. A comparison with a commercial cell with NiO-GDC electrode was carried out. Both cells were characterized by EIS and SEM-EDX, while the Ni-GDC electrode also by FIB-SEM 3D reconstruction. The electrochemical results show a different aging between the two types, despite a comparable final degradation. The resulting Ni particles are rather stable, whereas a GDC migration can be observed. Both cells were affected by Si contamination coming the glass seal, making the analysis complex. The presented concept opens the path to new possibilities for optimization of the electrolysis performance.

#### 3:40 PM

### (ICACC-S3-039-2025) Probing degradation phenomena in solid oxide cells using nanoscale techniques (Invited)

K. Develos-Bagarinao\*1

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Solid oxide cells (SOCs) are promising technologies that could contribute to the transition from a fossil-fuel-based infrastructure to a hydrogen-based economy. Among other issues such as cost reduction and stability, understanding the factors affecting the longterm performance of SOC devices is crucial towards promoting their commercial deployment. This talk will review the experimental results accumulated over the years and present important findings on various degradation phenomena revealed using a combination of nanoscale techniques, including high-resolution secondary ion mass spectrometry (SIMS) imaging, in conjunction with oxygen isotope exchange depth profiling and other advanced techniques such as scanning/transmission electron microscopy (S/TEM), for investigating both cell structures and model samples prepared using thin film deposition. Effects of processing methods and operating conditions on interfacial stability, oxide ion transport, and ionic conductivity are explored. Deactivation of reaction sites for main electrode processes due to poisoning by impurities as well as phase destabilization of common electrode materials (e.g., perovskite oxides such as  $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3.6}$ ) are also presented. Understanding these various degradation phenomena provides crucial insights into designing strategies for improving the stability of SOCs for practical applications.

### 4:10 PM

### (ICACC-S3-040-2025) Effect of Ni Content and Fuel Composition on Ni Migration in Ni-YSZ Electrodes

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1. Northwestern University, Materials Science and Engineering, USA

Ni migration in Ni-YSZ electrodes during solid oxide electrolysis is generally understood by Ni wetting angle variation over distance from the electrolyte. One possible explanation is a variation in the Ni/YSZ interface tension arising from electrowetting. However, the explanation is unclear as to migration occurred during electrolysis operation whereas no migration is observed during fuel cell operation. Here we attempt to quantify an electrowetting model for the Ni/YSZ interface, to predict the Ni/YSZ contact angle versus position. Results will present how the predicted contact angle varies with Ni-YSZ microstructure, cell operating conditions (such as current density, temperature, and H<sub>2</sub>/H<sub>2</sub>O ratio), and point of zero charge of Ni/YSZ interface. Estimates of how the Ni migration velocity varies with these parameters are based on models of Ni particle migration rates on YSZ surfaces. The predictions will be compared with experimental observations of Ni migration in Ni-YSZ/YSZ/Ni-YSZ symmetric cells, as a function of electrode Ni volume fraction and H<sub>2</sub>/H<sub>2</sub>O fuel compositions. Both factors appeared to contribute significantly to determining the extent of Ni migration. Experimentally, Ni-YSZ electrodes with 70 wt% initial NiO content exhibited Ni migration after 500 h electrolysis operation in 85% H<sub>2</sub>O at 1.0 A/cm<sup>2</sup>. Whereas for 50% H<sub>2</sub>O and 50 wt% NiO at 1.0 A/cm<sup>2</sup>, there was no evidence of Ni migration.

### 4:30 PM

### (ICACC-S3-041-2025) Room and high temperature tensile strength of ultrathin 3% yttria-stabilized zirconia (3YSZ) ceramic tapes for solid oxide fuel cells (SOECs)

I. Bombarda<sup>1</sup>; N. Langhof<sup>1</sup>; S. Schafföner<sup>\*1</sup>

1. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

High temperature electrolysis (HTEL) has several advantages compared to competing eletrolysis technologies, including a high efficiency at T = 850 °C when combined with an exothermic process. To reduce costs, increase lifetime and improve scale up production of electrolyte supported SOCs, a key property is the cell mechanical stability, which for electrolyte supported cells is mainly provided by the ceramic electrolyte. In this study, we investigated the tensile and ring-on-ring properties of ultrathin (t = 90  $\mu$ m) 3YSZ tapes at room and high temperature (T = 850 °C). A test setup and sample preparation procedure were developed for the tensile test. The tensile test concept was then adapted to a high temperature setup, allowing the tensile test at operating temperature with 90% valid samples. A 50 % strength drop was observed in tensile and ring-on-ring compared to room temperature. The high temperature tensile testing allowed the evaluation of a large effective volume and the identification of bulk defects, whereas with the ring-on-ring test only the surface defects could be assessed. The defects after the tensile test were measured and classified as non-critical, indicating subcritical crack growth.

### 4:50 PM

## (ICACC-S3-042-2025) Charge carrier relaxation phenomena in selected oxide ion conductors studied by impedance spectroscopy

M. Malys<sup>\*1</sup>; M. Struzik<sup>1</sup>; B. Lemieszek<sup>2</sup>; A. Cuper<sup>1</sup>; J. Mrowczynski<sup>1</sup>;

- M. Ratajczyk<sup>1</sup>; S. Molin<sup>2</sup>
- 1. Politechnika Warszawska, Faculty of Physics, Poland
- 2. Gdansk University of Technology, Laboratory of Functional Materials, Faculty of Electronics, Telecommunications and Informatics, Poland

An increase of the ac conductivity with increasing frequency, observed in ionic conductors, is accompanied by a finite decrease of the dielectric constant. In a range of materials, the dielectric function can be well described by the empirical functions of Cole–Cole or Havriliak-Negami, which in the limit of high frequencies give the power law frequency dependence of conductivity. The relaxation strength, the dc conductivity and the relaxation frequency obey the Barton-Nakajima-Namikawa relation. The coefficients relating the dc conductivity with the charge carrier relaxation, provides valuable information about the length scale and the time scale of nonrandom hopping, expressed respectively in units of jump length and average time between jumps of a hopping carrier. This concept has been tested in the case of several selected oxygen ion conductors (CeO<sub>2</sub> or Bi<sub>2</sub>O<sub>3</sub> based materials). The frequency dependence of conductivity and complex dielectric relaxation were combined in one model of the ac response. Accurate estimates of parameters were obtained when the complex equivalent circuit comprised contributions of all processes affecting the ac response. This research has been supported by the National Science Centre (NCN, Poland) DAINA 2 project number UMO-2020/38/L/ST8/00513.

### 5:10 PM

### (ICACC-S3-043-2025) Sodium carbonate ceria composite electrolytes for applications in low temperature solid oxide cells

M. C. Diaz Lacharme\*<sup>1</sup>; K. Monzillo<sup>2</sup>; A. Bartoletti<sup>3</sup>; E. Callone<sup>5</sup>; A. Gondolini<sup>3</sup>; S. Dirè<sup>4</sup>; V. Vaiano<sup>2</sup>; A. Donazzi<sup>1</sup>

- A. Gondolini<sup>+</sup>; S. Dire<sup>+</sup>; V. Valano<sup>+</sup>; A. Donazz
- 1. Politecnico di Milano, Department of Energy, Italy
- 2. Universita degli Studi di Salerno, Dipartimento di Ingegneria Industriale, Italy
- CNR-ISSMC, Istituto di Scienza, Tecnologia e Sostenibilitá per lo sviluppo dei Materiali Ceramici, Italy
- 4. Universita degli Studi di Trento, Italy
- 5. Universita degli Studi di Trento, Klaus Muller Magnetic Resonance Lab, Italy

Sodium carbonate ceria composites (CCCs) are a new class of ceramic materials that hold promise for utilization in solid oxide cells (SOCs). The structure of CCCs consists of nanoparticles of Samaria Doped Ceria (SDC < 50 nm) dispersed in a matrix of Na<sub>2</sub>CO<sub>3</sub>, which leads to a material with high protonic conductivity below 600°C. The morphology of the active phases, and the identification of the conductive pathway (either via the SDC/Na<sub>2</sub>CO<sub>3</sub> interface, or via carbonate bulk) are still debated. In this work, we study the electrochemical and structural properties of CCC electrolytes and complete SOCs with synergistic techniques. The electrolyte's conductivity is studied between 600 and 400°C with EIS as a function of the Na<sub>2</sub>CO<sub>3</sub> amount and of the firing temperature (up to 900°C), with dry and humidified H<sub>2</sub> and air, revealing ambipolar transport. Solid-state NMR analyses are applied to reveal the structural consequences of hydration. Raman and UV-DRS analyses provide insight in the ageing behavior, prior and after exposure to the reactive conditions. The intimacy of the SDC/Na<sub>2</sub>CO<sub>3</sub> contact and the thickness of the carbonate interface appear prominent in establishing the conductivity. Complete SOCs with LiNiO<sub>2</sub>-CCC and Ni-CCC electrodes are prepared combining die-pressing and screen-printing, and their performance is tested collecting I/V and EIS curves in electrolysis and fuel cell mode.

### <u>S5 Next-Generation Bioceramics and</u> <u>Biocomposites</u>

## S5- Ceramics and composites with antimicrobial/ antiviral properties

### Room: Ponce de Leon

Session Chair: Kalpana Katti, North Dakota State University

### 1:30 PM

### (ICACC-S5-006-2025) Glass/Ceramic Composite Coatings Embedding Silver Nanoparticles with Antipathogen Properties (Invited)

- C. Balagna\*<sup>2</sup>; F. Gattucci<sup>1</sup>; A. Luceri<sup>1</sup>; S. Perero<sup>1</sup>; M. Ferraris<sup>2</sup>
- 1. Politecnico di Torino, DISAT, Italy
- 2. Politecnico di Torino, Department of Applied Science and Technology, Italy

This study focuses on innovative glass/ceramic composite coatings embedding silver nanoparticles, developed to address emerging diseases caused by bacteria and viruses. These smart, sustainable nanostructured materials are designed to mitigate the effects of microbiological contaminants. Two techniques were employed: co-sputtering and the use of pre-ceramic polymeric precursors. The co-sputtered coatings feature silver nanoparticles well dispersed and anchored within a silica or zirconia matrix. This configuration ensures a controlled release of metallic ions, effectively preventing the adhesion, proliferation, and spread of various bacterial strains, fungi, and airborne viruses, including SARS-CoV-2. The co-sputtering technique offers versatility for coating various surfaces, including membranes, and scalability for industrial applications. Pre-ceramic polymeric precursors were also explored, offering advanced properties. These precursors transform into ceramic materials at low temperatures, generating minimal waste. Incorporating silver nanoparticles into these precursors represents a significant advancement for antimicrobial applications.

### 2:00 PM

### (ICACC-S5-007-2025) Investigating the composition-structureproperty relationships of novel antibacterial glass particles developed through a design of mixtures approach

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- 1. Dalhousie University, Biomedical Engineering, Canada
- 2. Dalhousie University, Department of Applied Oral Science, Faculty of Dentistry, Canada

Revealing the individual and synergistic effects of network modifiers in borate glasses is essential for advancing material optimization and innovation. In dentistry, utilizing such insights to design advanced biomaterials is a promising approach for effectively preventing and arresting dental caries, thereby improving oral health outcomes. By leveraging these insights, we can create sustainable, soluble materials that promote desirable host responses like remineralization and antibacterial efficacy. However, a significant gap remains in understanding how modifiers (e.g., Ag) impact borate glass structures and properties. In this study, we employed a Design of Mixtures (DoM) approach to investigate the individual and interactive effects of therapeutic ions within a borate glass network. Sixteen distinct glass compositions were synthesized and characterized for key chemical and physical properties, including density, glass transition temperature, percent crystallinity, and structural units. We identified correlations between these properties and the roles of individual modifiers and formers. This understanding enables precise modulation of glass systems, providing an opportunity to engineer materials that enhance desired responses, including caries prevention by controlling ion release through structural modifications.

### 2:20 PM

## (ICACC-S5-008-2025) Enhancing Antimicrobial Property of Fluorapatite Bone Scaffolds with Low-Dose Copper Doping

P. Elahi\*<sup>1</sup>; S. K. Steyl<sup>1</sup>; J. Shea<sup>1</sup>; V. Krishnamoorthi<sup>2</sup>; J. P. Beck<sup>3</sup>; J. Agarwal<sup>1</sup>; S. Jeyapalina<sup>1</sup>

- 1. University of Utah Health, Department of Surgery, USA
- 2. University of Utah Health, Department of Biomedical Engineering, USA
- 3. University of Utah Health, Department of Orthopedics, USA

Post-surgical infections significantly challenge bone graft survival, patient morbidities, and treatment costs. The rise of antibiotic-resistant bacteria highlights the need for bone scaffolds with inherent antimicrobial properties without compromising their biocompatibility. Osteogenic fluorapatite (FA) shows promise as a bone substitute. Our previous data demonstrated that 1-5 mol% copper-doped FA significantly reduced bacterial adhesion by 2- to 3-log folds compared to FA, though higher concentrations of copper may result in cytotoxicity. This study focused on the bacteriostatic properties and cytotoxicity of FA doped with 0-1 mol% copper. We synthesized 0, 0.25, 0.5, 0.75, and 1 mol% copper-doped FA using wet chemical precipitation method and characterized them using XRD, FTIR, and ICP-MS. Antimicrobial performance was evaluated against Staphylococcus aureus and Pseudomonas aeruginosa, while human osteoblast (hFOB 1.19, ATCC) cultures were used to assess cytotoxicity. Preliminary findings suggested that copper doping at 0.25-0.5 mol% could provide an optimal balance, significantly reducing bacterial adhesion while maintaining osteoblast viability. These results indicate that low-concentration copper-doped FA could function as a dual-purpose scaffold, offering both antimicrobial properties and support for bone regeneration in infection-prone surgical environments.

## S5- Biomineralization and tissue-material interactions

Room: Ponce de Leon

Session Chair: Cristina Balagna, Politecnico di Torino

### 3:20 PM

### (ICACC-S5-009-2025) Reliable in vitro models of cancer metastasis through next-generation tunable bio-nano composite scaffolds (Invited)

- K. S. Katti<sup>\*1</sup>; D. R. Katti<sup>1</sup>; J. Kim<sup>1</sup>; P. Ravi<sup>2</sup>; S. Ghosh<sup>1</sup>; A. Gaba<sup>4</sup>; P. Vyas<sup>3</sup>
- 1. North Dakota State University, Department of Biological Sciences, USA
- 2. North Dakota State University College of Engineering, Civil Construction and Environmental Engineering, USA
- 3. Sanford Medical Center Fargo, Orthopaedics, USA
- 4. Sanford Medical Center Fargo, Oncology, USA

Breast and prostate cancer incidents result in about 1M deaths worldwide each year. Both of these cancers have the propensity to metastasize to bone. Bone metastasis of prostate and breast cancer remains incurable due to the lack of studies at the bone metastasis site, resulting from difficulty in obtaining patient samples and failure of animal models. A novel nanoclay composite scaffold enables tuning of the composite's biological and mechanical properties. The tissue-engineered scaffolds are used to create testbeds of cancer metastasis by seeding patient-derived cancer cells on the bone-mimetic tissue-engineered composites. A specially designed horizontal-flow bioreactor enables the presence of physiologically relevant fluid-derived stress. The arrival of the tumor cells at the bone disrupts the Wnt/b-catenin pathway relevant for osteogenesis. This metastasis testbed is also used to screen anti-cancer drugs and to investigate new markers of metastasis and predict the severity of metastasis in patients. Mechanobiological investigations and FTIR and RAMAN spectroscopy are used to develop new biomarkers of metastasis progression. The cancer testbed is presented here as a next-generation tool to investigate fundamental cancer biology at metastasis, screen new drugs, provide a means for personalized medicine, and enable the discovery of new biomarkers for metastasis.

### 3:50 PM

## (ICACC-S5-010-2025) Modeling the cell-cell and cell-substrate interface in cancer bone metastasis

D. R. Katti\*1; K. S. Katti1; H. Gaikwad1; S. V1

1. North Dakota State University, Civil Construction and Environmental Engineering, USA

Prostate and breast cancer tend to metastasize to bone when the cancer is incurable. Cellular adhesion processes between cells and substrates such as bone are critical to metastasis. The adhesion is regulated by three cellular proteins: actins, integrins, and e-cadherins. The dynamic remodeling of actin cytoskeleton is observed in cellular processes during metastasis. Integrin enables cancer cells to adhere to the extracellular matrix. E-cadherin is instrumental in cell-cell adhesion and is necessary for tumor formation. Here, we present the mechanics of these proteins using steered molecular dynamics simulations and their roles in the mechanobiology of breast and prostate cancer bone metastasis. Actin filament polymerization and depolymerization critical to the cell-cell adhesion observed in tumor growth are modeled. The integrin studies elucidate the integrin activation mechanism on various surfaces, including the nanoclays used in in vitro models of cancer metastasis, the adhesion, and the subsequent cell signaling leading to cellular changes. The behavior of actins inside the cells is presented as the outside-in signaling mechanism of human cells. Further, e-cadherin-actin complex modeling provides a detailed view of the mechanics of cell-cell adhesion and the cell signaling leading to the e-cadherin junction formation. These studies provide mechanics-based cues to cancer cell progression.

### 4:10 PM

## (ICACC-S5-011-2025) Engineering curved strontium sulfate crystals

- C. Detwiler Gray\*2; A. Martin1; E. Samajpati3; A. Perez-Huerta3; V. Merk1
- 1. Florida Atlantic University, Chemistry & Biochemistry, Ocean & Mechanical Engineering, USA
- 2. Florida Atlantic University, Chemistry and Biochemistry, USA
- 3. The University of Alabama at Birmingham College of Arts and Sciences, Department of Geological Sciences, USA

Biomineralization creates biologically important support structures, including shells, exoskeletons, and bones. Some biomineralization processes involve transient amorphous precursor phases that are characterized by structural disorder and curved interfaces. Identification of amorphous precursors is crucial to understand crystallization pathways, yet there is a gap of knowledge surrounding the crystallization of earth alkaline sulfates. This study investigates biomimetic strontium sulfate (SrSO<sub>4</sub>) crystallization in the presence of poly(glutamic acid) using multiscale microscopy and vibrational spectroscopy. We hypothesize that poly(glutamic acid) promotes the formation of a polymer-induced liquid precursor (PILP) phase previously found in calcium carbonate and calcium phosphate minerals. Under the Scanning Electron Microscope, we observed round crystal shapes with granular texture. Biomolecule inclusion led to pronounced peak broadening in X-ray Diffraction and Raman spectroscopy. We studied the three-dimensional nanostructure and chemistry of the composites using Atom Probe Tomography, which revealed a helical arrangement of organic matter inside the inorganic lattice. Acknowledgements: VM is indebted to funding from the National Science Foundation (DMR-2137663). CDG thanks the Microscopy Society of America and FAU's OURI office for undergraduate research grants.

### <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

### **S6- Sodium-ion Batteries I**

Room: Coquina B

Session Chair: Chongmin Wang, Pacific Northwest National Lab

### 1:30 PM

### (ICACC-S6-056-2025) Shedding Light on Charge Compensation Processes and Structural Details of Battery Materials using Advanced X-ray Spectroscopic Methods (Invited)

M. Balasubramanian\*1

1. Oak Ridge National Laboratory, USA

There is significant interest worldwide to develop new battery systems for transportation, grid-storage, and other emerging applications. Development of new disruptive technologies will require tailoring advanced materials and/or incorporating additional chemical or electrochemical processes. In this talk, we will delve into the application of advanced X-ray spectroscopic methods to understand fundamental structure-property-function relationships of materials and systems relevant to electrochemical energy storage. Specifically, recent studies performed on lithium-ion battery systems that employ earth-abundant cathode active materials will be discussed.

### 2:00 PM

### (ICACC-S6-032-2025) Exploring Fluorine-Free Sodium-Ion Electrolytes and their Interface with Electrodes for Sodium-Ion Batteries (Invited)

C. Ban<sup>\*1</sup>

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Recent rapid advancement in sodium-ion batteries (NIBs) has shown excellent long-term performance at a large scale. However, NIBs utilize electrolytes that are fluorine-rich. The decomposition of these electrolytes produces highly corrosive and toxic HF and other fluorinated compounds. Thus, the resulting fluorine-containing compounds make recycling complicated and expensive. Moreover, the fluorine-containing precursors and electrolytes used in batteries also contribute to the additional cost of battery manufacturing. While extensive research still focuses on how to add more fluorine-containing additives in NIBs, our research aims to investigate the potential of using fluorine-free electrolytes and study the interface of using the possible fluorine-free electrolytes. In this presentation, we will talk about our strategies for developing fluorine-free electrolytes for sodium-ion batteries. We will also discuss the important role of the electrolyte-electrode interface in electrochemical properties and cycling life. The results of our materials discovery and characterization efforts provide valuable insights into better understanding the relationship between the electrolyte and electrode-electrolyte interface. This understanding can aid in the development of highly reversible sodium-ion batteries at an even lower cost.

### 2:30 PM

#### (ICACC-S6-033-2025) Electronic Structure and Electrochemical Mechanisms in Electrode Materials for Potassium Batteries (Invited)

L. Stievano\*1; L. Monconduit1

1. Universite de Montpellier, Institut Charles Gernardt Montpellier, France

Potassium-ion batteries (KIBs) represent a promising candidate for large-scale electrochemical energy storage systems. The use of KIBs exhibits several advantages compared to the conventional Li-ion technology; the abundance of K-containing resources combined with the use of Co-free cathode materials can reduce significantly the price of the final products. Furthermore, the fast diffusion kinetics of K<sup>+</sup> ions in liquid electrolytes might enable fast charge/discharge process. Several families of positive and negative electrode materials have been developed for KIBs: at the cathode site, one can mention Prussian-blue analogues (PBAs), vanadium fluorophosphates such as KVPO<sub>4</sub>F, and transition metal oxides, whereas at the anode site carbonaceous solids such as graphite and hard carbon seem the most promising and viable electrode materials. In this presentation, we will demonstrate how a combination of electrochemical methods, advanced characterisation techniques (applied under operando conditions when possible), and DFT-based theoretical approaches can reveal the electronic structure and electrochemical mechanisms in such families of anode and cathode materials for KIBs. This approach is crucial for designing novel materials that can be successfully implemented in KIBs.

### **S6-Sodium-ion Batteries II**

### Room: Coquina B

Session Chairs: Badri Narayanan, University of Louisville; Wan Si Tang, Underwriters Laboratories Inc

### 3:20 PM

### (ICACC-S6-034-2025) Understanding the Intersection of Solvation Structure and Interfaces for Next-Generation Na Metal Batteries (Invited)

R. Carter\*<sup>1</sup>; L. Morris<sup>2</sup>; C. Pyles<sup>1</sup>; A. Dunkelberger<sup>1</sup>; M. Swift<sup>1</sup>; J. Hart<sup>3</sup>; Z. Warecki<sup>1</sup>; C. Love<sup>1</sup>

1. US Naval Research Laboratory, USA

- 2. American Society for Engineering Education, USA
- 3. Nova Research Inc, USA

Na metal batteries have become one of the most attractive targets for beyond-Li electrochemical energy storage opportunities in recent years due to their low cost, high abundance, and sustainability when compared to popular lithium systems. The adoption of Na metal batteries has been limited, however, by their instability and poor cycle life. Recently, it has become clear that Na metal batteries behave distinctly Li requiring new electrolyte design strategies. We present the first compelling comparison of Na and Li solvation bridging length and time scales with DFT simulation, ultrafast spectroscopy, and in-situ optical cell investigation. Na inherently exhibits improved solvation behaviors leaving stable solid electrolyte interface (SEI) formation to facilitate a functioning Na metal batteries. We go on to investigate common electrolyte components (NaPF<sub>6</sub>NaTFSI, diglyme, and FEC) and find that Na-F is not analogous to Li-F in stabilizing Na metal. Without a known stable compound for Na stabilization, we explore the use of Li-F within a Na system. LiPF<sub>6</sub> added to Na electrolytes demonstrate improved electrochemical cyclability (EIS, coulombic efficiency) and morphology (SEM) and we identity Li-F via XPS and TEM analysis. We demonstrate a Na metal electrolyte (1M NaPF<sub>6</sub>, 0.1M LiPF<sub>6</sub> in diglyme) capable of harnessing Na improved solvation behaviors and plating morphologies.

### 3:50 PM

## (IACC-S6-049-2025) Fast Charge Transfer Pathway via Dielectric Interface

T. Teranishi<sup>\*1</sup>; Y. Higaki<sup>1</sup>; S. Kondo<sup>1</sup>; A. Kishimoto<sup>1</sup>; C. Sasaoka<sup>2</sup>;

- H. Hirabaru<sup>2</sup>; S. Katayama<sup>2</sup>
- 1. Okayama University, Japan
- 2. Nippon Denko Co., Ltd, Japan

A significant improvement in the high rate performance of lithium-ion batteries (LIB) to match that of supercapacitors is required, while maintaining their high energy density for next-generation power sources. One approach involves integrating dielectric nano interface, including the benchmark dielectric compound BaTiO<sub>3</sub> (BTO), into the active materials-electrolyte interface, which enables an ultrafast charge transfer pathway via the dielectric layer. A series of experimental results, along with

density functional theory and molecular dynamics (DFT-MD) calculations, have demonstrated the activation of this interfacial charge transfer pathway. For example, during charging, solvated lithium ions adsorb onto the dielectric surface, where they desolvate, allowing naked lithium to preferentially intercalate into the electrode bulk through the triple phase interface (TPI): the interface between dielectrics, active materials, and the electrolyte. The high rate capability was further investigated as a function of electronegativity of the doped cations in the fluorite  $ZrO_2$  matrix as a dielectric layer. The high rate capability displayed its maximum at the averaged electronegativity of the doped cation and Zr is approx. ~1.3. This phenomenon implied the balance between the magnitude of electrostatic attraction and repulsion determines the charge adsorption activity at the interface.

### 4:20 PM

### (ICACC-S6-036-2025) Design of Novel High-Performance Cathode Materials for Na-ion Batteries (Invited)

P. Kaghazchi\*1

1. Forschungszentrum Juelich, Germany

Sodium-ion batteries (SIBs) are the most promising replacement for lithium-ion batteries (LiBs) owing to the low price and availability of sodium. Cathode materials for SIBs have similarity to those for LIBs, including the most popular type, namely layered metal oxides (Na<sub>x</sub>MO<sub>2</sub>). However, capacity and stability of currently known Na<sub>x</sub>MO<sub>2</sub> materials need to be improved to meet the requirement for practical applications. In this work, multiscale modeling approaches combining electrostatic analysis, density functional theory (DFT) calculation, GW approximation, thermodynamics consideration, and finite element simulation have been applied to design novel  $Na_{x}MO_{2}$  materials. It is shown that calculated magnetic moment using DFT with hybrid exchange-correlation functionals can predict redox mechanism (i.e. capacity) of cathode materials. Moreover, it is shown that how multiscale-modeling approaches can be used to predict stability of cathode materials. Finally, a combined theoretical/experimental work on design of Na<sub>x</sub>MO<sub>2</sub> compositions with high capacity and stability is presented.

### <u>S7 19th Intl Symp on Functional</u> <u>Nanomaterials & Thin Films for Sustainable</u> <u>Energy Harvesting</u>

## S7- Functional coatings and innovative thin film techniques, e.g., ALD, PECVD- II

Room: Flagler C

Session Chair: Muhammet Toprak, KTH Royal Institute of Technology

### 1:30 PM

(ICACC-S7-032-2025) Beyond conventional lithography: ongoing efforts in the projects REMAP, e-APP, and TRANSMIT (Invited)

D. Colombara\*1; P. Anacleto2

- 1. Universita degli Studi di Genova, Italy
- 2. International Iberian Nanotechnology Laboratory, Portugal

Sustainable energy provision is critical. Yet, the sun provides far more energy than humanity will ever need. To unlock this potential, we need disruptive technologies that efficiently harvest sunlight on a massive scale. Current commercial photovoltaics (PV) struggle to meet this challenge sustainably. Silicon solar panels dominate the market and are based on an abundant material, but their production is highly energy-intensive. Conversely, thin-film solar panels (CdTe and CIGS), require less energy to produce but rely on rare elements, raising questions about short-term economic and ecological sustainability. Recently, advanced PV concepts like microconcentrator and semi-transparent PV have emerged. These can make use of CdTe and CIGS materials but are free (by design) from raw material constraints. To demonstrate these concepts in the lab, researchers have used optical projection lithography (OPL) to create patterns. However, OPL cannot scale to terawatt levels needed for widespread deployment. Indeed, it is essential to identify a fabrication route that ensures high semiconductor quality and throughput at competitive costs. Inspired by the work of Prof. Gary Friedman on ferrofluid lithography, a patent is pending on a disruptive microfabrication technique that could scale to terawatt levels economically. Here, efforts from three parallel projects are illustrated to make it a reality.

#### 2:00 PM

### (ICACC-S7-033-2025) Nanocrystalline Diamond: Synthesis, Characterization and Applications

A. Kumar\*1

1. University of South Florida, Mechanical Engineering, USA

It is imperative that the future of integrated nano and micro systems relies on the fundamental understanding of manufacturing structures, related processes and measurements across the scale, signal and domain boundaries. The presentation will demonstrate roles of nano materials, micro and nano processing tools, nano manufacturing processes and system durability related to successful realization of integrated systems. A discussion will be presented on the fundamental and applied science done on nanocarbon materials (nanocrystalline diamond and graphene) and microfabrication processes and characterization of mechanical, tribological, electronic transport, and bio-compatible properties. The unique properties of this nanocrystalline diamond (NCD) can make it a promising candidate for use as protective coating of machining tools, a hermetic, corrosion-resistant coating for biodevices, a cold-cathode electron sources, and structural materials in micro-and nanoelectromechanical systems (MEMS/NEMS). This talk will address the current on-going research on other carbon based materials (graphene and hybrid coatings) and its composite materials for emerging technology applications.

### <u>S8 19th Intl Symp on APMT for Structural &</u> <u>Multifunctional Materials & Systems</u>

# S8- Rapid prototyping, 3D printing, patterning, templates and self-assembly

Room: Flagler A

Session Chairs: Katalin Balazsi, Centre for Energy Research HAS; Hirokazu Katsui, National Institute of Advanced Industrial Science and Technology (AIST)

#### 1:30 PM

### (ICACC-S8-037-2025) Monolithic zirconia with quasi-composite properties

P. Makurunje\*1; J. Callaghan1; S. Middleburgh1

1. Nuclear Futures Institute, Bangor University, United Kingdom

Additive manufacturing presents a state-of-the-art technique for the fabrication of nuclear thermal propulsion systems. Additive manufacturing enables the fabrication of various space reactor designs without demanding complex tooling for the mission-critical components. In the present study, zirconia-based ceramics were prepared by additive manufacturing using digital light processed vat polymerisation. Prototypic fuel elements were prepared and simultaneous thermal analyses were performed to characterise the conversion of zirconiumbased photopolymerisation precursor to zirconia. Microstructural analyses were performed across different sintering temperature profiles. Shrinkage and density evolution data were obtained and explained the microstructures obtained. Thermal conductivity studies were performed on a laser flash analyser up to 1000 °C. Findings informed the thermo-mechanical studies for analysing the structural integrity of the fuel at varying temperatures. Flexural strength studies revealed how the deposited layers deflected crack propagation across the materials in a manner similar to how laminated composites behave. Monolithic zirconia processed by digital light vat polymerisation is capable of showing quasi-composite fracture properties.

#### 1:50 PM

### (ICACC-S8-038-2025) Sustainability in Additive Manufacturing: Recycling and other strategies

H. A. Colorado L.\*1

1. Universidad de Antioquia, Colombia

Additive Manufacturing (AM) is a highly adaptable technology capable of producing nearly any shape and accommodating a wide range of materials, particularly in extrusion-based methods and other techniques. This flexibility opens opportunities to repurpose solid wastes as raw materials for AM, promoting material circularity and offering a sustainable approach to pollution management. This presentation explores the role of solid waste in AM, along with other sustainability-related aspects of the technology. It highlights the benefits, current challenges, and future potential of these applications. With the global rise in ceramic waste, particularly in certain industries, AM presents a promising solution for sectors where such residues remain underutilized. The presentation will feature case studies, particularly in ceramics and composites, demonstrating how these multifunctional materials can incorporate substantial amounts of waste.

## S8- Novel forming/sintering technologies, near-net shaping

#### Room: Flagler A

Session Chairs: Junichi Tatami, Yokohama National University; Hisayuki Suematsu, Nagaoka University of Technology

#### 2:20 PM

## (ICACC-S8-033-2025) Fabrication of transparent $\rm YVO_4$ by orientation control and SPS (Invited)

T. S. Suzuki\*1; L. Liu1; J. Li2; K. Morita2

- 1. National Institute for Materials Science, Optical Ceramics Group, Japan
- 2. National Institute for Materials Science (NIMS), Japan

Transparent ceramics can maintain their transparency and structural integrity at elevated temperatures, making them valuable for high-temperature environments and applications. The green compacts having small residual pores prepared by colloidal processing is expected to enhance the densification. Furthermore, spark plasma sintering (SPS) is also effective way for densification in low sintering temperature. In ceramics with anisotropic crystal structure, in-line transmittance deteriorates due to birefringence due to the difference in refractive index at grain boundaries. Crystallographic orientation is effective for improving the in-line transmittance when it is necessary to suppress birefringence at grain boundaries. Orientation can be controlled by a magnetic field even in a diamagnetic and paramagnetic ceramics. YVO<sub>4</sub> particles with particle size of 126 nm were synthesized by hydrothermal method. The c-axis of YVO<sub>4</sub> was aligned by slip casting in a magnetic field. YVO<sub>4</sub> was densified by SPS at 1300 °C and 100 MPa. Sintering additives enhances the density. Orientation degree was increased with the increasing SPS temperature. 60% of the grains were aligned within the tilet angle less than 5 degree between the c-axis and magnetic direction. Crystallographic orientaion improved the tansparency because the birfringence was supressed by the reduction of difference in refractive index between adjacent grains.

#### 2:50 PM

### (ICACC-S8-034-2025) Improved Densification of SiC Ceramics by Three-Step Sintering (Invited)

#### Y. Kim<sup>\*1</sup>

1. WORLDEX Industry & Trading Co., Ltd., Republic of Korea

Silicon carbide (SiC) is renowned for its superior properties such as high stiffness, high hardness, and excellent chemical and thermal stability, which make it a promising candidate for use in various structural and functional applications. Densification of SiC ceramics can be made via liquid-phase sintering and solid-state sintering. Full densification is relatively easy in liquid-phase sintering by filling pores by liquid flow. However, it is difficult to process fully densified SiC ceramics by solid-state sinteing because of entrapped gases in closed pores. In this presentation, three-step pressureless sintering of monolithic SiC ceramics was investigated using submicron SiC powder and boron- and carbon-containing additives to achieve almost full density. A relative density of up to 99.5% was achieved by dwelling at three temperatures (T1, T2 and T3, T3>T2>T1). Furthermore, practical applications of SiC ceramics in semiconductor processing will also be explored.

#### 3:40 PM

# (ICACC-S8-035-2025) Innovative approaches to debind and sinter alumina (Al $_2O_3$ ) ceramics fabricated using direct ink writing

S. Bhandari\*<sup>1</sup>; O. Hanzel<sup>2</sup>; M. kermani<sup>3</sup>; V. M. Sglavo<sup>3</sup>; M. Biesuz<sup>3</sup>; G. Franchin<sup>1</sup>

- 1. Universita degli Studi di Padova Dipartimento di Ingegneria Industriale, Italy
- 2. Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovakia
- 3. Universita degli Studi di Trento, Ingegneria industriale, Italy

Direct ink writing (DIW) is a widely used additive manufacturing (AM) technique for producing complex ceramic shapes. Unlike other AM methods like vat photopolymerization or fused filament fabrication, DIW uses limited amount of oragnics thereby facilitating rapid debinding approaches. In this study, alumina inks with two ceramic loadings were prepared, and log-pile structures were printed using 0.41 mm and 0.84 mm diameter nozzles. The samples were dried at room temperature and then subjected to different rapid sintering sintering techniques: ultra-fast high temperature sintering (UHS), pressureless spark plasma sintering (PSPS), and fast-firing (FF). Both UHS and PSPS effectively densified the samples without defects in an Ar atmosphere in few seconds to minutes. However, fast-firing in air caused cracking, particularly with larger nozzles. Moreover, UHS and PSPS also produced nearly fully dense materials with refined microstructures, which are not attainable through conventional sintering. This study demonstrates the potential of novel sintering techniques to densify 3D-printed DIW structures, significantly reducing overall processing time and increasing throughput of the whole process.

### S10 Integrated computational-experimental modeling ad design of ceramics and composites

# S10- Molecular modeling of advanced materials structure and properties

Room: Coquina G

Session Chair: Jiamian Hu, University of Wisconsin-Madison

#### 1:30 PM

#### (ICACC-S10-001-2025) Ab-Initio Molecular Dynamic Simulations of the Conversion of Preceramic Polymers into Ceramics (Invited)

P. Kroll<sup>\*1</sup>

1. University of Texas, Arlington, USA

The thermal conversion of polycarbosilanes, polysilazanes, and polysiloxanes with tailored architecture results in high-performance ceramics such as SiC,  $Si_3N_4$ , and SiCO. We show atomistic details of fundamental reactions obtained from quantum-chemical (ab-initio) Molecular Dynamic Simulations. We observe intra-chain and interchain coupling, cross-linking, and elimination reactions. We discern the role of hydrogen in facilitating the rapid exchange of bonds. We analyze reactions that yield the incorporation of carbon into the polymer backbone (Kumada- or Yajima-like processes). Some outcomes are as expected, while others differ from common perceptions. Adjusting the elimination rates of gaseous species, we can also simulate the impact of reactive environments on the chemical composition of the products. We will show simulations that mimic pyrolysis under hydrogen or carbon dioxide atmospheres.

#### 2:00 PM

## (ICACC-S10-002-2025) Understanding Pyrolysis of Polysiloxane into Silicon Oxycarbide Using ReaxFF Molecular Dynamics

W. Li\*1; K. Lu1; M. Shaik1

1. University of Alabama at Birminghngham, USA

This study employs Reactive Force Field (ReaxFF) molecular dynamics simulations to investigate the high-temperature transformation of polysiloxane (PSO) into silicon oxycarbide (SiOC) ceramics. The simulations were conducted using the LAMMPS molecular dynamics package with the ReaxFF potential. The initial molecular model of PSO consisted of 100 monomer units, arranged in a periodic cubic simulation box to emulate bulk behaviors. Simulations were performed with a time step of 0.4 fs. The system was initially equilibrated at room temperature using an NPT ensemble. Subsequently, the temperature was increased to 3000 K, 4000 K, and 5000 K in steps, with each step involving 25,000 time steps for equilibration and data collection. Python scripts were employed to analyze the simulation outputs, particularly for identifying phase compositions and removing excess gas molecules formed during the simulations. This study reveals the importance of understanding the high-temperature behavior of PSO for optimizing the synthesis and enhancing the properties of SiOC ceramics. By utilizing ReaxFF molecular dynamics simulations, we can gain a comprehensive understanding of the chemical reactions and phase transformations that occur during the pyrolysis of PSO. This knowledge is essential for developing SiOC ceramics with tailored properties.

#### 2:20 PM (ICACC-S10-003-2025) Polymer Derived Ceramics Modeling: An Evolutionary Algorithm Driven Classical Molecular Dynamics Approach WITHDRAWN

M. Belhadj Larbi\*1

1. University of Missouri, Kansas City, Physics and Astronomy, USA

Modeling amorphous materials has many challenges, and for amorphous molecular solids the challenges are compounded. We propose a novel fully automated methodology for modeling this class of materials and here we focus on polymer derived ceramics (PDCs) drawn from within H/B/C/N/O/Si phase space that are grown as thin films via plasma-enhanced chemical vapor deposition. We specifically illustrate our process by producing models of amorphous hydrogenated silicon carbonitride (a-SiCN:H) and calculate the radial pair distribution function and the total energy. The core of our method lies in the integration of an evolutionary algorithm with classical molecular dynamics simulations that parameterize the bonding process to generate targeted structural models. Our method does not require an accurate interatomic potential and can mass produce models with a vast range of stoichiometries, which enables the systematic exploration of diverse structural configurations for a more comprehensive investigation of structure-property relationships.

#### 2:40 PM

#### (ICACC-S10-004-2025) A Combined Experimental and Theoretical Study on Benzyl (2-hydroxyethyl)(methyl)carbamate Synthesis for Analyzing Chemical Selectivity

J. M. Liu<sup>\*1</sup>; T. Shen<sup>2</sup>; L. Li<sup>2</sup> 1. Lambert High School, USA

2. Georgia State University College of Arts & Sciences, Chemistry, USA

Reaction selectivity is an important performance indicator in chemical and material synthesis, which plays an important role in obtaining high-purity substances. Traditional reaction selectivity mainly relies on a series of chemical compositions and multi-scale structural characterizations, even utilizing in-situ characterization to reveal the physicochemical origins of reaction selectivity. These methods often suffer from low efficiency and high costs. In this talk, we use the chemical synthesis of a typical organic compound, Benzyl (2-hydroxyethyl) (methyl)carbamate, which is an important biomolecule of protective antibodies and bioceramic precursor, as a case study. The product is characterized by NMR following the substitution reaction between N-(Benzyloxycarbonyloxy) succinimide and 3-Amino-1-propanol. First-principles studies including reaction potential energy surface, kinetic analysis, and electronic structure analysis are utilized to reveal the different product selectivity. We found that three-body structural stability play an important role in determining reaction selectivity.

# S10- Insights into advanced materials structures and transitions

### Room: Coquina G

Session Chair: Peter Kroll, University of Texas, Arlington

#### 3:20 PM

### (ICACC-S10-005-2025) Polycrystal Microstructure Informatics (Invited)

J. Hu\*1

1. University of Wisconsin-Madison, Materials Science and Engineering, USA

An important topic of materials research is to predict the processingmicrostructure-property relationship as well as the dynamical evolution of microstructures under complex/extreme environmental condition or external stimuli. In this talk, the presenter will introduce their recent works of applying graph neural network (GNN) to predict the microstructure-property relationship in polycrystalline materials, using giant magnetostrictive alloys Tb<sub>x</sub>Dy<sub>1-x</sub>Fe<sub>2</sub> and ceramic solid electrolytes Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> as examples. With benchmarking studies against conventional neural networks and other machine learning models, they demonstrate that the GNN approach simultaneously has low training cost, high prediction accuracy, high interpretability, and high transfer learning performance. Datasets generated from both physics-based modeling and the electron backscattered diffraction (EBSD) measurements were utilized. The presenter will then discuss their ongoing work of developing physicsinformed transformer neural network to predict the dynamical evolution of polycrystalline microstructures, with a goal to rapidly and accurately predict the microstructure patterns that are not captured due to limitation in the instrument and other constraints arising in numerical and real experiments. The presented works have been done in collaboration with M. Dai, M.F. Demirel, X. Liu, Y. Liang, W. Hao, D. Qi, and W.-W. Tung.

#### 3:50 PM

#### (ICACC-S10-006-2025) AI-Enabled Upscaling of Ab Initio Thermodynamics for SiC-3C(001) Surface Reconstructions

M. P. MacIsaac\*1; S. Bavdekar3; R. G. Hennig2; D. Spearot1; G. Subhash1

- 1. University of Florida, Mechanical & Aerospace Engineering, USA
- 2. University of Florida, Materials Science and Engineering, USA
- 3. Illinois State University, Mechanical Engineering, USA

Numerous applications of silicon carbide (SiC) in the field of electronics are critically dependent on the structural and thermodynamic properties of its surfaces and interfaces. The growth of SiC itself, as well as its use as a substrate for the epitaxial growth of other materials (e.g., graphene, alkali antimonides, etc.) requires a good understanding of the numerous surface reconstructions under varying environmental conditions. Disparities exist in the literature between experimental and ab initio findings, e.g., the most favorable surface predicted via DFT is not observed experimentally. This work attempts to reconcile these differences by bridging the gap between the quantum and micro scale studies with atomistic scale studies powered by machine-learned Ultra-Fast Force Fields (UF<sup>3</sup>) trained on ab initio data. Additionally, while most of the previous computational studies were performed with LDA functionals many decades ago, the ab initio calculations in this work employ the more accurate GGA functionals.

#### 4:10 PM

#### (ICACC-S10-007-2025) Understanding the Role of Entropy and Enthalpy Creating Mixed Carbide and Diborid Ceramics

X. Tang<sup>1</sup>; G. Thompson<sup>2</sup>; C. R. Weinberger\*1

- 1. Colorado State University, Department of Mechanical Engineering, USA
- 2. University of Alabama, Metallurgical & Materials Engineering, USA

One area where high entropy materials are now readily being explored is in the area of ceramics. Two main classes of materials are transition metal carbides with the rocksalt structure and the transition metal diborides with the AlB2 structure. However, there are gaps in our understanding of the thermodynamics of mixing of these complicated compounds which hinders our understanding of their synthesis. Thus, to explore how these materials might mix and what affects their mixing, we have utilized density functional theory calculations to determine the enthalpies of mixing, coupled with the quasi-harmonic approximation to obtain finite temperature free energies. These calculations elucidate the roles of atomic mismatch on enthalpies of formation and the competition between enthalpy, configurational entropy and vibrational entropy - all of which dominate in some regimes of composition and temperature space. These calculations and insights allow us to utilize the CALPHAD method to predict phase diagrams and temperatures for pure solid solutions.

### <u>S13 Development & Applications of Adv</u> <u>Ceramics & Composites for Nuclear Fission/</u> <u>Fusion Energy Sys</u>

# S13- Fuel, cladding, assembly, and core evolutions and performance modeling

Room: Coquina D

Session Chair: Gyanender Singh, Idaho National Laboratory

#### 1:30 PM

## (ICACC-S13-010-2025) Fracture modeling of TRISO Coating Layers (Invited)

W. Jiang\*1

1. NC State University, Nuclear Engineering, USA

The TRISO particle is a composite material which contains a uranium bearing kernel, enclosed sequentially by ceramic layers including a buffer, IPyC, SiC, and OPyC layers. TRISO particles are susceptible to potential failures under irradiation conditions in the reactor core, including overpressure failure, irradiation-induced IPyC cracking, debonding between coating layers, and buffer tearing. Although Weibull-based methods have been developed and analyzed to assess the integrity of TRISO fuel particles, these methods fall short of providing a deeper understanding of the failure mechanisms. A high-fidelity modeling approach based on fracture mechanics theory is proposed to produce accurate and consistent failure predictions. In this talk, we will focus on fracture mechanics-based failure probability calculations, as well as a phase field fracture modeling approach to simulate crack initiation and propagation in the composite layers of buffer, IPyC, and SiC materials.

#### 2:00 PM

## (ICACC-S13-011-2025) Modelling TRISO Nuclear Fuel Using Peridynamics (Invited)

T. A. Haynes<sup>\*1</sup>

1. University of East Anglia, Engineering, Mathematics & Physics, United Kingdom

Tri-structural isotropic (TRISO) fuel for high temperature reactors (HTRs) consists of a fissile kernel coated by a porous buffer and a sandwich of SiC between two layers of pyrolytic carbon (PyC). During both the initial rise to power and subsequent operation, these layers experience a complicated array of residual stresses from manufacture, thermal strains and creep. Peridynamics is a non-local structural-mechanical technique able to capture the initiation, retardation, branching and coalescence of cracks in brittle materials. Bond-based peridynamics, implemented in Abaqus, is uniquely placed to leverage the benefits of both peridynamics and finite element analysis. By combining the techniques, it is possible to predict both cracking within each layer and the delamination of layers, together with the impact upon overlying layers and the SiC coating, which acts as the primary containment for fission products in the HTR. Of particular interest is the impact of cracking in the buffer layer upon the overlying SiC and the role of residual stresses in delamination of the buffer and kernel. By combining advanced modelling techniques with experimental measurements, the inherent safety benefits of TRISO fuel can be assured. This will help enable HTRs to provide low-carbon electricity generation and process heat, contributing to a sustainable net-zero society.

#### 2:30 PM

## (ICACC-S13-012-2025) Simulating irradiation-enhanced diffusion in advanced ceramic nuclear fission fuels (Invited)

M. W. Cooper\*1; C. Matthews1; A. Schneider1; J. Rizk1; A. D. Andersson1

1. Los Alamos National Laboratory, USA

Fission nuclear fuel performance and the degradation of fuel properties are governed, in many respects, by the irradiation-induced formation and diffusion of point defects and clusters in the lattice. For example, the diffusion of fission gas and vacancies through the lattice controls gaseous swelling and release, which are key performance metrics. Understanding these processes in advanced ceramic fuel forms, like UN and UC, will benefit several fission reactor concepts, particularly fast-spectrum reactors and microreactors. We present atomic scale calculations of the diffusion mechanisms of host and impurity (Xe) defects in advanced ceramic nuclear fuels (UN and UC). The atomic scale predictions of the stability and diffusivity of point defect and clusters in these systems have then been implemented in cluster dynamics simulations to predict irradiation-enhanced defect concentrations, and Xe/self-diffusivities. The importance of in-reactor conditions and varying chemistry will be discussed, as will the role of certain defects, such as antisites. The impact of these predictions on fuel performance code development will also be shown.

#### **S13- Material technologies for advanced reactors** Room: Coquina D

Session Chair: Michael Cooper, Los Alamos National Lab

#### 3:20 PM

### (ICACC-S13-014-2025) Low temperature and pressure synthesis of novel inert matrix or microencapsulated fuel forms

N. Rani<sup>1</sup>; D. Bhardwaj<sup>1</sup>; L. Snead<sup>1</sup>; D. Sprouster<sup>\*1</sup>

1. Stony Brook University, Material Science and Chemical Engineering, USA

We describe our recent efforts in fabricating monolithic MgO, and MgO containing TRISO and BISO particles, through low pressure sintering. We find that sintering and densification can occur at exceedingly low pressures (as low as 2MPa) to form large dense monolithic compacts. In this presentation, we detail our MgO compact fabrication, characterization (including thermophysical, mechanical and microstructural) and optimized processing subsequently used to fabricate dense Inert matrix fuel compacts. The inclusion of BISO and TRISO particles up to several volume percent with low-to-no cracking demonstrates a potential pathway to fabricate novel inert matrix or microencapsulated fuel forms for advanced reactors.

#### 3:40 PM

### (ICACC-S13-015-2025) Evolution of radiation damage and 3D porosity in a proton irradiated nuclear graphite material

M. Jiang<sup>1</sup>; C. Densham<sup>2</sup>; F. Pellemoine<sup>3</sup>; D. Liu<sup>\*1</sup>

- 1. University of Oxford, Engineering Science, United Kingdom
- 2. Rutherford Appleton Laboratory, United Kingdom
- 3. Fermi National Accelerator Laboratory, USA

Nuclear graphite plays the critical role of neutron moderator, reflector and structural component in several nuclear fission reactor designs. They also serve in High Energy Physics (HEP) as production targets including in the Neutrinos at the Main Injector (NuMI) beamline and Long-Baseline Neutrino Facility (LBNF) at FermiLab, as hadron absorber in Tokai to Kamioka (T2K) at Japan Proton Accelerator Research Complex, and as the target material in muon facilities such as the ISIS Neutron and Muon Source, the J-PARC Muon Source and the PSI Swiss Meon Source. Therefore, it is important to understand radiation induced damage and microstructural changes in nuclear graphite. This work investigated the radiation damage and porosity evolution of POCO ZXF-5Q graphite that has been irradiated with high energy protons. Six locations across the nuclear graphite sample with proton beam fluence and temperature gradients have been studied using Raman spectroscopy and focused ion beam-scanning electron microscopy tomography. A novel method was developed to evaluate the total radiation damage in the material based on the G-band shift in the Raman spectroscopy measurements and results are compared with open literature related to ion and neutron irradiation. It was found that micro-porosity decreases with increased radiation damage and this was compared with other grades of nuclear graphite.

#### 4:00 PM

### (ICACC-S13-016-2025) Multimodal characterization of neutron irradiation effects in glassy carbon

J. D. Arregui-Mena\*<sup>1</sup>; T. Koyanagi<sup>2</sup>; D. Cullen<sup>2</sup>; M. Zachman<sup>2</sup>; Y. Lin<sup>2</sup>; Y. Katoh<sup>2</sup>

- 1. Oak Ridge National Lab, Nuclear Materials Science & Technology Group, USA
- 2. Oak Ridge National Laboratory, USA

Glassy carbon is an allotrope of carbon that has the potential to be used applications in nuclear applications due to its remarkable properties. Glassy carbon is classified as non-graphitizable material due to its inability to be graphitized through conventional thermal treatments. Neutron irradiation of graphite has been thoroughly investigated, but the consequences of neutron-induced defects in non-graphitizable materials have been limited. Through a combination of multiscale characterization techniques, this research seeks to uncover the effects of irradiation on glassy carbon. Advanced microscopy techniques were used to characterize samples irradiated at two neutron doses, which are: a low dose of  $1.97-2.24 \times 10^{25}$  n/m<sup>2</sup> (> 0.1 MeV) and high a high dose in the range of  $6.47 \times 10^{25}$  n/m<sup>2</sup> to  $1.08 \times 10^{26}$  n/m<sup>2</sup> (> 0.1 MeV). This research will enhance the knowledge of the impact of neutron irradiation on glassy carbon and provide insights into other carbon-based materials.

#### 4:20 PM

#### (ICACC-S13-017-2025) SiC-SiC CMCs & Graphite in Nuclear Reactors: Design & Construction Rules in ASME BPV Code Sec. III, Div. 5 for Nonmetallics - 2025 Edition Revisions

M. G. Jenkins\*1; S. T. Gonczy2; J. W. Geringer3; Y. Katoh4

- 1. Bothell Engineering and Science Technologies, USA
- 2. Gateway Materials Technology, USA
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4. Oak Ridge National Laboratory, USA

US DOE is supporting use SiC-SiC CMCs and graphite to enhance fuel performance and improve accident tolerance in high-temperature reactors (HTRs) because these materials are tolerant to the relevant irradiation and chemical environments. Because SiC-SiC CMCs and graphite are nonconventional materials, they are of special concern because the mission of the US Nuclear Regulatory Commission (NRC) is to license and regulate the nation's civilian nuclear reactors, reactor designs and reactor materials. NRC is legally required to use consensus codes and standards as integral parts of the regulatory process. Therefore, the ASME Boiler and Pressure Vessel (BPV) Code Section III "Rules for Construction of Nuclear Components" (including accepted materials) is included in the NRC regulations. Division 5 on HTRs of Section III has supported a working group on graphite and ceramic composites since 2008. For SiC-SiC CMCs to be incorporated into future HTRs, they must be included in ASME BPV Code as acceptable materials. A progress update is provided on revisions for the 2025 edition of Design and Construction Rules in ASME BPV Code that specifically address use of graphite and SiC-SiC CMCs in core and core components.

#### 4:40 PM

#### (ICACC-S13-018-2025) Thermal Expansion of Nuclear Graphite Materials at High Temperatures with In-situ Neutron Diffraction

- H. Ling\*1; E. Obbard1; D. Liu2; A. Paradowska3; M. Jiang2
- 1. University of New South Wales, Australia
- 2. University of Oxford, United Kingdom
- 3. Australian Nuclear Science and Technology Organisation, Australia

Graphite exhibits highly anisotropic thermal expansion, with a room temperature coefficient of thermal expansion (CTE) of approximately -1.5 x  $10^{-6}$  °C<sup>-1</sup> parallel to the basal plane and 27 x  $10^{-6}$  °C<sup>-1</sup> perpendicular to it. These CTE values generally increase with temperature and follow a non-linear function. The bulk CTE of nuclear-grade Gilsocarbon in pline is around 7 x  $10^{-6}$  °C<sup>-1</sup> and is lower than what is practed by a fully dense, isotropic polygranular structure. This discrepancy is attributed to microstructural crack closure in the material. Thus, understanding of the complex thermal expansion behaviour of different polygranular graphite materials is crucial for ensuring their dimensional stability as reactor core material, preventing stress-induced degradation, and maintaining effective heat transfer. This study has investigated the anisotropic thermal expansion of five grades of fine-grained and coarse-grained nuclear-grade graphite materials. CTE values were measured over a temperature range from room-temperature to  $1600^{\circ}$ C. Specifically, this study has employed a high-temperature in-situ neutron diffraction method using the Kowari diffractometer at the Australian Centre of Neutron Scattering. The samples were heated in a niobium vacuum furnace, replicating the high temperatures reactor core materials are subjected to in both current and advanced reactor technologies.

### <u>S15 9th International Symposium on</u> <u>Additive Manufacturing and 3-D Printing</u> <u>Technologies</u>

#### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies- Vat Photopolymerization 2

Room: Coquina A

Session Chairs: Michael Stuer, Empa; Martin Schwentenwein, Lithoz GmbH

#### 1:30 PM

### (ICACC-S15-010-2025) Fabrication of highly transparent yttria 3D structures by DLP-based additive manufacturing (Invited)

#### H. Yun\*

1. Korea Institute of Materials Science, Republic of Korea

High-quality transparent Yttria (Y<sub>2</sub>O<sub>3</sub>) can be produced using various shaping techniques, including dry pressing, gel casting, and slip casting. However, the geometric control limits of shaping processes would hinder the utilization and application of transparent Y<sub>2</sub>O<sub>3</sub>. We herein propose digital light processing (DLP)-based additive manufacturing (AM) as one of the best solutions to this structural drawback. In this study, 3D-structured transparent Y<sub>2</sub>O<sub>3</sub> ceramic was achieved via DLP-based AM technology assisted by vacuum sintering, and the critical factors governing the transparency were revealed. As sintering additives, zirconia and lanthana were utilized to regulate grain growth. Printing parameters including layer thickness and UV light intensity were optimized to control printing accuracy. Following pre-sintering in air and vacuum sintering treatments, the transparent  $Y_2O_3$  ceramics attained a high transmittance reaching 98.7% of the theoretical limit by achieving a fine-grained dense microstructure. Polished with newly developed 3D polishing

technology, the 3D  $Y_2O_3$  lens exhibits superior optical imaging capability. This study demonstrates that overcoming the geometric control limitation of  $Y_2O_3$  by ceramic AM offers excellent promise for expanding the utilization of  $Y_2O_3$  in various applications.

#### 2:00 PM

### (ICACC-S15-011-2025) 3D printing of bio-based photocurable ceramic slurries prepared with second-life glass-based materials

M. Porcarello<sup>\*1</sup>; M. Salvo<sup>1</sup>; F. Smeacetto<sup>1</sup>; S. Anelli<sup>1</sup>; M. Sangermano<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology, Italy

This study explores the potential for repurposing waste glass materials in the field of 3D printing of slurries via Vat photopolymerization technologies, using biobased photocurable formulations. The formulations were prepared with acrylated epoxidized soybean oil (AESO) and reactive diluent isobornyl acrylate (IBOA). Waste materials like mineral wool and glass from the vitrification of ash from municipal waste incinerators were milled and sieved under 25 µm. The powders were morphologically characterized using field emission scanning electron microscopy (FESEM) and thermally using dynamic scanning calorimetry (DSC), hot stage microscopy (HSM) and dilatometry. Afterwards, the powders were mixed with AESO formulations to prepare photocurable slurries with ceramic loadings ranging from 40 to 60 wt%. Rheological and photo-rheological analyses were carried out to establish printing parameters including exposure time and layer thickness. Then, porous like structure were 3D printed using masked-stereolithography printers. Subsequently, thermal treatments were performed to consolidate the printed objects, removing the resin component and yielding glass-ceramic structures. The results indicate significant potential for manufacturing porous-like glass-ceramic materials through this method, with promising results for sustainable material reuse and advanced manufacturing processes.

#### 2:20 PM

# (ICACC-S15-012-2025) Effect of filler particles on the composition and properties of 3D printed polymer-derived ceramics

A. Kulkarni<sup>\*1</sup>; H. Yazdani Sarvestani<sup>1</sup>; A. Sohrabi<sup>3</sup>; T. Lacelle<sup>2</sup>;

- V. Karamzadeh3; A. Shashoua3; Y. Martinez-Rubi2; M. Jakubinek2; B. Ashrafi1
- 1. National Research Council Canada, Aerospace, Canada
- 2. National Research Council Canada, Quantum and Nanomaterials,
- Canada
- 3. McGill University, Canada

Ceramic materials are renowned for their high compressive strength, thermal stability, and chemical resistance, making them invaluable in various applications. However, their inherent brittleness and low damage tolerance limit their structural use. To address these challenges, polymer-derived ceramics (PDCs) offer a promising solution by overcoming the shape constraints typical of traditional ceramic processing. This study focuses on the formulation of commercial preceramic polymer (PCP) resins, to produce UV-curable preceramics suitable for 3D printing via vat photopolymerization. The 3D printed geometries are subsequently pyrolyzed to form strong, lightweight ceramic components. Tailoring of the composition and properties is achieved through the use of additives, such as filler particles in the resin formulation, which influences the composition of the ceramic. The composition of the final ceramic also dictates the high temperature stability and mechanical properties. Here we assess the effect of different additives on the final ceramic by comparing the ceramic yield, the composition and the mechanical properties of lattice structures. The combination of PCPs with vat photpolymerization 3D printing enables the creation of complex ceramic lattices, demonstrating a cost-effective and a facile route for manufacturing customized, high-performance ceramic composites.

#### 2:40 PM

#### (ICACC-S15-013-2025) Additive Manufacturing of Vibration Absorbing Ceramics for Rotating Detonation Engines

B. Lam<sup>\*1</sup>; B. Pajo<sup>1</sup>; C. Martinez<sup>1</sup>; R. Trice<sup>1</sup>

1. Purdue University, MSE, USA

Combustion in rotating detonation engines produce rhythmic vibrations in the kilohertz range with combustion temperatures well above 2200°C observed. Due to the harsh environment during RDE service, ceramic inner and outer bodies would be favored for this application. However, ceramics are brittle and linear elastically propagate the energy of the detonations, contributing to premature failure. Of interest here is to design glass/ceramic composites that can absorb part of the detonation energy by tuning the glass transition temperature of the glass to the operational temperature and frequency of the combustion of RDEs. In this presentation, additive manufacturing using a digital light projection technique will be explored as a potential method of producing parts out of a SiO<sub>2</sub>/mullite-material system. Successful ink development, printing, and post-processing shows the potential for additive manufacturing being a viable manufacturing method for this material system. Preliminary data will be presented to show damping (via internal friction) versus temperature for the SiO<sub>2</sub>/mullite system.

### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies- Vat Photopolymerization 3

#### Room: Coquina A

Session Chairs: Hui-Suk Yun, Korea Institute of Materials Science; Fiona Spirrett, Osaka University

#### 3:20 PM

### (ICACC-S15-014-2025) Refined powders in additive manufacturing: Challenges and opportunities (Invited)

E. Rosado<sup>2</sup>; R. Moreno<sup>2</sup>; T. Graule<sup>3</sup>; M. Stuer<sup>\*1</sup>

- 1. Empa, Advanced Materials and Surfaces, Switzerland
- 2. Instituto de Ceramica y Vidrio, Spain
- 3. Empa, Laboratory for High Performance Ceramics, Switzerland

For all the interest additive manufacturing has earned across industrial fields, basic challenges must still be addressed before its widespread adoption can be realized. Particularly, the promise of arbitrary shape complexity in additive manufacturing could not yet be achieved. Changing part dimensions and complexity often cause process development costs and delays, diminishing the benefits of additive manufacturing in dynamic industrial settings. While part individualization is possible once a slurry system has been optimized for a specific part typology (e.g. product), the slurry formulation is generally not robust enough to accommodate significant changes (e.g. dimensions, complexity), rapidly leading to processing defects. This imposes recurrent slurry formulation and process optimization efforts to address the defects and ensure for the reliable shaping of high-quality ceramic parts. With efforts underway to turn towards the use of refined powders, these challenges may even be enhanced as the use of refined (nanoscale) powders comes with its own set of difficulties. In this presentation, the motivation for refined powders in microstructural engineering will be discussed and the resulting impact on the additive manufacturing process and produced parts described, before providing some outlook on future research directions.

#### 3:50 PM

### (ICACC-S15-015-2025) Multi-material ceramic/ceramic and metal/ceramic components through vat photopolymerization

- M. Schwentenwein\*1; S. Geier1; J. Schlacher3; S. Nohut1; R. Bermejo2
- 1. Lithoz GmbH, Austria
- Montanuniversitaet Leoben, Institut fuer Struktur- und Funktionskeramik, Austria
- 3. Montanuniversitaet Leoben, Austria

This talk presents the status quo of multi-material AM of ceramics based on lithography-based ceramic manufacturing (LCM), a technology belonging to the family of vat photopolymerization (VPP) techniques. Different material combinations have been investigated including hydroxyapatite (HA)/tricalcium phosphate (TCP), porous/ dense alumina, porous/dense HA, alumina/zirconia-toughenedalumina (ZTA), and copper or silver in combination with glass ceramic. In more detail, this contribution will showcase the use of this multi-material AM approach to combine ZTA sandwiched between pure alumina, yielding a characteristic strength higher than 1 GPa on the laminate multi-material system, compared to 650 MPa in the monolithic alumina. It will also present the outstanding thermal shock resistance of such AM produced multi-material components owing to the embedded compressive layers, which leads to a significant performance enhancement compared to the monolithic reference. This article also discusses the main issues and future possibilities of ceramic-ceramic and metal-ceramic multilayer fabrication by LCM technology. The obtained results show that this technology holds great potential to path the way from classical single material structures to multi-material and functionally graded ceramics.

#### 4:10 PM

### (ICACC-S15-016-2025) Challenges of printing of large ceramic parts by SLA 3D printing

E. Louradour<sup>\*1</sup>; C. Manière<sup>2</sup>

- 1. 3DCERAM SINTO, Process, France
- 2. ENSI CAEN, CNRS, France

SLA 3D printing is one of the most relevant and promising techniques to produce technical ceramic parts. The growing demand for complex and large shaped products makes SLA 3D printing process the ideal technique to answer this need and confirm its industrial deployment as a new standard shaping process. With the help of a printer that allows it (C1000/C3601 3DCERAM), the printing of large parts with very thin to very thick cross-sections is possible thanks to a good mastery of the different stages of the manufacturing process: formulation of ceramic slurries, machine and printing parameters, etc. However, to get the de-binded parts that do not show deformation or cracks remains a challenge. This study will describe the ability of SLA 3D printing to manufacture parts with highly variable cross-sections and the latest work to satisfactorily de-bind them. Zirconia will serve as an example material because of its multiple applications, but also Si3N4, whose use in the space, medical or electronics fields is constantly increasing

#### 4:30 PM

#### (ICACC-S15-017-2025) Additive Manufacturing of Novel Ceramic Armour Structures using Vat-Photopolymerization: A comparative study on Alumina, ZTA, and ATZ

B. Ozkan<sup>\*1</sup>; A. Goulas<sup>1</sup>; A. Ketharam<sup>1</sup>; A. Kanna<sup>1</sup>; P. Vasudevan<sup>1</sup>; B. Vaidhyanathan<sup>1</sup>

1. Loughborough University, Department of Materials, United Kingdom

Ceramic materials like Alumina, ZTA, and ATZ are increasingly preferred for ballistic armor due to their high hardness, low weight, and excellent impact resistance. Traditional manufacturing methods limit shape complexity and customization, restricting their application. This study explores the use of Direct Light Processing (DLP), a form of VAT Photopolymerization, to 3D print these ceramics, ballistic performance of the 3D printed samples. The study presents a significant advancement in the creation of complex, lightweight, and conformal ceramic armor structures. These findings highlight the potential for additive manufacturing to produce tailored, high-performance ceramic armors for both defense and civilian applications, offering new opportunities for customized ballistic protection.

#### 4:50 PM

#### (ICACC-S15-018-2025) High Temperature Ceramic Heat Exchanger for Re-Entry Systems through Additive Manufacturing

N. Zheng\*1; J. Gou1

1. University of Central Florida, Mechanical and Aerospace Engineering, USA

With increasing rocket launches over the recent years, there is growing interest in reusability of launch vehicles. Returning vehicles experience ablation on surface due to aerothermal heating imposed on them during the atmospheric entry, and the temperatures at the leading edge can be as high as above 2,000C. These vehicles required a heat regulator to ensure the surface temperatures are within operating tolerances and reduce the maintenance needs upon return. The ceramic heat exchanger has a honeycomb structure of consecutive matrix panels aligning to one another in a stairway pattern. Due to the complexity and capability of scaling, the structure was additively printed through polymerization of an alumina-based ceramic resin utilizing digital light processing (DLP) and then undergoing pyrolyzing to form the final structure. The part was sintered at 1,510C in a single firing schedule spanning approximately 75 hours. The work will present the design and geometry of the prototype, shrinkage of part after pyrolysis, material characterization, and a simulation and analysis of heat transfer and circulation of cooling fluid to maintain temperatures. The simulation was conducted using COMSOL Multiphysics where diffusing of heat through the solid ceramic panel and a cooling fluid was introduced.

#### 5:10 PM

#### (ICACC-S15-019-2025) Exploring the Potential: Wireless Embedded Ceramic Sensors using Additive Manufacturing

N. Reed\*1; J. B. Shivakumar3; R. Srinivasaraghavan Govindarajan1;

- S. C. Perry<sup>2</sup>; K. Coote<sup>1</sup>; E. Rojas-Nastrucci<sup>3</sup>; D. Kim<sup>1</sup>
- 1. Embry-Riddle Aeronautical University, Aerospace Engineering, USA
- 2. Embry-Riddle Aeronautical University, Mechanical Engineering, USA
- 3. Embry-Riddle Aeronautical University, Electrical Computer Science and Systems Engineering, USA

Additive manufacturing (AM) has enabled and accelerated the development of structural components with embedded sensors. The unique AM process allows for extensive access to the internal structure of complex parts, something unattainable with traditional manufacturing methods. However, despite this, creating ceramic structures with embedded sensors remains a significant challenge. The advantageous temperature resistance and stiffness of ceramic parts present distinct challenges when attempting to process a structure to incorporate an embedded sensor. In this work, we explore the development of ceramic structures embedded with additively manufactured sensors to accurately measure the internal properties of the substrate at elevated temperatures. Utilizing the vat photopolymerization process, a wireless ceramic sensor base is printed in-situ inside a ceramic substrate. After the sensor and substrate are completely fabricated and post-processed, a permittivity-based

resonator and antenna are printed inside the ceramic to complete the sensor. After post-processing, the completed sample can perform wireless sensing while retaining the beneficial properties of the underlying ceramic material. This novel fusion of embedded AM ceramic sensor fabrication with wireless sensing technologies enables highly customizable in-situ sensing of structures previously unachievable with traditional techniques.

### **<u>S16 Geopolymers Inorganic Polymers and</u>** <u>Sustainable Construction Materials</u>

#### S16- Novel applications of geopolymers I

Room: Ballroom 1-2

Session Chair: Enrico Bernardo, University of Padova

#### 1:30 PM

### (ICACC-S16-008-2025) Organic-based synthesis of geopolymers and conversion to ceramics (Invited)

D. Samuel<sup>2</sup>; D. do Carmo Silva<sup>2</sup>; W. M. Kriven<sup>\*1</sup>

- 1. University of Illinois at Urbana-Champaign, USA
- 2. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA

Alkali geopolymers are a facile forming route for alkali aluminosilicate ceramics because they are formed as fluids and crystallize upon heating to about 1000 °C. This work investigated the synthesis of geopolymers with organic bases rather than inorganic alkali hydroxides. This avoids the use of alkali cations entirely and greatly widen the range of ceramics formable via geopolymers. The successful organic base tested was guanidine, for its ability to form geopolymers with Al<sub>2</sub>O<sub>3</sub> : SiO<sub>2</sub> ratios of 1:2 and 1:4 as well as 3:2 to match the composition of mullite. Guanidine was successful, causing reaction at room temperature and producing bodies with atomic structures and microstructures similar to the equivalent sodium geopolymer compositions. Yttrium silicate and zinc silicate geopolymerica compounds were formed via guanidinium hydroxide charge balancing. A CO<sub>2</sub> laser sintering method is extremely efficient in terms of processing time. While an oven may take hours to reach the desired temperature, a laser can achieve the same temperature in just a few seconds. After laser sintering, a notable contraction of the mullite precursor composition, geopolymer sample was observed, which can indicate a good densification and proved the effectiveness of the method used. The microstructure of the grains was observed to take the form of needles which were evenly dispersed across the entire surface of the sample.

#### 2:00 PM

#### (ICACC-S16-010-2025) Elimination of malachite green from aqueous and saline water by laterite-derived Na-polyferrosialate and polyferrophosphosialate geopolymers (Invited)

S. Tome\*1; C. Rüscher1

1. Leibniz University Hannover, Mineralogy, Germany

In this study, two laterites (LA)-based geopolymers were synthesized using alkalination (GPAL) and phosphoric acid-activation (GPAC) approaches and applied to scavenge malachite green (MG) dye from aqueous (non-saline) and saline water. The adsorption kinetics data were best described by the pseudo-first-order (PFO) model wherein the adsorption rate, denoted by rate constant (k1), increased with an increase in ionic strength (salinity). The equilibrium data were best modelled by the Sips isotherm. GPAL had a higher maximum adsorption capacity (Qms) than GPAC in both aqueous (non-saline) and saline water. The adsorption swithout NaCl, from 12.4 to 54.1 mg/g and from 57.1 to 92.0 mg/g for GPAC and GPAL, respectively. The adsorption capacities were increased in saline solution relative to aqueous solutions without NaCl, from 12.4 to 54.1 mg/g

and from 57.1 to 92.0 mg/g for GPAC and GPAL, respectively. These results indicate that alkaline-based geopolymers are better candidates for scavenging MG dye from water, especially in saline environments.

#### S16- Novel applications of geopolymers II

Room: Ballroom 1-2 Session Chair: Pozhhan Mokhtari, University of Illinois at Urbana-Champaign

#### 3:20 PM

#### (ICACC-S16-011-2025) Development of Electro Chemical Bonding For Refractory Castables

R. A. Pattillo<sup>\*1</sup>

1. Reno Refractories, Inc., Research, USA

Newly developed bonding techniques for application in castables used in high temperature industrial processes provide superior properties. These materials are proving to extend campaign life compared to the best low/no cement materials. The use of electrically active components generates electric fields that alter the normal particle interactions during bond formation. Test results are presented to support the improvements claimed.

#### 3:40 PM

## (ICACC-S16-012-2025) Development of an intumescent inorganic coating on steel substrates

W. Ncho\*1

1. UNIVERSITE, IRCER, France

The challenge of environmental protection is a fundamental issue in all industries. Organic polymers play an important role in the French nuclear industry. They are used in many safety-related applications and in large quantities to fight corrosion and fire. However, they are less durable and require a lot of energy to maintain. Geopolymer-based coatings are a promising alternative due to their excellent properties, such as mechanical strength and fire resistance (up to 1500 °C). The aim of this work is to produce a high-temperature resistant and intumescent geopolymer-based coating on steel plates. Geopolymer foam, dense geopolymers as well as multilayer geopolymer systems with different porosities were prepared with two different metakaolins, and cast on steel plates previously blasted with corundum for 4 min. Geopolymer coatings with intumescent additives were prepared and sprayed on the samples previously prepared on the steel plates. The adherence is around 2 MPa. Fire resistance were carried out with a flame at 800°C. The results showed that the samples geopolymer coatings allow to reach only on the backside test flame a temperature maximum of 600 °C after 30 min. The multi-layer permits to reduce this temperature at 400 °C with intumescent additive. Aging tests of samples are currently being carried out as well as the challenge of intumescence.

#### 4:00 PM

## (ICACC-S16-013-2025) Feasibility of using geopolymer technology in SiC powder synthesis process (Invited)

W. Lee\*1; Z. Yang1; Y. Tsai3; Y. Lin2

- 1. National Taipei University of Technology, Institute of Mineral Resources Engineering, Taiwan
- 2. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan
- 3. National Yang Ming Chiao Tung University, Department of Civil Engineering, Taiwan

Silicon carbide (SiC) is extensively used in lots of industries due to its high temperature, oxidation, and wear resistance. However, traditional synthesis methods, such as chemical vapor deposition, sol-gel, and carbothermal reduction, face challenges like high temperatures, expensive raw materials, and complex processes. This study focuses on the impact of geopolymer technology on SiC powder synthesis, focusing on parameters like synthesis temperature, carbon-to-silicon ratio, nucleating agent addition, and ion removal. The results show that geopolymer technology improves SiC crystallinity after the carbothermal reduction reaction. TEM analysis showed clear crystal faces with twin crystal morphology. After using optimal parameters to fabricate the geopolymer green body and synthesize at 1600°C for 4 hours, the crystallinity of SiC will be increased and a shift from twin to single crystals. Further enhancements, including seed crystal addition and alkali metal ion removal before synthesis, increased SiC content to 99%. This study shows the successful synthesis of high-quality SiC powder from industrial by-products, paving the way for its broader application in various industries.

#### 4:30 PM

#### (ICACC-S16-014-2025) Comparative Testing of the Wear Resistance of Na-Based Geopolymer Composites Filled with Basalt Glass and Glass-Ceramic Microspheres

Y. Zubko\*1; Y. Zubko3; W. M. Kriven2

- 1. University of Illinois Urbana-Champaign, Materials Science and Engineering, USA
- 2. University of Illinois at Urbana-Champaign, USA
- 3. Micro Basalt Innovations Canada Corp., Canada

The results of comparative testing according to ASTM C501-21 standard for the wear resistance of composite material samples based on a sodium geopolymer filled with microspheres of basalt glass and glass-ceramics are presented. These microspheres were obtained by the method of superheated melts. It was established that, as a result of high-temperature annealing of basalt glass microspheres, a series of phase transitions occur, leading to a significant restructuring of the microstructure of the basalt microspheres, caused by the appearance of microcrystalline inclusions. As a result of this modification, basalt glass-ceramic microspheres are obtained, which have higher density and microhardness. Comparative testing shows that, with the same degree of filling, samples containing basalt glass-ceramic microspheres have, on average, 20 % higher wear resistance, compared to those containing basalt glass microspheres. The composite material based on basalt glass-ceramics also has higher thermal stability and may be of interest to specialists developing wear-resistant composite products operating at elevated temperatures.

#### 5:00 PM

#### (ICACC-S16-015-2025) Design of alumino-silicate refractory matrices in the context of climate change: sustainability approach (Invited)

#### E. Kamseu<sup>\*1</sup>

1. MIPROMALO, Research, Cameroon

Elie Kamseu<sup>a</sup>, Paolo Veronesi<sup>a</sup>, Isabella Lancellotti<sup>a</sup>, Cristina Leonelli<sup>aa</sup> Department of Engineering "Enzo Ferrari", Modena, Via P. Vivarelli 10, 41125, Italy <sup>b</sup>Local Materials Promotion Authority, Nkolbisson, Yaounde, P.O. Box 2393, Cameroon dRCER, UMR 7315, University of Limoges, Limoges, 12 Rue Atlantis, France Abstract: The work proposes cold-setting method for the design and production of alumino-silicate refractories with energy saving and low emission of CO2. The cold-setting process proposed is based on shrinkage-free theory and the management of the expansion coefficient of refractory oxides from natural raw materials. Refractory composites designed are capable to withstand high temperature and thermal gradient. A-rich-kalsilite, Mullite, Tialite and Mullitecordierite based refractory matrices are designed with alternatives cold-setting processes with desirable porosity in the way to achieve dense and porous refractories. The mechanism of the formation and consolidation of cold-setting refractory matrices highlight the role of colloidal silicate and alumina in partial replacement of alkali-based colloidal solution. Consequently refractoriness, shrinkage, thermal resistance, are improved with the achievement of optimum microstructure.

### **<u>S17 Advanced Ceramic Materials and</u> <u>Processing for Photonics and Energy</u>**

# S17- Advanced Ceramic Materials and Processing for Photonics and Energy IV

#### Room: Coquina H

Session Chairs: Giovanni Fanchini, University of Western Ontario; Fiorenzo Vetrone, INRS, Université du Québec

#### 1:30 PM

#### (ICACC-S17-022-2025) Developments in Tubular Oxide Nanomaterials for Sensing Applications (Invited)

O. K. Varghese\*1; D. Waligo1; M. Paulose2

- 1. University of Houston, Department of Physics & Texas Center for Superconductivity, USA
- 2. University of Houston, Department of Physics, USA

Among a wide range of low dimensional material architectures discovered to date, the nanotube architecture stands out due to the unique properties exhibited by materials in this geometry and the development of scalable methods for fabrication. This geometry provides the materials tremendous surface area and tunable electrical and optical properties via manipulation of geometrical features. For this reason, the nanotube geometry has been extensively explored for applications involving semiconductors, especially where surface/interfacial interactions are relevant. The charge carriers in a semiconducting nanotube can always stay in the vicinity of the surface and take part in the surface/interfacial reactions, which can help them make these processes efficient. Recently, we developed a new nanotube material using anodic oxidation. The material showed distinct properties highly suitable for sensing chemicals for emerging energy related applications. This presentation is aimed at discussing its unique sensing characteristics.

#### 2:00 PM

#### (ICACC-S17-023-2025) Development of a Silicon Nitride Platform for Next-Generation Photonic Devices (Invited)

B. Ahammou<sup>\*1</sup>; N. Dalvand<sup>2</sup>; Y. Ouldhnini<sup>1</sup>; A. Radi<sup>1</sup>; B. Le Drogoff<sup>4</sup>; K. K. Ghuman<sup>1</sup>; J. Margot<sup>3</sup>; M. Ménard<sup>2</sup>; M. Chaker<sup>1</sup>

- 1. INRS, Energie materiaux télécommunications, Canada
- 2. Ecole de technologie superieure, Canada
- 3. Universite de Montreal, Physics, Canada

Silicon nitride (SiN) is a key ceramic material for photonic integrated circuits, offering ultra-low optical losses, a wide spectral transparency, and CMOS compatibility. Its ability to function across visible to mid-infrared wavelengths, coupled with superior optical power handling and reduced propagation losses compared to silicon-on-insulator platforms, makes SiN essential for applications such as telecommunications, biosensing, and quantum photonics. The development of a robust SiN-based optical platform is crucial for advancing these technologies. The flexibility of SiN enables its use in both thin and thick waveguides, each tailored to specific applications. Thin SiN waveguides are ideal for passive filters and low-loss waveguides, while thick SiN layers offer strong optical confinement, necessary for applications such as nonlinear optics, mid-IR photonics, and frequency combs. However, producing thick SiN layers faces challenges, such as cracking due to high tensile stress when grown using Low-Pressure Chemical Vapor Deposition and high optical absorption losses when synthesized by Plasma-Enhanced Chemical Vapor Deposition caused by hydrogen incorporation. Our work combines experimental and computational approaches to address these limitations, optimizing stress control and deposition processes.

#### 2:30 PM

## (ICACC-S17-024-2025) Using Organic Conjugated Polymers to Recycle Waste Heat (Invited)

E. Orgiu\*1

1. Institut National de la Recherche Scientifique (INRS), EMT Centre, Canada

With world's reserves of fossil fuels being depleted rapidly, researchers are working towards the quest for new and more environmentally friendly sources of energy. Furthermore, it is estimated that >60% of the energy is lost in the form of waste heat, resulting in useless dissipation and environmental pollution. Hence, it iappears clear that recycling waste heat is of utter importance, and for this reason, more and more attention is being paid to thermoelectric materials, i.e., materials that are capable of converting a heat gradient into electricity. In this presentation I will give a few examples on how to use conjugated polymers to make organic thermoelectric generators. On the one hand, I will talk about the versatility of inkjet printing technology with a commercial PEDOT:PSS ink to evaluate the thermoelectric performances of films deposited on different substrates (polyimide foils, glass, and silicon oxide). The substrate wettability and the printing direction were found to strongly impact the resulting thermoelectric performances. Moreover, to investigate the thermoelectric performances of a fully inkjet-printed flexible thermoelectric device, we compared the role of e-beam evaporated vs. inkjet-printed electrodes. In addition, I will present a novel polymer with a joint polaronic and radical conductivity which brings to a higher conductivity which is pivoltal to achieving a high thermoelectric figure of merit.

#### 3:20 PM

#### (ICACC-S17-025-2025) Advances in Catalyst Design for Efficient Hydrogen Production: From Electrocatalytic Membranes to Solar-Driven Systems (Invited)

M. Siaj\*1

1. Universite de Sherbrooke Faculte de Genie, Chemical engineering, Canada

This talk covers recent advances in designing advanced catalysts for hydrogen production, focusing on electrochemical and photoelectrochemical systems. We highlight the potential of transition metal chalcogenides (e.g., MoSe<sub>2</sub>, NiCoSe<sub>2</sub>) and hybrid nanostructures (e.g., MoS<sub>2</sub>/CdS, CdS/Au/SnO<sub>2</sub>) for efficient hydrogen evolution reactions (HER). Special attention is given to binder-free electrocatalyst membranes, which offer high performance with low overpotentials and durability through vertically aligned porous architectures. Additionally, cryogelation and carbonization processes enhance catalyst effectiveness. In photoelectrochemical systems, plasmonic nanoarrays and core-shell heterojunctions increase photoconversion efficiency, as seen in CdS/Au/SnO<sub>2</sub> and MoS<sub>2</sub>/CdS structures. These developments in materials design support scalable hydrogen production, advancing the shift to renewable energy.

#### 3:50 PM

### (ICACC-S17-026-2025) Specialty glass materials and fibers for biophotonics and sensing (Invited)

- S. Russo<sup>1</sup>; M. Nagar<sup>1</sup>; J. T. Pandayil<sup>2</sup>; N. Boetti<sup>2</sup>; D. Janner<sup>\*1</sup>
- 1. Politecnico di Torino, DISAT, Italy
- 2. Fondazione LINKS, Italy

The advancement of bioresorbable glasses have enabled promising advancement in the fields of biophotonics. Indeed, those glasses have allowed to translate some biomedical techiques, both for therapy and diagnostics, to move from the application from outside the body to the inside of the body. This potentially overcomes the limitations of the current fiber optics based on silica. Aside from that, the decoration and application of coatings and nanomaterials to the surface of traditional fibers have enabled to develop very sensitive detection systems based on fiber optics. Those systems are at the basis of point-of-care/bedside sensing for therapy and diagnostics in the biomedical field. We will present an overview of these glass materials and fibers for biophotonics and sensing starting from state of the art in research to some perspectives for the future in terms of research on materials and fabrication techniques.

#### 4:20 PM

# (ICACC-S17-027-2025) Casimir nanoparticle levitation with broadband perfect magnetic conductor metamaterials (Invited)

V. Giannini\*

1. TII, Advanced Materials, United Arab Emirates

Casimir-Polder forces are natural candidates to tackle the phenomenon of levitation but are usually attractive forces. Here, we present nanoparticle levitation only based on the design of a metamaterial showing an effective perfect magnetic behavior on a broad range of frequencies. The nanoparticle's potential resulting from the combination of the Casimir-Polder force and its weight allows anharmonic oscillations for the nanoparticle in general and harmonic ones for energies close to the potential minimum. We show that the characteristic frequency of the latter depends linearly on Planck's constant.

#### 4:50 PM

### (ICACC-S17-028-2025) Silicon nitride substrates for power electronics

- E. Zschippang\*2; A. Wolfrum2; L. Schmidtner2; J. Hoerig1; M. Herrmann2
- 1. Fraunhofer-Center für Silizium-Photovoltaik CSP (ISE), Germany
- 2. Fraunhofer IKTS, Germany

Silicon nitride materials show excellent mechanical properties and high thermal shock resistance. In addition, the thermal conductivity of silicon nitride  $(Si_3N_4)$  materials can be increased to up to 100 W/(m\*K) and more by adjusting the chemical composition and microstructure. It is this combination of properties that makes  $Si_3N_4$ substrates particularly suitable for high-performance power modules based on SiC semiconductors. In this presentation the influence of different powder qualities and sintering conditions on the microstructure and hence thermal conductivity of  $Si_3N_4$  materials will be shown. Based on the materials developed, substrates were manufactured by sintering large blocks and multi-wire sawing. These substrates were characterized with regard to their thermal conductivity as well as their mechanical and electrical properties, and the results are now presented and discussed.

### **S18 Ultra-High Temperature Ceramics**

### S18- Response in Extreme Environments

#### Room: Coquina F

Session Chairs: Lisa Rueschhoff, Air Force Research Lab; Sea-Hoon Lee, Korea Institute of Materials Science

#### 1:30 PM

#### (ICACC-S18-033-2025) Mechanical performance, oxidation behavior, and thermal shock resistance of additively manufactured short carbon fiber-reinforced zirconium diboride (Invited)

L. M. Rueschhoff\*1; C. Wyckoff2; J. Kaufman2

- 1. Air Force Research Laboratory, USA
- 2. UES, Inc., USA

Zirconium diboride is an ultra-high temperature ceramic (UHTC) of interest for the typical UHTC properties of high melting temperature and oxidative resistance, all at a comparative low price and density. As typical with ceramics and UHTCs, processability and performance (both mechanical and high temperature oxidation) are often limited. Here, we present a method to additively manufacture zirconium diboride with short carbon fiber reinforcements for enhanced mechanical performance and thermal shock resistance. The material extrusion technique of direct ink writing allows for near-net shaping of a highly-loaded (52 vol.% ceramic and up to 10 vol.% fiber) feedstock inks, resulting in in high density (~ 95%) after pressureless sintering. Characterization of the sintered composites reveals a dependence of mechanical properties and oxidation behavior on sintering temperature. A detailed analysis of microstructures before and after oxidation and thermal shock exposure (achieved via oxyacetylene torch), along with room-temperature bending strength will be presented.

#### 2:00 PM

(ICACC-S18-034-2025) Universal trends in spectral emittance of oxides and carbide at ultrahigh temperatures (Invited)

P. E. Hopkins<sup>\*1</sup>

1. University of Virginia, USA

Mitigating the thermal loads at high and ultrahigh temperatures in the extreme environments associated propulsion and hypersonic flight require materials with requisite radiative heat transport properties. Here we present the measurements of the spectral absorptivity/emissivity and emittance of a series of rare-earth doped oxides, zirconates and metal carbides at temperatures up to their melting point through a combination of infrared variable angle spectroscopic ellipsometry to measure the intrinsic optical properties of the ceramics, and laser heating-based radiometry for emittance measurements. In the oxides, we show blackbody like emissivity in the mid-infrared due to phonon mode absorption, which broaden the near-perfect-like emissivity into the near-IR at increased temperature. In the visible and near-IR, we observe a nearly universal increase in graybody like emittance of the rare earth oxides up to their melting points. In the metal carbides, we show that the temperature dependent emissivity of metal carbides either increases or decreases up to their melting point depending on the electronic configuration and surface roughness, with all measured values for emittance converging close to melt. We show similar trend in measured emittance of high entropy carbides.

#### 2:30 PM

#### (ICACC-S18-035-2025) Torch Testing of Polymer Derived Ultra-High Temperature Ceramics Matrix Composites Prepared from Air Force Preceramics

J. Ponder\*<sup>1</sup>; J. Deijkers<sup>1</sup>; A. Advincula<sup>1</sup>; J. Delcamp<sup>2</sup>; M. B. Dickerson<sup>2</sup>; T. Pruyn<sup>2</sup>

1. UES, A BlueHalo Company / Air Force Research Laboratory, USA

2. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

As aerospace applications increasingly demand materials capable of withstanding extreme conditions, preceramic materials that generate ultra-high temperature ceramics (UHTCs) for fibers, coating, and ceramic matrix composites (CMCs) will be vital to future advancement. Processable PCP that generate UHTCs in even moderate yield are not available. Air Force Preceramics (AFPCs), are a new class of liquid PCPs that generate metal carbides in high yield upon pyrolysis. Here we utilize this emerging class of materials for the preparation of polymer derived ultra-high temperature ceramics matrix composites (UHTCMCs) and subsequently study their durability when subjected to extreme environments. In addition to composites using Zr- and Hf-based AFPCs, we have prepared composites using state-of-the-art commercial Si-based PCPs to allow for direct comparison. Microscopy was utilized to visualize how different infilled and pyrolyzed PCP materials interact with and fill carbon fiber tows. Post oxyacetylene torch testing analysis of the composite panels allows for an in-depth analysis of the macro and microstructure while diffraction and spectroscopy methods are used to understand the final ceramic composition. Ultimately, we report liquid UHTC forming PCPs with infill yields comparable to commercial SiC formers and demonstrate their use for high temperature protection.

#### 2:50 PM

#### (ICACC-S18-036-2025) Internal stress and hydrogen permeability in carbon-doped TiZrN coatings fabricated by laser carburization

S. Kim\*1; E. Hong2; S. Lee1; J. So1; H. Lee3

- 1. Korea Institute of Materials Science, Republic of Korea
- 2. Korea Testing Laboratory, Republic of Korea
- 3. Pusan National University, Republic of Korea

Internal stress plays a crucial factor in determining the lifetime of hydrogen permeation barrier coatings, as it influences the hydrogen isotopes diffusion and crack propagation. Here, we fabricated carbon-doped TiZrN coatings under different laser outputs, and investigated the changes in hydrogen permeability due to carbon compound formation and internal stress induced by laser shock peening. XPS and Raman analyses showed that the doped carbon substituted nitrogen sites in TiZrN to form carbides (TiC, ZrC) or existed interstitial site. By confirming the sp2/sp3 ratio, ID/IG ratio, and TEM-SAED patterns, it was observed that an amorphous carbon-embedded (Ti, Zr)(C, N) structure formed at laser outputs above 40%. The internal stress in coatings increased from 4.323 GPa before carburization to a maximum of 5.620 GPa. The increase in residual stress led to a reduction in hydrogen permeability by up to 69%, 57%, and 24% at 573 K, 673 K, and 773 K, respectively. This study advances the understanding of carbon compound formation and internal stress in TiZrN coatings under different laser output. It demonstrates that the formation of residual compressive stress due to laser shock peening significantly influences the hydrogen permeability by inhibiting hydrogen isotope diffusion and crack propagation in coatings

#### 3:30 PM

### (ICACC-S18-037-2025) UHTC Research Activities in South Korea (Invited)

S. Lee\*<sup>1</sup>; J. So<sup>1</sup>

1. Korea Institute of Materials Science, Republic of Korea

In Korea, various research efforts are underway for the development of ultra high-temperature ceramics (UHTC). The Korea Institute of Materials Science (KIMS) is optimizing unit processes related to UHTC, including the powder synthesis, dispersion, shaping, densification, and manufacturing of Ceramic Matrix Composites (CMC), as well as performance evaluation in extreme environments. The Korea Institute of Ceramic Engineering & Technology (KICET) is conducting research related to large-scale CMC manufacturing and performance evaluation in extreme environments, operating two UHTC-related centers: a fiber commercialization center and a composite materials manufacturing center. The Korea Atomic Energy Research Institute (KAERI) is engaged in the manufacturing of UHTC coatings using Chemical Vapor Deposition (CVD) and Chemical Vapor Infiltration (CVI) processes. The Korea Institute of Energy Research (KIER) has the capability related to the manufacturing of UHTC and SiC CMCs using the melt infiltration (MI) process. Jeonbuk National University have arc jet plasma wind tunnels with capacities of 0.4MW and 2.4MW and vacuum plasma spray machine (VPS) for UHTC coating, using these facilities to study UHTC coating and ablation properties under various conditions. Soongsil University is carrying out research on the optimal composition calculation of multiphase UHTC.

#### 4:00 PM

### (ICACC-S18-038-2025) Influence of $\rm Al_2O_3$ coatings on the oxidation behavior of $\rm ZrB_2$

J. E. Förster\*1; W. Fahrenholtz2; G. Hilmas2; P. Mechnich1; R. Naraparaju1

- 1. DLR German Aerospace Center, Institute of Materials Research, Germany
- 2. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA

Properties such as a high melting point >3000°C and a low density of 6.09 g/cm<sup>3</sup> project ZrB<sub>2</sub> as a suitable candidate for sharp leading edges or the thermal protective system (TPS) of hypersonic missiles and re-entry vehicles. The formation of a porous ZrO<sub>2</sub> scale and volatile B<sub>2</sub>O<sub>3</sub> glass at temperatures above 1500°C offers no longterm protection against oxidation. Protective overlay coatings such as Nb and HfO<sub>2</sub> have shown an improvement in oxidation resistance of ZrB<sub>2</sub>. In this study, Al<sub>2</sub>O<sub>3</sub> coatings have been investigated as a new potential candidate for protective overlay coatings on ZrB<sub>2</sub>. The coatings were applied by means of slurry deposition (Reactive Bonded Aluminum Oxide (RBAO)). Subsequently, the coated specimens were oxidized at 1500°C, 1600°C, and 1700°C for up to 60 min in a tube furnace under controlled atmosphere. On one hand, the Al<sub>2</sub>O<sub>3</sub> scale reacted with the liquid B<sub>2</sub>O<sub>3</sub> and formed a solid solution  $Al_{18}B_4O_{33}$  at the surface. The stabilized glass prevented the  $B_2O_3$ evaporation and reduced the oxygen diffusion to the oxidation front of ZrB<sub>2</sub> as long as it remained at the surface. On the other hand, the precipitation of secondary ZrO<sub>2</sub> induced the formation of a dense ZrO<sub>2</sub> oxide scale at the surface. The dense oxide scale provided protection against oxygen diffusion to the oxidation front of ZrB<sub>2</sub> even though the protective Al<sub>18</sub>B<sub>4</sub>O<sub>33</sub> and B<sub>2</sub>O<sub>3</sub> left the surface. The results will be presented and discussed in detail.

#### 4:20 PM

#### (ICACC-S18-039-2025) Oxidation of Hafnium Diboride - Silicon Carbide at 1500°C in Air; Effect of Compressive Stress

A. DeGregoria<sup>1</sup>; M. Ruggles-Wrenn\*<sup>1</sup>; G. Pry<sup>1</sup>

1. Air Force Institute of Technology, Aeronautics & Astronautics, USA

The long-term oxidation behavior of HfB<sub>2</sub> and of HfB<sub>2</sub>-20 vol% SiC was studied. Test samples were oxidized at 1500°C in air. Exposure times were 0, 0.5, 1, 2, 3, 6, 9, 12, 15, 30, 45, and 90 h. Crystal structure and composition of the surface scales were analyzed using x-ray diffraction and SEM with EDS. For HfB<sub>2</sub> the oxide scale consists predominantly of porous HfO2. For HfB2-20 vol% SiC the oxide scale is composed of a borosilicate glass outer layer and a porous HfO<sub>2</sub> layer. Weight gain and growth of oxide scale with exposure time were measured. Oxidation kinetics were determined using the weight gain as well as the scale thickness measurements. Parabolic rate constants were calculated for both materials. Addition of SiC dramatically inhibited the oxidation of HfB<sub>2</sub>. The effects of compressive stress on oxidation of HfB2-20 vol% SiC were also examined. Samples were oxidized while under compressive stress of 50-150 MPa for up to 30 h at 1500°C in air. Compressive stress had little effect on the growth of oxide scale. The oxidation data were analyzed in terms of mechanistic models for the oxidation of monolithic and SiC-containing refractory diborides. For HfB<sub>2</sub>-20 vol% SiC, the model predictions agreed well with experimental data. For HfB<sub>2</sub>, the model underpredicted the scale thickness, but accounted for weight gain reasonably well except for the longest exposure time of 90 h.

#### Poster Session B

Room: Ocean Center

#### 5:00 PM

#### (ICACC-PB001-2025) Carbon Reinforced Boron sub-Oxide Nanocomposite- Abridged visual poster summary

#### J. Kenny\*1

1. AWE plc, Non Nuclear Components, United Kingdom

It was possible to make a nanocomposite of Boron Suboxide  $(B_6O)$ and Boron Carbide (B<sub>4</sub>C) formed via the reaction of the B<sub>6</sub>O with carbon (C) deriving from reduced Graphene Oxide (rGO). This material could see uses in neutron moderation and absorption, as well as armour applications. This nanocomposite was formed by blending the B<sub>6</sub>O with rGO in aqueous suspension before filtering and consolidating it via Spark Plasma Sintering (SPS). It was shown that the pure  $B_6O$  sintered at 1850 °C, densified to ~95% of the samples theoretical density (TD), exhibited a comparable hardness to near-fully dense B<sub>4</sub>C made through similar methods (~35 GPa at ~95% of TD for  $B_6O$ , compared to ~32.5 GPa at >98.5% TD). In 1 wt.% GO additions, it was possible to detect  $B_6O$  and  $B_4C$  using X-Ray Diffraction when the composite was sintered at 1570 °C for 15 mins. After 30 mins of sintering, the sample almost completely transformed to B<sub>4</sub>C, thereby proving the hypothesis of the study. Furthermore, it was possible to prove that none of the significant indicators of shock induced amorphisation were present in any of the CaRBON samples. During neutron irradiation testing, the samples were exposed to a neutron fluence of  $39.6 \pm 3.41 \text{ n/cm}^2$  with energies of 13.7  $\pm$ ~1.5 MeV. By the end of the test, all samples had a radioactivity of 0.2 mSv. Post irradiation analysis revealed no signs of radiation-induced damage across the tested samples.

#### (ICACC-PB002-2025) Mechanisms of Oxide Film Formation for Enhanced Corrosion Resistance on FeCrAl Alloy Surfaces in Aggressive Environments

H. Kang\*1; K. Park2; D. Kim3; Y. Yoon1

- 1. Gachon University, Materials Science and Engineering, Republic of Korea
- 2. Kongju National University, Division of Advanced Materials Engineering, Republic of Korea
- 3. Auburn University, USA

The formation of oxide films on metal surfaces is of critical importance in enhancing corrosion resistance, particularly in harsh environments that are characterized by high temperatures, humidity, and acidity. This study examines the mechanisms by which protective oxide films are formed on FeCrAl alloy surfaces and their role in corrosion resistance. A selective etching process involving HCl and HNO<sub>3</sub>was employed to preferentially dissolve Fe ions, thereby enriching the surface with chromium. This process facilitated the formation of a dense Cr<sub>2</sub>O<sub>3</sub> oxide film, which effectively inhibited electron transfer and prevented the dissolution of metal ions in corrosive environments. The resulting oxide layer demonstrated notable stability and retained its protective characteristics in acidic environments. Furthermore, the etching process increased surface roughness, which enhanced hydrophobicity and minimized water contact, as predicted by the Cassie-Baxter model. This study demonstrates that the Cr-rich oxide film formed through selective etching significantly improves the corrosion resistance of FeCrAl alloy surfaces. The findings offer valuable insights into the design of high-performance corrosion-resistant metal surfaces for applications in fuel cells, chemical processing equipment, and marine structures.

## (ICACC-PB003-2025) Effect of cellulose nanofiber addition on powder injection molding process

S. Kobayashi\*1; T. Osada<sup>2</sup>

- 1. Tokyo Metropolitan University, Mechanical Systems Engineering, Japan
- 2. Tokyo Metropolitan University, Japan

Powder Injection Molding (PIM) process is suitable for fabricating small and complex shaped ceramics or metal parts with high production volume. In this study, in order to improve the PIM process, cellulose nanofibers(CNF) were focused. There are problems such as deformation during debinding and sintering due to the addition of a large amount of binder. On the other hand, the strength of the green compact decreased with decreasing binder contents. In this study, cellulose nanofibers were added with a binder during mixing in order to improve the handling of green compacts, and decrease the deformation during debinding and sintering. Effects of CNF contents on the mechanical properties were investigated.

#### (ICACC-PB004-2025) A machine learning-driven approach to predict mechanical degradation in fiber-reinforced composite laminates associated with matrix cracks

M. Fikry²; F. Mirza4; J. Mack4; N. Martono<sup>1</sup>; K. TAN4; V. Vinogradov3; S. Ogihara\*<sup>1</sup>

- 1. Tokyo University of Science, Japan
- 2. Tokyo University of Science, Mechanical Engineering, Japan
- 3. Newcastle University, United Kingdom
- 4. University of Akron, USA

Matrix cracks in fiber-reinforced composite laminates reduce stiffness and induce residual strains, compromising structural integrity. Existing analytical approaches, though effective, often struggle with the computational demands and complexities of large datasets. This study leverages machine learning models, including linear regression, polynomial regression, and random forest, to efficiently predict mechanical degradation associated with matrix cracks. The objective is to capture the relationships between crack density, stiffness reduction, and residual strains in fiber-reinforced composites, specifically focusing on two different materials: carbon fiber reinforced polymer and glass fiber reinforced polymer in cross-ply and angle-ply laminates. The models prioritize experimental data while integrating analytical data from the recently extended and refined variational stress analysis to enhance prediction accuracy. Results show that the random forest model provides reliable predictions, effectively capturing non-linear interactions and offering deeper insights into stiffness reduction and residual strain. Future work will apply this approach to more complex composite structures and other damage modes, including delamination.

#### (ICACC-PB005-2025) Phthalonitrile Functionalized Resoles: High Char Yield Resins for Carbon/Carbon Composites

- N. Chaussoy<sup>1</sup>; D. Brandt\*<sup>1</sup>; J. Gerard<sup>2</sup>
- 1. CEA, DAM, Le Ripault, F-37260, France
- 2. IMP, INSA Lyon, France

Recently, phthalonitriles have gained interest due to their very good thermostability and high char yield making them interesting candidates for carbon/carbon (C/C) composites fabrication via precursor infiltration and pyrolysis (PIP) method. However, phthalonitrile resins are generally solid at room temperature and often have a narrow processing window. In this work, synthesis methods allowing access to phthalonitrile resins were developed from 2,3-dicyanohydroquinone. These methods propose to consider together phenolic chemistry (phenolic reactive positions and aldehyde) and self-crosslinkable phthalonitrile chemistry (hydroxyl-mediated from phenolic and nitriles). It was thus possible to synthesize liquid resins at room temperature, leading to polymeric networks with a good thermostability and very high char yield ( $\geq$  70 %).

# (ICACC-PB006-2025) Experimental and numerical investigation of damage process in adhesively bonded composite scarf joints

#### S. Oshima\*1; S. Kobayashi2

- 1. Tokyo Metropolitan University, Department of Aeronautics and Astronautics, Japan
- 2. Tokyo Metropolitan University, Mechanical Engineering, Japan

The damage process in adhesively bonded composite scarf joints was investigated from the initial stage of loading to the final failure. The damage accumulation in scarf joints with different scarf angles and stacking sequences made of carbon fiber reinforced plastics was characterized by several in situ techniques, such as optical microscopy, high-speed photography, and acoustic emission testing. In addition, progressive damage analysis was carried out to analyze stress distributions depending on the damage state using the finite element method with stress triaxiality-dependent yield and damage constitutive models. Transverse cracks appeared in composite adherends in the initial stage of loading because of local stress concentration near the end of the 0° layers. The final failure was triggered by the interfacial crack growth between the 0° and 90° layers initiated from the transverse cracks. Numerical simulation results showed that the presence of transverse cracks largely affects the stress distribution in the adhesive layer.

#### (ICACC-PB007-2025) Application of AE Measurement to Crack Tip Location and Damage Mode Evaluation on Mode-I and Mode-II Tests for CFRP

T. Sakai\*1; K. Miura1

1. Saitama University, Japan

For the Double Cantilever Beam (DCB) and End Notched Flexure (ENF) test, it is necessary to measure the crack length to calculate fracture toughness in Mode-I and Mode-II, respectively. In this research, we measured the crack length in the DCB and ENF tests by using the acoustic emission (AE) method. The crack tip positions were identified by the AE arrival time difference with removing noises and using the precise analyze method as the Akaike Information Criterion. As a result, the position of the crack tip obtained by the arrival time difference of the AE during the DCB test showed equal or more precise value than the position obtained by microscope observation, therefore, the AE method can be used for measurement of the crack tip position. In the ENF test, AE could observe the internal cracking behavior before the fracture, however, microscope observation could not catch that cracking behavior. Furthermore, the damage mode could be specified from the frequency analysis of the AE waveform measured during the DCB and ENF test.

#### (ICACC-PB008-2025) Improvement of Deep Drawability of Carbon Fiber Reinforced Thermoplastics in Dome Shape

#### S. Kobayashi\*1

1. Tokyo Metropolitan University, Mechanical Engineering, Japan

The processing conditions for dome-shaped deep drawing of carbon fiber reinforced thermoplastic (CFRTP) were investigated to improve the drawability. Blank holder pressure was investigated using springs. The results showed that wrinkles were reduced and drawability was best when 1/2 Spring was used. The thickness and laminate configuration of the laminates were examined. The results showed that the plate thickness in this test was 2.0 mm, and that the smaller the fiber orientation angle of the adjacent layers, the better the drawability. Compression test results showed that fabric laminates exhibited sharp load drops due to damage extension in the in-layer and thickness directions.

#### (ICACC-PB009-2025) Quantitative evaluation of fiber straighten effect on axial compressive strength of unidirectional carbon fiber reinforced plastic

M. Ueda\*1; R. Nishi1; N. Ichihara1

1. Nihon University, Japan

The axial compressive strength of a high-strength unidirectional carbon fiber reinforced plastic is about half of the compressive strength. The reason for the low compressive strength is the matrix since the matrix properties determine the axial compressive strength. The fiber waviness is inherent in the carbon fiber reinforced plastic because of the small diameter of the carbon fibers. Axial compressive loading to the unidirectional carbon fiber reinforced plastic causes the matrix shear deformation due to the fiber waviness. The matrix loses its fiber-supporting capability with increases in the axial compressive load, resulting in compressive failure. The fiber waviness, as well as matrix property, plays an essential role in determining the axial compressive strength. The smaller fiber waviness is required to increase axial compressive strength. In this study, the axial compressive strength of a unidirectional carbon fiber reinforced plastic is evaluated, considering the actual fiber waviness. The improvement of the axial compressive strength of unidirectional carbon fiber reinforced plastics was quantitatively evaluated depending on the extent of fiber waviness.

#### (ICACC-PB010-2025) Characterization of mode I fracture behavior in aging-treated A7075/CFRP adhesive-bonded joints using acoustic emission method

Y. Zusho\*1; S. Kobayashi2

- 1. Tokyo Daigaku, Department of Aeronautics and Astronautics, Japan
- 2. Tokyo Metropolitan University, Mechanical Engineering, Japan

When carbon fiber reinforced plastics (CFRP) are used as structural materials for aircraft, they are generally joined by mechanical fastening using bolts and nuts or rivets. However, mechanical fastening is considered to have problems with stress concentration in the perforated area, which can be the starting point of the fracture. Therefore, adhesive bonding, which does not require drilling, is desirable. Adhesive bonding can reduce the weight because rivets are not required, and it is also expected to improve aerodynamic smoothness, fatigue resistance, and damage resistance. Considering adhesive joints between CFRP and metals, galvanic corrosion, a phenomenon in which metals corrode rapidly due to a large potential difference between the materials, is an important issue. In this study, adhesive-bonded joints of A7075 aluminum alloy and CFRP were examined to investigate the effect of galvanic corrosion on mode I fracture toughness. Homogeneously and heterogeneously bonded joints were fabricated and subjected to accelerated corrosion aging by salt spraying. Double cantilever beam (DCB) tests combined with the acoustic emission (AE) method were conducted to characterize the change in the mode I fracture behavior of adhesive-bonded joints over time due to corrosion.

### (ICACC-PB011-2025) Development of a densification process for metal BJT compacts with fine grains

K. Kariya\*1; T. Osada1; S. Kobayashi1

1. Tokyo Metropolitan University, Mechanical Engineering, Japan

Binder jetting (BJT) metal additive manufacturing uses the binder to selectively bind metal powders and build metal parts in three dimensions. Since BJT has low equipment costs and is highly scalable, BJT has attracted attention as a new fabrication technique in the metal additive manufacturing process. However, parts printed by the BJT process are difficult to be high density. Conventional densification methods involve high temperatures and long sintering. However, this method results in larger grains and lower strength. Therefore, densification with fine grains is necessary. This study suggests densification process for metal BJT composites with fine grains. However, a sintered compact at low temperatures has an interconnected pore. Interconnected pore in a low-temperature sintered compact must be eliminated because HIP can't ensure density if there are interconnected pores. Therefore, we attempted to eliminate the interconnected pore by coating the pre-sintered compact with a slurry of fine powder. The fine powder on the surface becomes high-density even at low sintering temperatures. And it will eliminate interconnected pore. As a result, pre-sintered temperature at low temperatures will be high density by HIP. It will be fine-grained specimen was obtained.

#### (ICACC-PB012-2025) Effect of Surface Textures on Mechanical and Osteogenic Properties of Alumina Toughened Zirconia Composites

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Biomaterials such as artificial tooth roots and implants are used in high load-bearing areas, and therefore, materials with excellent loadbearing capacity and biocompatibility are required. In recent years, zirconia has attracted attention as a biomaterial because of its superior esthetic and mechanical properties compared to titanium. This study used Alumina Toughened Zirconia (ATZ) with approximately 20 mass% alumina. ATZ is a bioinert material that does not bond with bone after implantation in vivo, resulting in a higher initial failure rate and longer time to fixation than conventional titanium implants. In this study, we attempted to improve the bioactivity of ATZ by controlling the surface properties. We also expect creating a one-piece zirconia implant that utilizes the surface properties. In this study, the effects of surface morphology changes on cell adhesion, proliferation, and differentiation were also investigated, as well as the evaluation of mechanical properties of surface modification.

#### (ICACC-PB013-2025) Development and Evaluation of Low Environment Impact Fabrication Methods for Zirconia CIM Parts

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Zirconia (ZrO<sub>2</sub>) has excellent mechanical properties, but its brittleness and high hardness make it difficult to manufacture complex shapes. This study focuses on Ceramics Injection Molding (CIM), a very effective technology to mass produce complex shaped parts with high dimensional accuracy at a competitive cost. Organic compounds are used as binder components. During the debinding process, greenhouse gases may be generated, which may lead to an environmental burden. Considering this problem, the objective of this study is to develop an environmentally friendly CIM system for achieving the SDGs. In this study, we focus on polylactic acid (PLA), a biomass-derived biodegradable polymer that is one of the most important renewable resource-based biodegradable polymers because of its thermoplasticity, hydrolyzability, and superior mechanical properties. On the other hand, due to its poor flowability, biodegradable carnauba wax (CW) and stearic acid (SA) were used as lubricants. These waxes have relatively low melting points and dissolve easily during mixing to improve flowability. Thermogravimetric analysis (TGA) was conducted to investigate the thermal decomposition behavior of the binders during debinding. This suggests that the process of SA pore formation is important in debinding. The relative density of the sintered compact was more than 99% and a dense component was obtained.

## (ICACC-PB014-2025) Ceramic coating of fibre reinforced polymers using separate powder injected laser application

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In the aerospace industry, lightweight construction with highperformance materials has been historically one of the most important requirements. In airplanes it enables payload capacity or operating range to be increased. The focus on lightweight design will be intensified by climate targets as well as by a transition away from fossil fuels towards renewable energies such as the use of hydrogen. In particular in the field of distribution and storage of hydrogen (e.g. pipelines, storage tanks), a lightweight design is of crucial importance. Fibrereinforced plastics (FRP) are already widely used for such lightweight applications due to their mechanical properties: They are characterized by high strength and stiffness. However, synthetic resins are also characterized by their low melting and decomposition temperature compared to metals. A combination of a FRP core and a metal sleeve is conceivable, but this combination is challenging to be manufactured. A promising approach to achieve such combination is the direct coating of FRP using Separate Powder Injected Laser Application (SPILA). SPILA can be used to coat FRP directly with metallic alloys and afterwards with ceramic materials. In this context, the feasibility of coating by means of SPILA for different FRP is investigated using aluminum as a coating material on the inner layer and Al203 on the outer layer.

### (ICACC-PB015-2025) Fabrication and Characterization of Lightweight Composite Conductors

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The increasing complexity of wiring components in modern electrified aircraft presents significant challenges in reducing overall weight while maintaining energy efficiency. Consequently, there is a growing interest in designing high-conductivity, lightweight conductors. This study investigates copper-coated carbon nanotube (Cu/CNT) yarn composites, fabricated through electroplating, as a potential solution. Our previous results indicate that Cu/CNT composites offer improved performance, potentially surpassing traditional copper in electrical and mechanical properties. The chemical and structural properties of the copper layer on the unprocessed CNT yarns were evaluated after five hours of electroplating by scanning electron microscopy (SEM) and X-ray diffraction (XRD). Four-probe electrical resistance monitoring was used to measure the electrical conductivity of the composite wires. These analyses suggest the formation of copper species such as Cu<sub>2</sub>O, CuCO<sub>3</sub>, and Cu<sub>x</sub>C, consistent with previous theories. Cold-drawn and annealed Cu/CNT yarns achieved an electrical conductivity of 61.6 MS/m, exceeding the International Annealed Copper Standard (IACS) by 6.21%. A custom 3D-printed mounting rig was developed to improve sample throughput and ensure a uniform copper coating on CNT yarns. After four hours of electroplating, a 26.7-foot-long Cu/CNT yarn was produced, with an average copper layer thickness of 0.5 mm.

# (ICACC-PB016-2025) Design and characterization of promising SOC electrolytes with mixed $H^+/O^{-2}$ conductivity for co-electrolysis

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SOCs are promising technologies to obtain clean energies from renewable sources and vice versa. Moreover, SOCs are also being applied for  $CO_2/H_2O$  co-electrolysis to obtain synthetic fuel and reduce  $CO_2$  emissions. However, the extreme operating conditions, i.e., high temperatures and reducing atmospheres, contribute to the degradation of the cell components. Therefore, the development of new materials is required to achieve a good electrochemical performance and long-term stability. (Zr,Ce,Y)O<sub>2</sub> fluorites are wellknown commercial electrolytes due its O<sup>-2</sup> diffusion. Otherwise, (Sr,Ba)(Zr,Ce)O<sub>3</sub> perovskites have been gaining attention due their H<sup>+</sup> conductivity and CO<sub>2</sub> tolerance. The combination of both oxides is expected to improve the coelectrolysis performance. This work presents SOC electrolytes based on (Ca,Sr,Ba)(Zr,Ce,Y)  $O_3$  perovskites for H<sup>+</sup>/O<sup>-2</sup> conductivity. They were obtained by SSR. The crystallographic properties of powders were studied by XRD, while the microstructure of pellets was observed by SEM. Electrolyte conductivity was studied by TPM, between 200 and 800 °C under wet (2 % of water vapor) and dry synthetic air by slow heating/cooling rates (i.e., quasi equilibrium conditions). Sr(Ce,Y)  $O_3$  evidenced a mixed H<sup>+</sup>/O<sup>-2</sup> conductivity conductivity between 400 and 600 °C, however, density and conductivity values are low compared to state-of-the-art materials.

### (ICACC-PB017-2025) Characterization of Sm(Ba,Ca)Co $_2O_5$ as possible air and fuel electrodes for IT-SOCs

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Intermediate Temperature Solid Oxide Cells (IT-SOCs) are promising electrochemical devices capable to obtain clean energies from renewable sources, and vice versa, between 600 and 800 °C. Fuel flexibility, long-term stability, electrochemical behavior, etc., are critical parameters during materials selection and microstructural desing for IT-SOC components. Currently, material science and engineering are focused to improve the electrochemical perfomance of the air electrode. Sm(Ba,Ca)Co<sub>2</sub>O<sub>5</sub> have been proposed as air electrodes for IT-SOCs due their remarkable oxygen electrode activity. These double perovskites present a layered structure with fast oxygen diffusion and high conductivity. However, these have not been studied as fuel electrodes for symmetric and/or reversible IT-SOCs. This work presents the characterization of the crystallographic, thermodynamic and electrochemical properties of Sm(Ba,Ca)Co<sub>2</sub>O<sub>5</sub> under diluted oxidizing/reducing/oxidizing atmospheres. During reducing cycle, the double perovskites were decomposed and segregated in other compounds, and the polarization resistances were higher than pristine sample. After reoxidation process, polarization resistance values were higher than pristine sample, due some oxides in the grain boundary and/or particle surface. More experiments are required to establish if Sm(Ba,Ca)Co<sub>2</sub>O<sub>5</sub> air electrode could be applied in symmetric IT-SOCs.

### (ICACC-PB018-2025) Impact of Accelerated Degradation on CO2 Separation Performance of Zeolite Adsorbents

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To achieve the 1.5°C target of the Paris Agreement, reaching carbon neutrality by 2050 and implementing negative emissions thereafter are essential. Alongside decarbonizing electricity, conserving energy, and fuel switching, carbon capture, utilization, and storage (CCUS) from point sources is crucial. The CO2 capture market is projected to grow significantly, becoming about 20 times larger by 2050 than in 2020. For the full-scale implementation of CO2 capture technologies, more cost-effective and energy-efficient CO2 separation materials are needed. However, there is no standardized evaluation method for these materials, making performance comparisons difficult. Additionally, most tests are short-term and conducted under ideal conditions, lacking data on long-term durability. Supported by NEDO, our research institute aims to establish a standardized evaluation method for the CO2 separation performance of adsorbents and develop an accelerated degradation test for durability assessment. In this presentation, we describe an accelerated degradation test for physical adsorbents. We prepared degraded zeolite 13X by cycling adsorption with a CO2/H2O/N2 gas mixture and desorption via heating at a rate of over 100 times per day using a specialized test apparatus. The specific surface area, adsorption isotherm, and breakthrough curve of this degraded adsorbent were evaluated and will be discussed.

#### (ICACC-PB019-2025) Advancing Standards-Transforming Markets: ASTM International Standards for Properties & Performance of Advanced Ceramics

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Advanced ceramics figure prominently in global innovation trends. Properties and performance of brittle bodies such as advanced ceramics and glasses are challenging to measure accurately and precisely unless the proper techniques are used. Such techniques are embodied in the full-consensus standards (e.g., test methods, practices, guides, terminology) of ASTM Committee C28 on Advanced Ceramics which, since 1986, has developed nearly 50 standards to determine properties and performance of monolithic and composite ceramics as well as coatings and constituents that may apply to some glasses. These standards provide details for determining mechanical, physical, and thermal properties and performance, as well as characteristics for processing, thereby providing accurate, reliable, repeatable and complete data. Users, producers, researchers, designers, and academicians who are involved in ASTM Committee C28 write, update, and validate standards through round robin test programmes. This poster includes a pictogram of Committee C28 standards and how to obtain them as either individual or collection of standards. Also included is a listing of other related ASTM committees. Finally, some examples of the tangible benefits of standards for advanced ceramics demonstrate their practical application help illustrate that advancing standards can transform markets.

# (ICACC-PB020-2025) Phenolic- and PEEK-derived C/C-SiC – Tensile and flexural strength after low-cycle fatigue at temperature up to 350 $^\circ C$

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C/C-SiC combine beneficial properties, like a low density (~ 2 g/cm<sup>3</sup>), high hardness, thermal shock, wear resistance and damage tolerance. It can be found in several applications, e.g. in the automotive sector as ceramic brakes or in aerospace as nozzle material. Besides of C-fibers, C/C-SiC consist of a C, SiC and Si matrix. Due to CTE mismatches, during cooling from the fabrication temperature (> 1420 °C), residual stresses remained. Relieving these stresses can increase the strength of C/C-SiC. In this study we focused on low cycle fatigue (LCF). All C/C-SiC samples were fabricated by the liquid silicon infiltration process (3k-HT-fibers, plain weave, 55 vol-% fibers) with powdered resins (Novolak and PEEK). Initial flexural strengths of 234 MPa (PEEK-based) and 173 MPa (Novolak-based) and tensile strengths of 144 MPa (PEEK-based) and 74 MPa (Novolak-based) were measured. For both materials the strengths remaining constant after cyclic loading at 350 °C (50 % of UTS), but the stiffness decreases. Increasing the preload to 90 % (one cycle) show also no effect on the tensile strength of the PEEK-based C/C-SiC. However, the flexural strength increases of about 24 % from RT to 350 °C. Residuals stresses were calculated, microstructures studied and fractured surfaces analyzed in order to find reasons for somehow surprising behavior of the C/C-SiC after LCF.

## (ICACC-PB021-2025) Graphene effect on the mechanical properties of the ceramic matrix composites

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Ceramic composites reinforced with carbon allotropes such as graphene, carbon nanotubes, and fullerenes have demonstrated improvements in mechanical properties as fracture toughness, and rupture strength in various studies. However, these gains are not uniform across all properties and can vary multifactorially, influenced by factors such as grain size and matrix composition. The reinforcement materials can contribute positively due to their excellent mechanical properties, but also negatively due to agglomeration, geometry, and positioning. Additionally, the density, porosity, phase transition, and sintering temperature of the composites are important parameters that must be controlled. Thus, a series of alumina + zirconia samples reinforced with graphene was produced to investigate the influence of these parameters on the mechanical, microstructural, and structural properties of the composite. The analysis of the results indicated that using concentrations of up to 1.60% by weight of graphene provided an increase in fracture toughness and rupture strength. In contrast, microhardness values increased for concentrations of up to 0.80% by weight. The diffusion of carbon into the matrix, crack deflection effects, densification, and the agglomeration of the reinforcement material were observed to understand the improvements in the properties of the produced composite.

#### (ICACC-PB022-2025) Composites Materials Handbook 17

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The intent of the Composite Materials Handbook 17 (CMH17) Vol 5A—Ceramic Matrix Composites is to provide the information and guidance necessary to characterize, design, fabricate, and implement ceramic matrix composite components for commercial aircraft applications. Where available proven industry best practices and lessons learned are also included. The CMH17 sponsor is the FAA (Federal Aviation Administration). The presentation/ poster describes the CMH-17 organization, the objectives and activities of the Working Groups that create and maintain the handbook content and provide an overview of the newer revision to come. The 5 Working Groups are: 1) Data Review, 2) Testing, 3) Materials & Processes, 4) Design and Analysis, and 5) Engine Applications. A new revision is being drafted, with the goal to release Vol 5B in 2025. A draft table of contents will be available.

#### (ICACC-PB023-2025) Silicon Nitride-Invar Joining

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Silicon nitride is widely used across various industries, including aerospace, engine components, cutting tools, vacuum furnaces, and bearings, due to its excellent wear resistance, high toughness, and thermal shock resistance. However, its challenging machinability limits broader applications. To address this, developing a low-residual stress joining method that mitigates the significant thermal mismatch between silicon nitride and metals is crucial. This study aims to investigate a cost-effective, scalable, and relatively simple method for joining silicon nitride to Invar42. A surface pretreatment based on aluminium was applied to the silicon nitride to improve wettability, followed by joining to Invar42 using S-bond\* 400 alloy under different temperatures and heating conditions. This work evaluates the mechanical properties of the joints at both room and 300 °C, examining the influence of the surface pretreatment procedure and the resulting joints' microstructure.

### (ICACC-PB024-2025) Advanced Joining Technologies at J-Tech@ PoliTO

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This work provides an overview of advanced joining technologies carried out at J-Tech@PoliTO, an interdisciplinary research center at Politecnico di Torino, Italy. The center's activities include custom joint development for composites, polymers, metals, ceramics, and glasses using techniques such as brazing, adhesive joining, and soldering. Additionally, this work summarizes advanced welding methods, such as laser welding and friction stir welding (FSW), along with high-temperature mechanical testing. Non-destructive evaluation techniques, including CT-scan and Impulse Excitation Technique (IET), are also discussed in relation to the joining processes.

# (ICACC-PB025-2025) Machinable SiC composites for elevated temperature tribological applications: A promising alternative to traditional SiC ceramics

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SiC-based ceramics are preferred for wear components in harsh environments. However, difficulty in shaping and sintering limits its usage. Persistent research is required to develop quick and cost-effective machinable SiC composites with superior wear resistance. In this regard, SiC composites with (up to 30vol%) TiB<sub>2</sub> and/ or ZrN reinforcement are sintered at considerably lower sintering temperature of 1800 °C using ten vol% Y2O3-AlN additives by spark plasma sintering. In sintered composites,  $\beta \rightarrow \alpha$  SiC phase transition is restricted. Fracture toughness increased with increase in reinforcement content. Electrical conductivity of SiC composites increased with increase in conductive boride/nitride content. All investigated SiC composites are successfully machined by wire-EDM and material removal rate increased with reinforcement content. Furthermore, the reciprocating sliding wear behaviour of sintered SiC-ZrN and/or TiB<sub>2</sub> composites is assessed at room temperature and 600 °C. Results demonstrate atleast one order of lower wear at 600 °C compared to room temperature. Wear mechanisms changed from fracture-induced wear at room temperature to tribo-oxidation at 600 °C. In conclusion, effective machining and improved high temperature wear performance of investigated composites demonstrate their potential for expanding the application regime of SiC ceramics.

#### (ICACC-PB027-2025) Development of Aramid-Fabric Composite Hinges for Origami Structures

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Over the last decade, research has been conducted into origami as an engineering solution to facilitate large structures which must store in a small transit volume. Within this area, the development of loadbearing origami structures with hinges that allow for a full range of motion to accommodate for panel thickness while maintaining strength and minimizing deformation have proven to be difficult to manufacture, characterize, and simulate. This study develops new methods for creating an aramid and flexible region within a cured composite structure using high-strength fabrics and removable matrix materials to both transmit loads experienced throughout the structure and allow for a full 180° movement capability. The properties of the hinges made using this method are then tested and compared, showcasing both their strength and fatigue limits within expected loading scenarios. Finally, a simulation of an example load-bearing origami structure are compared to ensure proper characterization and performance for future applications. This research allows for the creation of new structures which not only compact into a significantly smaller area than in its deployed state but will also be able to resist high loads both in- and out-of-plane for the structure.

#### (ICACC-PB028-2025) Enhanced CMAS Resistance and Thermal Properties of Rare Earth-Doped Gadolinium Zirconate for Advanced Thermal Barrier Coatings

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Yttria-stabilized zirconia (YSZ) has been extensively utilized as a thermal barrier coating (TBC) for gas turbines; however, it exhibits significant limitations in phase stability, sintering behavior, and resistance to calcium-magnesium-alumino-silicate (CMAS) at temperatures exceeding 1200°C. To address these challenges, various materials have been developed, many are known to lack sufficient mechanical properties for commercial applications. In this study, several compositions of gadolinium zirconate (GZ) doped with rare earth elements were synthesized as candidate materials for TBC. We evaluated the thermal properties, including thermal conductivity, durability, and CMAS resistance, and found that GZ demonstrated similar mechanical properties alongside superior CMAS resistance compared to YSZ.

### (ICACC-PB029-2025) Joining and Coating of Oxide-CMC by Preceramic Polymers

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In many energy fields, oxide-CMC devices endure harsh conditions such as high temperatures and oxidation. This work aims to identify optimal coating and joining materials based on oxide preceramic precursors for oxide-CMC. Oxide preceramic polymers adhesion and cohesion on oxide-CMC have been improved by adding functionalized fillers like Al2O3 nanoparticles and fibers. The process involves curing at 180°C and pyrolysis at 1200°C in air. The morphology, microstructure, and mechanical properties of the joined oxide-CMC will be assessed.

#### (ICACC-PB030-2025) A Multi-Scale Hierarchical PHFGMC Framework for Predicting Mechanical Properties of C/C-SiC CMCs

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The mechanical performance of Carbon/Carbon-Silicon Carbide (C/C-SiC) ceramic matrix composites (CMCs) is critical for high-temperature structural applications. This study presents a multi-scale hierarchical framework utilizing the Parametric High-Fidelity Generalized Method of Cells (PHFGMC) to predict the mechanical properties of C/C-SiC CMCs. The framework leverages the PHFGMC, extended to concurrently operate at both micro and meso scales, making it a valuable tool for enhancing the CMC manufacturing process. The microstructural composition and spatial arrangement of the multi-phase C/C-SiC material significantly influence its mechanical response. The refined PHFGMC framework offers a balance between computational efficiency and detailed representation of the local microstructure, capturing

essential material characteristics without excessive computational demand. Scanning Electron Microscope (SEM) and Computed Tomography (CT) surveys are incorporated to generate multi-scale nested PHFGMC micromechanical models for predicting effective orthotropic properties of a single layer. The proposed modeling approach can be adaptable to the design of a wide variety of CMCs with diverse weaving architectures. It can be further developed to incorporate nonlinear behaviors and damage modeling, potentially broadening its application scope in CMC design and optimization.

### (ICACC-PB031-2025) Borate bioactive glasses modified by Co ions

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Borate bioactive glasses (BBGs) are novel and interesting ceramic materials. BBGs are produced by substituting silica ions with boron ions in the glass network. Boron is a vital trace element that plays significant roles in the human body. In this study borate bioactive glasses were synthesized and characterized. The primary objective was to asses the influence of the synthesis method on the bioactivity and structural properties. The glasses were made in binary oxide system doped with cobalt ions using both traditional melting and the sol-gel method with four different organic boron precursors. The glass composition was 40B<sub>2</sub>O<sub>3</sub>-54CaO-5CoO mol%. Structural analysis (FTIR, XRD) was conducted to evaluate the character of the materials as well as phase composition. X-ray absorption spectroscopy (XAS) was employed to investigate the local structure of cobalt ions. An apatite-forming ability of the BBGs after immersion in simulated body fluid was examined using SEM/EDX, FTIR, ICP-OES methods. XRD analysis verified that all samples exhibited an amorphous structure. FTIR analysis showed borate units in materials. FTIR, SEM and ICP-OES confirmed the bioactivity of borate bioactive glasses after incubation in simulated body fluid. This work was supported by the "Excellence Initiative - Research University" program for AGH University.

### (ICACC-PB032-2025) Co-sputtered antibacterial and antiviral composite coatings with Ag nanoparticles for air filters

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The recent spread of the Coronavirus disease and the resulting global economic and health crisis have heightened the scientific community's focus on incorporating antimicrobial and antiviral materials into everyday life. In this context, the European NanoBloc project was initiated to provide reliable antimicrobial, antifungal, and antiviral coatings applicable to a wide range of textiles and surfaces for various end uses. Research at POLITO has focused on developing silicaand zirconia-based coatings using the eco-friendly co-sputtering technique for air filtration systems. Silver nanoparticles were incorporated to impart antibacterial and antiviral properties to the coatings, with a particular emphasis on their application in air filter systems. These coatings demonstrated a controlled and sustained release of silver ions, effectively inhibiting the growth of bacteria and fungi. Their high thermal stability made them ideal for thermal regeneration and sterilization processes, without compromising their antimicrobial and antiviral effectiveness. Additionally, antiviral tests on the composite coatings confirmed their strong efficacy against the Human Coronavirus. The coatings developed are wellsuited for industrial scaling. The initial results from this work have shown promising potential in advancing the development of functional materials for various applications.

# (ICACC-PB033-2025) Advanced freeze-dried chitosan hydrogel scaffolds enhanced with strontium-doped bioactive glass and resveratrol

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Chitosan-based hydrogels are highly attractive biomaterials due to their high water content, swelling, gradual degradation and biocompatibility, making them ideal for drug delivery systems. They can also be easily modified with biologically active substances. This research focuses on freeze-dried chitosan hydrogel scaffolds enriched with resveratrol at 2%, 5% and 10% concentrations and strontium-doped bioactive glass A2Sr5 (40 mol% SiO<sub>2</sub>, 49 mol% CaO, 6 mol%  $P_2O_5$ , and 5 mol% SrO<sub>2</sub>). This study assessed the impact of these bioactive substances on the scaffolds physicochemical, mechanical and biological properties. Materials were incubated in simulated body fluid to evaluate swelling and mineralization. Morphology and structure were analyzed using SEM microscopy and FTIR spectroscopy. Antioxidant properties were tested with ABTS radicals. Mechanical properties were measured using a tensile testing machine and the release profile of bioactive substances was analyzed. Biological studies were conducted on RAW 264.7 murine macrophage cells. Obtained results showed that resveratrol and strontium-doped bioactive glass significantly influenced the materials structure and properties. The hydrogel scaffolds demonstrate promising potential for tissue engineering applications. This work was supported by the National Science Centre, Poland (Grants no. 2023/49/N/ST11/02999).

# (ICACC-PB034-2025) Innovative injectable chitosan-based hydrogels enriched with strontium-doped bioactive glass and retinol

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Chitosan-based hydrogels, due to their unique properties, find wide applications in various scientific fields, particularly in the biomedical and pharmaceutical sectors. The objects of the present study are injectable chitosan-based hydrogels enriched with retinol at concentrations of 2%, 5%, and 10%, as well as high-calcium bioactive glass doped with strontium A2Sr5. The study was conducted to evaluate the effect of the active substance used on the physicochemical, mechanical, rheological and biological properties of the hydrogels. The materials were incubated in SBF solution to evaluate their mass loss. Rheological studies were performed in a function of time and frequency, and mechanical parameters were tested using a tensile testing machine. Self-healing of the materials was evaluated using optical microscopy while biological studies were performed on the RAW 264.7 murine macrophage cell line. The developed and obtained hydrogels have promising potential for use as innovative injectable materials for tissue engineering for bone and cartilage regeneration. This work was supported by the National Science Centre, Poland (Grants no. 2023/49/N/ST11/02999).

### (ICACC-PB035-2025) CuO as a modifier of bioactive borate glasses

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Bioactive borate glasses (BBGs) possess unique properties for tissue engineering. Due to their compositional flexibility, BBGs are suitable as inorganic carriers for therapeutic ions, such as copper, which promotes angiogenesis and has antimicrobial properties. The properties of these glasses are influenced by the coordination and oxidation states of the transition metal ions within the glass matrix. In this study BBGs were obtained by melting and the sol-gel method with various boron precursors. The glass composition was 80B2O3-(16-x)CaO-4P2O5-5CuO mol%. Phase composition and crystallization tendency were analyzed using XRD, while FTIR provided structural characteristics. The oxidation state and coordination of copper were investigated through UV-Vis spectroscopy and XAS. A simulated body fluid (SBF) assay was performed to determine the in vitro bioactivity. SEM-EDS was conducted to analyze the morphology and chemical composition of the samples, while ion release kinetics were investigated using ICP-OES. XRD analysis proved the amorphous nature of the materials with slight crystallization of boric acid. FTIR spectra show the presence of boron in both tetrahedral and trigonal coordination. Both FTIR and SEM-EDS showed the formation of an apatite layer after incubation in SBF. ICP-OES confirms the bioactivity of the glasses. This work was supported by the "Excellence Initiative - Research University" program for AGH University.

### (ICACC-PB036-2025) Bioactive polymer - ceramic composites for rapid osteoinduction of human adipose-derived stem cell

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Adipose-derived stem cells (ASCs) are a readily accessible source of multipotent cells, serving as an alternative to bone marrow-derived stromal cells (BMSCs) for osteoblast differentiation. Despite their potential, ASCs have a lower osteogenic capacity than BMSCs. We introduce innovative strategies for enhancing osteogenic differentiation of human ASCs by culturing them on bioactive growth surfaces, supplemented with specific additives in osteogenic medium, and applying fluid shear stress. Human ASCs were cultured on PLGAbased composites with 50 wt% sol-gel bioactive glasses (SBGs) from the SiO2-CaO±P2O5 system, either unmodified or modified with 5 wt% ZnO or SrO. The osteogenic medium contained recombinant human bone morphogenetic protein. Culturing ASCs on SBG-PLGA composites, along with medium supplements, increased the expression of early and late osteogenic markers. Modifications with SrO or ZnO further enhanced osteogenic gene expression compared to unmodified SBGs. Additionally, applying fluid shear stress amplified the osteogenic effects. Our proposed strategies for ASC differentiation hold promise for the delivery of osteoblastic cells or mineralized osteoblasts for cell-based bone regeneration therapies. This work was partially supported by NCN Poland Grant no. 2023/51/B/NZ5/01403 and the "Excellence Initiative - Research University" program for AGH University

### (ICACC-PB037-2025) Phosphate Functionalized Graphene Oxide for Bone Regenerative Engineering

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Graphene oxide (GO) is a highly oxidized form of graphene that contains various oxygen functional groups, consisting mostly of hydroxyl and epoxy groups. These oxygen-rich groups provide desirable biomedical characteristic such as an auto-degradation pathway in aqueous environment, protein adsorption, cell attachment and proliferation,  $Ca^{2+}$  ion adsorption, and greater interactions with matrices for more efficient load transfer. Calcium phosphate graphene (CaPG), a recent novel derivative of GO contains covalently tethered polyphosphates to its backbone and has been shown to release inducerons, including  $Ca^{2+}$  and  $PO_4^{3-}$ , as an alternative to growth factors for the induction of stem cell differentiation, in vivo. PLGA/CaPG microspheres were fabricated through an oil-inwater emulsion/solvent technique at 1 and 5 wt%. SEM confirmed a smooth surface of the microspheres, and the presence of CaPG within matrices was confirmed by TGA. A higher hydrophilicity was also observed via a contact-angle assays for the CaPG-containing matrices. Lastly, live/dead staining and MTS assays displayed the scaffolds' capability of supporting the viability and metabolic activity, respectively, of human bone marrow stem cells. The incorporation of CaPG has shown great promise in enhancing the properties of a bio-engineered matrix. However, further research is required to study CaPG's applications in clinical applications.

#### (ICACC-PB038-2025) Advanced performances of fibre optic sensors by combination of nanostructured metal oxides and polymeric electrospun nanofibers

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At present, early diagnosis and treatment of cancers through biomarker detection in body fluids represents one of the greatest challenges in biomedical research given the health, social and economic impact. The gold standard approaches rely on complicated, operator-dependent and time-consuming tests that require large volumes of samples and reagents. Therefore, there is an urgent need of a reliable, compact and operando monitoring platform with a low limit of detection (LOD) through a simple liquid biopsy. This contribution presents the research activities conducted in the frame of the FOCAL project, which aims at the design of a biophotonic platform based on optical fibre sensors combined with functional nanomaterials and microfluidics for non-invasive early diagnosis of cancer. Nanostructured substrates based on metal oxides are combined with electrospun polymeric fibres to enhance the sensitivity of optical fibres and provide an effective surface for cell adhesion, creating an in vitro model with an integrated sensing element. Metal oxide nanoparticles characterized by high refractive index (such as TiO<sub>2</sub>) will be dispersed into the polymeric nanostructured substrates to further improve the performance of the biosensor and reach a final LOD at the femto-molar level.

#### (ICACC-PB039-2025) Magnesium Phosphate Functionalized Graphene Oxide and PLGA Composite Matrices for Enhanced Bone Regenerative Engineering

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Bone defects affect millions of people annually, making bone tissue of particular interest for developing treatments. Current strategies are lacking in complete, successful solutions due to their drawbacks. The field of Regenerative Engineering has shown promise in healing complex tissues of the body, including critical-sized bone defects, which are difficult to heal despite surgical intervention. In this work, we fabricated composite microsphere-based matrices by incorporating a novel Magnesium Phosphate Graphene (MgPG) within PLGA (Poly(lactic-co-glycolic acid) and studied them for their morphological, chemical, and physical characteristics for bone regeneration in vitro. We evaluated the cytocompatibility and osteogenic potential of these composite matrices, which showed high cell viability and osteogenesis. Further, we evaluated markers of the canonical Wnt signaling pathway via RT-qPCR and demonstrated that potentially Wnt may contribute to the enhanced osteogenicity MgPG. Thus, these scaffolds demonstrated potential for osteogenesis and proliferation that are highly desired for regeneration of critical-sized defects. With further studies, these MgPG matrices may prove to be ideal, delivering bioactive molecules to the defect site to aid in bone regenerative engineering.

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#### (ICACC-PB040-2025) Classification and Interpretation of Intermediate Feature Representations of Silicon Nitride Microstructures using t-SNE

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The microstructure of silicon nitride  $(Si_3N_4)$  is complex, but it contains information related to mechanical properties such as bending strength and fracture toughness. Previously, we utilized deep learning to predict the mechanical properties from microstructure images of Si<sub>3</sub>N<sub>4</sub>, demonstrating precise prediction. However, the basis for the predictions from the obtained deep learning model was unclear, making it difficult to evaluate the validity of these predictions from a structural perspective. This study focused on the intermediate feature representations (IFRs)extracted from the deep learning network and aimed to evaluate the effectiveness of the model by correlating these with structural factors. Since IFRs can only be expressed in a high-dimensional space, we utilized t-distributed stochastic neighbor embedding (t-SNE), one of the AI techniques known for dimensionality reduction while preserving microstructural information, to plot the IFRs in a 2D space. The structural factors related to the two axes were then examined. Although direct interpretation of the axes in the 2D plot was difficult, it became clear that pore size and distribution, as well as the size and shape of Si<sub>3</sub>N<sub>4</sub> grains, played a role in data classification after applying axis rotation. This technique offers new potential for interpreting properties' predictions using deep learning.

#### (ICACC-PB041-2025) Prediction of size dependency of strength scatter in ceramics using extreme value statistics for defect distribution

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Strength scatter and size dependency due to the brittleness and microstructural heterogeneity of ceramic materials are major barriers to their use as structural components. To address these issues and design reliable ceramic components, it is desirable to understand the strength scatter caused by the stochastic distribution of defects and to predict the strength of the component. In this study, we proposed a numerical simulation method to predict the strength scatter of ceramics and its size dependency based on internal microstructural data obtained using X-ray computed tomography and scanning electron microscopy with a local fracture mechanics model. In particular, the sizes of pores, which are the major fracture origins, were organized based on the generalized Pareto (GP) model, a type of extreme value statistic, and focused only on candidate fracture origins. The prediction of strength scatter was examined for alumina fine ceramics under four bending test conditions to demonstrate the effectiveness of the proposed simulation method. The predicted strengths were in good agreement with the experimental ones. By taking advantage of the characteristics of the GP model and using the number density information of defects, it was confirmed that the proposed method can be applied to discretized analytical models with arbitrary element sizes.

#### (ICACC-PB042-2025) Dispersion Stabilization of Magnetorheological Slurries for Applications in Chemical Mechanical Planarization

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This study introduces an innovative magnetorheological (MR) slurry comprising ceramic abrasive particles and carbonyl iron particles (CIPs) that respond to magnetic fields and are dispersed in the CMP slurry. This MR slurry enables real-time control of polishing processes through magnetic field manipulation, resulting in more precise and uniform material surface polishing compared to conventional CMP methods. The primary focus of this research is to effectively disperse the abrasive and CIP powders and assess their dispersion impact on polishing efficiency. We propose the use of a polyelectrolyte to aid in the powder dispersion. DLVO calculations and DFT numerical simulations were employed to elucidate the dispersion mechanisms when the polyelectrolyte is added. Our examinations include assessments of how the aqueous slurry dispersion affects planarization efficiency, as measured by material removal rate and substrate surface roughness.

#### (ICACC-PB043-2025) Nanocomposite-Typed Energy Harvesters Assisted by Relaxor Ferroelectric Polymer Matrix

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Piezoelectric nanocomposites composed of a polymer matrix and ceramic fillers hold potential for use in flexible, wearable, and self-powered electronic devices. However, the inherent differences between ferroelectric polymers and ceramics at the piezoelectric interface pose challenges in creating efficient hybrid nanocomposites without unwanted polarization and artifacts. This study investigates the influence of a relaxor ferroelectric terpolymer matrix on piezoelectric output, which can improve the energy harvesting and sensor performance of piezoelectric composite devices that utilize nanocomposite generators with lead zirconium titanate filler nanoparticles. The proposed terpolymer matrix exhibits enhanced dielectric properties and reduced ferroelectric interference, enabling better poling to align the polarization of piezoelectric ceramic fillers compared to a conventional ferroelectric copolymer matrix. As a result, relaxor ferroelectric polymers may offer advantages over traditional ferroelectric polymers as the matrix material in hybrid polymer-ceramic piezoelectric nanocomposites. This research provides valuable insights into the physical interactions at the interface between polymer matrices and ceramic fillers in flexible piezoelectric nanocomposite applications.

#### (ICACC-PB044-2025) Enhanced Piezoelectricity of Piezo-ceramic/ composite and Its Applications to Flexible Energy Harvesters

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Flexible piezoelectric energy harvesters (f-PEHs) which can generated the sustainable and long-lasting energy source has attracted a great interest because it can harvest the electricity from the tiny mechanical deformations that are more accessible in almost everywhere. Recently, for enhancing current and charge performance of f-PEHs, many researchers have proposed the various inherently excellent piezoelectric nanomaterials and polymers using a simple and cost-effective process. Herein, we will describe perovskite-structured piezo-ceramic BaTiO<sub>3</sub> (BTO) nanomaterials using various synthesis processes such as hydrothermal, solid-state reaction, anodization, picosecond laser ablation. We also demonstrated the flexoelectric-boosted electromechanical properties of piezoelectric nanoparticles using an induced built-in strain gradient in heterogeneous core-shell nanostructure for enhancing the intrinsic piezoelectricity of pure BTO nanoparticles. Next, we have demonstrated the enhanced poling efficiency in nanocomposite made of poly(vinylidene fluoride-co-trifluoroethylene) and porous BTO nanofibers. Finally, we will describe the high-temperature workable f-PEH comprising the KNN-based ceramics and a thermally stable polyimide (PI) matrix which can be a promising candidate for developing f-PEH and self-powered sensors working in high-temperature environments.

#### (ICACC-PB045-2025) Development of Direct Plasma Treatment Process to Enhance the Powder Density of Ceramic Slurry

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The forming process utilizing ceramic materials predominantly employs resin, with slurry contributing as the primary component. Notably, the density of the ceramic powder incorporated within the slurry is a critical parameter for minimizing shrinkage and deformation during the post heat processing stages of formed products. These challenges can be effectively mitigated through the production of uniformly dispersed high-density slurries. However, conventional ball milling method require relatively extended processing times to form functional groups on the surface of ceramic powders and may result in deformation of the powder particles. Consequently, it is required to develop alternative production process of ceramic slurry suitable for high-mix low-volume (HMLV) scenarios. In this study, a novel method is proposed for enhancing the dispersion and powder content of fluid ceramic slurry through direct plasma treatment. Unlike previous studies, ionization of the water is achieved using Ar plasma only, resulting in a significant improvement in the dispersion of the slurry compared to the control group. Notably, the use of a rotational process chamber facilitates the formation of the slurry into a thin film, thereby expanding the interaction area with the plasma. This process, combined with appropriate agitation, proves effective in producing high-density ceramic slurry.

### (ICACC-PB046-2025) Utilization of Silt from gold mine waste for Silt-Polyester composite (SPc)

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The continuous increase of gold mine wastes poses threats to the environment. One of the possible ways to mitigate these hazards is to valorize the wastes for industrial or municipal applications. In this study, the silt from gold mine waste in Northern Mindanao, Philippines, was explored as the potential filler to a Silt-Polyester composite (SPc). The coarse materials of the silt were removed by screening. The undersize of 38-micron particles were chosen as the size fraction for the composite. This size fraction contains at least 53% SiO<sub>2</sub>, 9% Al<sub>2</sub>O<sub>3</sub>, 8% Fe<sub>2</sub>O<sub>3</sub>, 9% MgO and 7% CaO. Four different solid loadings were investigated for their effects on the flexural and tensile strengths of the composites. Results showed that the 3wt% Silt-Polyester composite showed the highest flexural and tensile strengths, and are better than the pure polyester counterpart. It also exhibited the highest mean flexural modulus at ~1,828MPa. However, the 7wt% SPc showed the highest mean Young's modulus at ~1,159MPa. Thus, incorporating silt from gold mine waste as a filler to the polyester matrix can improve the tensile and flexural strengths of Silt-Polyester composites at a lower cost since the filler is coming from mine waste.

#### (ICACC-PB047-2025) Unlocking the Potential of Agricultural Waste: Novel Micro-Mesoporous Silicates from Agricultural Residues

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This paper explores the potential of agricultural waste as a source for innovative materials. Specifically, rice husk ash (RHA) is investigated for its use in producing micro-mesoporous silicate particles (MMSP). These materials, characterized by their unique pore structure, offer exceptional properties such as high surface area and adsorption capacity. The paper outlines the synthesis process, including acid leaching, sodium silicate extraction, and sol-gel methods, along with advanced templating techniques. It highlights the potential applications of MMSP in various fields, including water treatment, catalysis, and possible energy storage (thermal management materials). Future research should focus on optimizing synthesis, functionalizing MMSP, developing large-scale production, and exploring novel applications to fully realize their potential

# (ICACC-PB048-2025) Hydrophobic Surface Modification of MgO for thermal management interfaces in Electric Vehicle Batterie

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With the growth in electric vehicles worldwide, thermal management interfaces (TMIs) have become increasingly important for preventing fire accidents and enhancing battery safety. TMIs refer to materials designed to efficiently transfer and dissipate heat generated by batteries, which requires high thermal conductivity. Among various types of fillers for TMIs, Al<sub>2</sub>O<sub>3</sub> has been commonly utilized, but its high density and low thermal conductivity make it less appropriate for TMIs. As a promising alternative for  $Al_2O_3$ , MgO has been actively studied due to its commercial applicability, relatively low density, and high thermal conductivity, which can be expected to replace Al<sub>2</sub>O<sub>3</sub> and significantly improve TMIs performance. However, the hydrophilicity of MgO can lead to degradation through reactions with H<sub>2</sub>O, resulting in undesired phase transformations with lower thermal conductivity. To solve this problem, fluorine was used to impart hydrophobicity to the MgO surface. The hydrophobic coating was developed through a sol-gel process using Fluorine Alkyl Silane. This coating provides Si-C and C-F groups, which enhances hydrophobicity as confirmed by contact angle measurements. The developed hydrophobic MgO as a filler for TMIs is expected to enhance the safety of battery systems by preventing undesired phase transformations and improving stability.

### (ICACC-PB050-2025) Post-oxygenation under high pressure of superconducting EuBCO and GdBCO coated conductors

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REBCO (Re=Y, Eu, Gd) coated conductors (CC) have a lot of application opportunities: grid cables, fault current limiters, high-field magnets of energy storage and fusion devices, NMR systems, wind mills, cyber security management systems, different electronic devices, motors and generators for electrical and hydrogen aviation, etc. But efficient application of CC needs further increase of current carrying capacity. One of the ways to reach this can be overdoping by oxygen of the REBCO structure of CC which can be attained by pressure-temperature treatment under oxygen. Before oxygenation experiments the Cu surfaces layers were chemically removed from CC. Oxygen pressure waried in the range 1 - 160 bar and temperatures between 300-800 °C. From some EuBCO-CC and GdBCO-CC the 2 mm thick surface Ag layer was chemically removed before oxygenation as well. Signatures of overdoping were observed for many treated samples. Treatment under 100 bar of O<sub>2</sub> for 3 h of GdBCO\_CC (with Ag layer) at 600 °C led to an increase in J<sub>c</sub> (77 K, 0 T) from 2.57 to 2.67 MA/cm<sup>2</sup> and of GdBCO\_CC (without Ag layer) at 300 °C to an increase in  $J_c$  (77 K, 0 T) from 2.10 to 2.28 MA/cm<sup>2</sup>. It was accompained with a decrease in the c-parameter of Gd123 from 1.17351 to 1.17310 nm in the both cases.

#### (ICACC-PB051-2025) Combined Effects of Displacement Damage and Transmutation on the Thermal Diffusivity of CVD-SiC

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The study presented is part of a wider effort to evaluate NITE-SiC/SiC as a candidate structural material in the Liquid Sandwich Vacuum Vessel (LSVV) concept for ARC-class fusion energy devices. The LSVV design proposes the use of a non-conductive structural material shell made Silicon Carbide composites like Nano Infiltration Transient Eutectic Phase Silicon Carbide Matrix reinforced with Silicon Carbide fibers (NITE-SiC/SiC) enclosing a conductive liquid (like molten lead). This assembly is contained within the liquid immersion blanket. We will present the results of the first stage of an experiment to study the combined effect of displacement damage and transmutation on the thermal diffusivity of SiC prepared by chemical vapor deposition. 4 samples of CVD-SiC are prepared and irradiated with Si2+ and combinations of the gaseous transmutants (H+ and He2+). All dual and triple ion irradiations will be performed sequentially in this first stage. The PI3TGS device at the Massachusetts Institute of Technology is used where, Transient Grating Spectroscopy (TGS) is applied in-situ during the Si2+ ion irradiation to determine the changes in the thermal diffusivity of the irradiated layer as a function of dose. Transmission Electron Microscopy will then be used to link the observed changes in the thermal diffusivity to the microstructure of the material.

#### (ICACC-PB052-2025) Effects of Oxide Formation on Corrosion Resistance of Structural Materials in Chlorine-Based Salt Environments

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With the increasing focus on nuclear power, research is advancing on innovative fourth-generation reactors that aim to reduce the risk of nuclear accidents. This study explores the effects of oxide film formation on the corrosion resistance of structural materials, specifically Fe- and Ni-based alloys, in chlorine-based salt environments relevant to Molten Salt Reactors (MSRs). MSRs, an emerging technology in nuclear power, offer significant advantages such as enhanced safety and efficiency using molten salts as coolants. However, the aggressive nature of chlorine-based salts necessitates the development of materials with robust corrosion resistance. The research investigates how the Cr and Mo content in SUS316L, Hastelloy C-276, and Hastelloy N alloys influences the formation of protective oxide films and overall corrosion behavior. The alloys were exposed to high temperatures of 800°C to simulate the harsh conditions within MSRs. SUS316L, with low Mo content, suffered from significant grain boundary corrosion, while Hastelloy N, low in Cr, experienced surface corrosion. In contrast, Hastelloy C-276, with its high Cr and Mo content, exhibited superior corrosion resistance, highlighting the importance of these elements in protecting structural materials in chlorine-based salt environments.

#### (ICACC-PB053-2025) Innovative Swaging-Drawing ATF Tube with Zr Nitride Formation for Enhanced Thermal Stability Evaluation under LOCA Conditions in PWR

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In the years following the Fukushima nuclear accident in 2011, operations of Pressurized Water Reactors (PWRs) will continue to be validated using Accident-Tolerant Fuels (ATF) technology, which is scheduled for implementation until 2028. Nuclear fuel tubes in power plants must withstand both accident scenarios and extreme conditions, prompting research into surface coatings and compositional modifications to enhance the safety of Zr alloy tubes during Loss-of-Coolant Accidents (LOCAs). A research team from Korea has demonstrated excellent thermal stability under LOCA simulation conditions using swaging-drawing technology, a core process in ATF development. An ultra-thin stainless steel (SS) tube, approximately 70 micrometers thick, underwent swagingdrawing both internally and externally. Subsequently, thermal stability was evaluated under LOCA conditions at 1,200°C, where the formation of zirconium nitride (Zr-nitride) at the SS-Zr interface inhibited oxidation. Furthermore, theoretical analysis confirmed that power generation output remained unaffected despite the high neutron absorption cross-section of the iron-based alloy. This innovative swaging-drawing triple tube is thus a promising candidate for ATF applications in PWRs, offering both thermal stability and accident resistance under LOCA conditions.

#### (ICACC-PB054-2025) Interlaboratory Study of Flexural Strength in Additively Manufactured Alumina

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We report the results of an international interlaboratory study (ILS) of the flexural strength of alumina fabricated across six laboratories using the same lithography-based ceramic additive manufacturing (AM) technology. The mechanical testing of all the specimens,

142 in total, was performed at NIST according to the well-established four-point bending method standardized for traditional ceramics. Overall, the existing ASTM standard for the four-point bend testing proved adequate for AM ceramics, with several modifications to the specimen requirements to account for the specifics of AM processes. Critical flaws that caused failure were identified in all but two cases using optical fractography augmented with the imaging of fracture surfaces by SEM. The flexural strength data, analyzed following the Weibull statistics, exhibited considerable variation among the specimen sets manufactured by different laboratories. This variability correlated with the presence of many distinct critical flaws. We identified seven types of flaws that accounted for the failure of 94 % of specimens. We discuss the nature of these flaws and their relation to the printing and post-processing conditions. This study contibutes toward the development of standards for AM ceramics, with current initiatives ongoing jointly within ASTM and ISO Standards Development Organizations.

#### (ICACC-PB055-2025) Binder Jetting of Glass Grinding Waste

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Glass grinding waste is typically disposed of in landfills, as it has no further application or value. This waste is a slurry with approximately 80 wt% solid content, consisting of fine particles of glass and abrasive materials. We will present our initial results on the additive manufacturing of 3D objects from grinding waste produced in automotive float glass manufacturing using binder jetting technology. Hot-stage microscopy was employed to determine the debindering and sintering thermal parameters of the 3D-printed objects. Detailed characterization of the sintered 3D-printed samples was performed using SEM imaging, XRD, and Raman spectroscopy. The XRD and Raman spectroscopic analysis results indicate that wollastonite is the dominant crystalline phase in the sintered 3D-printed objects. A 3D-printed, sintered object with a compressive strength of up to 9.12 MPa, characterized by the presence of open surface porosity, was successfully produced from the glass grinding waste.

#### (ICACC-PB056-2025) Fused Filament Fabrication of Silicon Carbide: Effects of Printing and Sintering Parameters on Material Properties

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The aerospace industry has an increasing need for lightweight, high-performance materials that can withstand extreme environments. Silicon carbide (SiC) is a strong candidate for various aerospace applications with its desirable material properties such as high thermal stability, high strength, high hardness, and low density. This work focuses on the additive manufacturing of SiC via fused filament fabrication (FFF). Additive manufacturing enables the production of parts with complex geometries while reducing waste and fabrication time. Understanding how different print settings as well as how the post-printing sintering process influence the material's performance is crucial for optimizing its applicability. This study investigates the effect that various printing parameters (number of shells, infill type, and infill percentage) and varying sintering schedules (differences in holding time) have on the resultant microstructure, mechanical, and thermal properties.

#### (ICACC-PB057-2025) Exploring the limits of rapid sintering: The impact of nozzle diameter and sintering atmopshere on fused filament fabricated Al<sub>2</sub>O<sub>3</sub> ceramics

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Fused filament fabrication (FFF) remains one of the most widely used rapid prototyping techniques for fabricating complex structures. This is mostly due to the extensive use of inexpensive and custommade printers specifically designed for polymer printing. However, the bottleneck of the whole process lies in the very slow thermal debinding and sintering that are usually employed to obtain dense and defect-free ceramics. In this study, filaments with ~79 wt.% of Al<sub>2</sub>O<sub>3</sub> powder was embedded in a commercial thermoplastic blend to obtain a filament suitable for FFF. Thereafter, the filament was used to print gyroids with with three different nozzle diameters (0.4, 0.6 and 0.8 mm). All the samples were solvent debinded in acetone before carrying out the thermal debinding and sintering in a single step using novel rapid sintering techniques such as ultra-fast high temperature sintering (UHS) and fast firing (FF). The findings in this study will highlight the effect of geometric limitations and sintering atmosphere on the rapid sintering for FFF-printed alumina structures, suggesting that both the factors plays a critical role in determining the viability and structural integrity of the final product.

# (ICACC-PB058-2025) Microstructural evolution and phase analysis of SS410-Al2O<sub>3</sub>-SiC multilayered functionally graded composite fabricated through laser cladding

- A. Murugesan\*1
- 1. Indian Institute of Technology Kharagpur, School of Nanoscience and Technology, India

In this study, a functionally graded metal-ceramic composite structure comprising SS410, Al2O<sub>3</sub>, and SiC particles with varying composition, structure, and properties in a single deposit was successfully fabricated using direct energy deposition (DED). The composition ranged from 90% SS410 with 10% (xAl2O<sub>3</sub> + ySiC) to 10% SS410 with 90% (xAl2O<sub>3</sub> + ySiC), where x = 70% and y = 30%in a layered FGM design. The microstructure, phase evolution, and mechanical properties of the components with different composition gradients were characterized by microscopy, energy-dispersive spectroscopy, wavelength-dispersive spectroscopy, X-ray diffraction, and microhardness tests. The investigation revealed complex phases such as C0.12Fe0.79Si0.09, M7C3, and Fe3Si, formed due to the interaction between SiC and SS410 during the cladding process. Microstructural analysis showed a transition from columnar dendrites at the bottom zone of the cladding to a cellular structure and carbide particle agglomerates in the middle zone, with finer grains at the top. This gradation in microstructure correlated with an increase in microhardness, ranging from 299 HV at the bottom to 966 HV at the top. The hardness enhancement was due to solid solution strengthening from C and Si, originating from the decomposition of SiC and the precipitation of intermetallic phases

#### (ICACC-PB059-2025) Design and Development of 3D Printed PEEK and Nylon Composites

- A. Thorne<sup>1</sup>; A. Elhassan<sup>\*1</sup>; S. Gupta<sup>1</sup>
- 1. University of North Dakota, USA

Additive manufacturing (AM) has emerged as a vital component for manufacturing complex structures. In this poster presention, we will present some of the recent development in manufacturing of nylon and PEEK composites. We will present detailed microstructure and mechanical behavior of the designed composites. It is expected that these composites can be used for functional and structural applications.

#### (ICACC-PB060-2025) Utilization of Robotic Arms in Non-Planar 3D Printing

#### M. G. Hardiman\*1; C. Dewey1; D. Kim1

1. Embry-Riddle Aeronautical University, Aerospace Engineering, USA

Recent research has shifted toward additive manufacturing to improve efficiency in the production of complex structures, especially those for in-space applications. Standard 3D printers have typically been used for additive manufacturing; however, they are limited in printing certain geometry and orientation and are often incompatible with the desired materials. This research aims to utilize systems of robotic arms with six degrees of freedom and refine manufacturing procedures to produce composite parts with a high level of consistency. This system is capable of non-planar printing without supports. With a modular design, different printing heads can be swapped out and the robotic arms can be relocated to fit specific printing requirements. The printing heads can print with various materials, including hybrid thermoplastic-continuouscomposite-fiber filaments. Experimentation includes varying print parameters such as extrusion rate, motor speed, and robotic path. Results are analyzed with respect to structural integrity and part irregularities. Identification and characterization of surface irregularities will be done utilizing a digital microscope and optical profilometer. Structural testing will include tensile, compression, shear, stress, and strain tests. This research allows for automated production and improved consistency in parts produced through additive manufacturing, suitable for usage in the aerospace industry.

### (ICACC-PB061-2025) Sustainable Construction: An Innovative Geopolymer-Pozzolanic Hybrid Binder

S. S. Hossain\*1

1. Texas A&M University, Department of Civil and Environmental Engineering, USA

The construction industry is urgently searching for sustainable materials that can help lower carbon emissions and reduce energy consumption. This research presents an innovative Geopolymer-Pozzolanic Hybrid Binder (GPHB) as a promising solution, utilizing metakaolin and alkali activators, supplemented with zeolite for enhanced properties. Calcium oxide (~4 wt.%) is introduced to initiate a pozzolanic reaction, which synergistically complements the geopolymeric reaction. This unique combination enables effective curing at ambient conditions, eliminating the need for the energy-intensive heating processes typically associated with geopolymer production. Zeolite provides additional silica and alumina, improving the binder's durability and density, while calcium oxide enhances early strength development through pozzolanic interactions. Experimental results indicate that this GPHB achieves enhanced compressive strength, reduced water permeability, and increased resistance to chemical attacks, making it an ideal candidate for diverse construction applications. This research highlights the potential of geopolymer-pozzolanic hybrid binders as a sustainable and high-performance alternative to traditional construction materials, contributing to a more environmentally friendly and resilient built environment.

### (ICACC-PB062-2025) Effect of curing temperature on mixtures of clayey waste with hydraulic cement for geothermal pavements

- L. C. Hernández García\*1; H. A. Colorado L.<sup>2</sup>
- 1. Universidad de Antioquia, Antioquia, Colombia
- 2. Universidad de Antioquia, Colombia

The need for clean energy has led to the development of geothermal pavement technology. This, along with the objective of reducing material consumption and reusing excavation, demolition, and construction waste, has motivated this research. This study reviews the mechanical, physical, and chemical behavior of three clayey residues mixed with hydraulic cement and cured in cabins that maintain a constant temperature and humidity for 7 days. Each cabin has a different temperature: 40°C, 28°C, and 10°C. It was found that, unlike hydraulic concrete mixtures, soil-cement mixtures exhibit endothermic rather than exothermic reactions, which results in variations in their strength and resilience.

#### (ICACC-PB063-2025) Physical-Mechanical Properties of Permeable Concrete in Hardened State made with recycled aggregates

E. Murillo Mosquera\*1

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This research is about the physical-Mechanical Properties of Permeable Concrete in Hardened State. The control variables were the maximum particle size of the aggregate, the water-cement ratio, and the percentage of aggregate used. The samples included some with 100% recycled concrete and some with 100% non-recycled concrete (new raw materials). The nominal maximum diameter used was 12.7 mm; and the water/cement ratio used was 0,35; for the permeable concrete manufactured with natural aggregate, the same percentage, water/cement ratio and maximum aggregate size were used. Scanning electron microscopy, voids content, compressive strength, and permeability tests were included. The results and their correlations in properties, microstructure, and application are discussed in detail.

### (ICACC-PB064-2025) Glass-Enhanced Bricks: An Additive Manufacturing Approach

- C. Revelo Huertas\*2; H. A. Colorado L.1; C. F. Vieira2
- 1. Universidad de Antioquia, Colombia
- 2. State University of the North Fluminense, Advanced Materials Laboratory, Brazil

Additive manufacturing, a process that involves creating objects layer by layer from a digital design, offers a promising solution for repurposing waste materials. This study focuses on utilizing recycled glass bottles to produce bricks through a technique known as Robocasting (RC). By incorporating 30% ground glass waste into a yellow clay mixture sourced from Campos dos Goytacazes, Brazil, we were able to create bricks with unique and customizable shapes. To optimize the material's properties and reduce water content, we experimented with various additives, including citric acid, cornstarch, and sodium silicate. The resulting bricks were subjected to rigorous testing to assess their density, shrinkage, and compressive strength. X-ray fluorescence (FRX) analysis was conducted to characterize the raw materials while scanning electron microscopy (SEM) provided insights into the microstructure of both the raw materials and the manufactured samples. The integration of glass waste into ceramic production through additive manufacturing not only improves the properties and performance of the final products but also contributes to a more sustainable future by reducing environmental waste.

### (ICACC-PB065-2025) Crystallographic changes due to sintering temperature of calcium phosphates synthesized by products

S. M. Restrepo Arcila\*1; H. A. Colorado L.2; M. Márquez1

- 1. Universidad Nacional de Colombia, Materials and nanotecnology, Colombia
- 2. Universidad de Antioquia, Colombia

Three materials were synthesized from a bioleaching process using a Colombian phosphoric rock with a 5% by weight P content determined by XRF and AA. This mineral was treated with sulfuric acid, obtained from the microorganism strain AT ATCC 13977, which solubilizes sulfur in a 9K medium in a 5-liter reactor. The acid used in the reactions presented a concentration between 48000 and 100000 mg/L, measured by UV-Vis method. The liquid product of the solubilization was characterized in a Thermo Scientific Genesis 10 UV spectrometer, using the 4500-PC spectrophotometric method at a wavelength of 470 nm, obtaining a range between 74% and 100% of solubilized P. The concentration of Ca was determined in ppm using the titrimetric method. The synthesized materials were obtained by a chemical precipitation method, using the product of solubilization as a source of P, Mg and Ca. The synthesis was carried out at an initial pH of approximately 5.2, at a temperature of 25°C, and was reacted with a Ca(OH)<sub>2</sub> solution obtained from the calcination of eggshells and subsequent hydration at a concentration of 5%, until a pH of 10 was reached with an agitation of 300 rpm. Subsequently, the materials were dried and subjected to heat treatment at 400, 600, 800, 1000 and 1200 °C. These materials were characterized by XRD and FTIR spectroscopy to identify the crystallographic changes at each temperature.

## (ICACC-PB066-2025) Anti-oxidation UHTC coatings obtained by plasma spraying

#### A. Charrue\*1

1. Commissariat a l'energie atomique et aux energies alternatives Siege administratif, France

The plasma spray process is particularly well suited to produce protective coatings. The coatings are built through the successive layering, in the form of lamellae, of melted particles. Due to the energy available within the plasma jet, it is possible to shape any material with a melting point, including those with the highest melting temperatures. Therefore, the process is well suited to shape ultra-refractory materials (UHTCs, Ultra High Temperature Ceramics). This study focuses on four UHTC-based coatings as ZrB<sub>2</sub>, ZrC, HfB<sub>2</sub> and HfC obtained by plasma spraying under an inert atmosphere. It is conducted in the context of new space applications where carbon/carbon composites need protection against oxidation at temperatures above 2000°C for several minutes. The samples were evaluated at high temperatures and under an oxidizing atmosphere using the MESOX facility (air plasma), located at the focal point of the 6 kW solar furnace in Odeillo, and under an oxidizing plasma jet with Vulcain set-up. Different oxidation mechanisms, ablation phenomena and interactions with the substrate will be discussed based on SEM, XRD, EDS and SXES analyses.

#### (ICACC-PB067-2025) Effects of WC addition on the microstructure and mechanical properties of (Hf,Nb,Ta,Ti,Zr) B<sub>2</sub>-(Hf,Nb,Ta,Ti,Zr)C dual phase high entropy ceramic

- R. Hassan\*1; W. Fahrenholtz1; G. Hilmas1
- 1. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA

(Hf,Nb,Ta,Ti,Zr)B<sub>2</sub>-(Hf,Nb,Ta,Ti,Zr)C dual phase high entropy ultra-high temperature ceramics were synthesised by a single step boro-carbothermal reduction route. After synthesis, 2.5 wt%, 5 wt%, or 10 wt% WC was added before densification. After spark plasma sintering at 2000 °C, WC dissolved completely into the dual phase for the 2.5 wt% and 5 wt% additions, preferentially going into the carbide phase. However, a monoboride phase rich in W appeared in the microstructure for the composition with the 10 wt% WC addition. This secondary phase was uniformly distributed throughout the microstructure, but its presence did not affect the grain size of the primary boride or the carbide phases. The effects of WC dissolution, and the W-rich monoboride phase on the room temperature hardness, elastic modulus, fracture toughness and flexural strength, were then studied and compared among the compositions.

## (ICACC-PB068-2025) Rare-Earth Doping of Zirconium Diboride for Extreme Environments

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- 1. UES, A BlueHalo Company, USA
- 2. Air Force Research Lab, Materials and Manufacturing Directorate, USA

Zirconium diboride  $(ZrB_2)$  is a material of interest for extreme environments due to its high melting point, but degradation from oxidation at ultra-high temperatures limits its applications. Here, rare-earth (RE) oxides and borides have been added to  $ZrB_2$  to stabilize the oxide phases that form, limiting the detrimental effects of thermal shock and volumetric phase changes. The addition of the RE compounds will aim to increase the emittance of both the  $ZrB_2$  and the resulting oxide, decreasing the overall temperature of the material in a given high heat flux condition by increasing the radiative heat losses. To inform the selection of the RE compounds studied, density functional theory calculations have been used to calculate the dielectric function and the emissivity of RE compounds as a function of frequency. The effect of silicon carbide inclusion on the stability of the RE phases is investigated. RE doped  $ZrB_2$  and  $ZrB_2$ -SiC pellets have been fabricated and subjected to static oxidation and oxyacetylene torch testing to evaluate the properties of the resulting oxide, such as mechanical stability, surface roughness, emittance, and microstructure.

# (ICACC-PB069-2025) Friction and wear of carbon fiber reinforced $\rm ZrB_2$ based UHTCMC-materials on steel, C/C-SiC and C/C

N. Langhof<sup>\*1</sup>; M. Mor<sup>2</sup>; M. Meiser<sup>1</sup>; A. Vinci<sup>3</sup>; S. Schafföner<sup>4</sup>; D. Sciti<sup>5</sup>

- 1. University of Bayreuth, Ceramic Materials Engineering, Germany
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- Ceramics, Italy
- 3. CNR ISSMC, Italy
- 4. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany
- 5. National Research Council of Italy, ISSMC (former ISTEC), Italy

Ultra-high temperature ceramic matrix composites (UHTCMCs) can withstand challenging conditions at high temperatures > 2000 °C and heat fluxes. ZrB<sub>2</sub> is one of the most promising materials due to its low density (~6 g/cm<sup>3</sup>). C-fiber reinforced  $ZrB_2$  damage tolerant CMC and considered for applications in the field of aerospace, hypersonic vehicles, propulsions and friction materials as well. In order tests the tribological behavior of UHTC-ZrB2/SiC brake pads under high loads, the materials were evaluated on a self-designed test rig with a fly wheel of 800 kg. The UHTCMC-pads with Granoc HM C-fiber reinforcement (short fibers and fabric, 35 vol. %) were fabricated by mold casting, layup and hot pressing. The matrix contains about 90 vol.% ZrB2 and 10 vol.% SiC. A steel, a C/C and a C/C-SiC disc were selected as counterparts. The coefficient of friction, the wear and the temperature of the friction couples were measured, applying an initial sliding speed of 20 m/s and braking pressures < 3 MPa. In general, the COF was between 0.8 and 0.3. The pads and discs show temperatures up to 600 °C, especially with C/C-discs. The COF drops instantly from 0.7 to 0.3 if the temperatures exceed 450 °C. The pads and discs materials were compared with references and studied frictional surfaces, compositions and microstructures.

#### (ICACC-PB070-2025) The effect of compositional homogeneity on the thermomechanical properties of solid solution carbides for nuclear thermal propulsion

- L. Hansen\*<sup>1</sup>; E. Payne<sup>1</sup>; A. Nadermann<sup>1</sup>; S. J. Zinkle<sup>2</sup>
- 1. The University of Tennessee Knoxville Tickle College of Engineering, Department of Nuclear Engineering, USA
- 2. University of Tennessee, USA

NASA is investigating the use of refractory solid solution carbides containing uranium carbide as a means of creating a robust nuclear fuel form for Nuclear Thermal Propulsion (NTP) which would allow twice the specific impulse of traditional chemical propulsion. However, the thermomechanical properties of solid solutions consisting of zirconium, niobium, tantalum, and titanium carbides are needed to achieve acceptable technology readiness levels. Solid solution carbides were sintered via Spark Plasma Sintering (SPS) and characterized to investigate homogenization via x-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS). It was observed that the powder preparation process had a significant effect on the chemical homogeneity of the solid solution carbides even after sintering to near ideal density. The effects of cation species and homogeneity on the sintered solid solution carbide's thermomechanical properties was investigated by comparing properties such as hardness and thermal conductivity.

### (ICACC-PB071-2025) Phase stability of transition metal carbides with rare-earth zirconates

#### R. P. Magdum\*1; G. Hilmas1; W. Fahrenholtz1; D. Lipke1

1. Missouri University of Science and Technology, Materials Science and Engineering, USA

Rare-earth zirconates and high-entropy carbide are being investigated for thermal barrier coatings and ultra-high temperature ceramics applications. This poster illustrates thermochemical phase stability of different transition metal carbides with rare-earth zirconates for ultra-high temperature applications. Transition metal monocarbides with metals from groups IV, V, and VI were prepared by carbothermal reduction. Rare-earth oxides were reacted with zirconia powders after high-energy milling and reaction in a furnace to form rare-earth zirconates. These rare-earth zirconate and transition metal carbide powders were mixed and densified using spark plasma sintering. The phase analysis of the powders and ceramics was performed by X-ray diffraction. Scanning electron microscopy with energy dispersive X-ray spectroscopy was used for examination of different element distribution in the microstructure of the densified ceramics. The outcomes from this study will advance the use of rare-earth zirconates as thermal barrier coatings for high entropy carbide ceramics.

#### (ICACC-PB072-2025) Thermal Properties of (Hf, Mo, Nb, Ta, Zr) C Ceramics with Varying Zr Content

- E. A. Pritchett<sup>\*1</sup>; S. M. Smith<sup>1</sup>; G. Hilmas<sup>1</sup>; W. Fahrenholtz<sup>1</sup>
- 1. Missouri University of Science and Technology, Materials Science and Engineering, USA

High-entropy carbides are suitable materials for extreme environments because they have high melting temperatures and maintain strength at temperatures up to at least 1800°C. Thermal property control of high-entropy carbides is a novel concept, and the focus of this research is to minimize thermal conductivity. Carbothermal reduction will be used to synthesize carbide powders containing equimolar amounts of Hf, Mo, Nb, and Ta with Zr content ranging from 0-20 atom percent. The resulting powders will be densified by spark plasma sintering. Thermal diffusivity will be measured by the laser flash method up to 2000°C. Scanning electron microscopy will be used to characterize the microstructures. X-ray diffraction and energy dispersive spectroscopy will be used to determine which phases were present and the metal ratios. The poster will focus on the effect of Zr on the resulting thermal properties and microstructure for each composition.

# (ICACC-PB073-2025) Synthesis of high entropy monoboride $(Mo_{0.25}W_{0.25}Cr_{0.25}Ta_{0.25})B$ powders with abundant twinsfrom oxide.

L.  $Li^{*1}$ ; J.  $Zou^1$ 

1. Wuhan University of Technology, Materials Science and Engineering, China

High entropy monoborides powders are mainly prepared from metal and boron powders which can be costly. In this study, a novel approach starting from mixed oxides, boron carbide, and graphite was first developed to synthesize quaternary monoboride powders by combining multiple boro/carbothermal reductions (MBCTR). As an exemplar, ( $Mo_{0.25}W_{0.25}Cr_{0.25}Ta_{0.25}$ )B powders with purity up to 94.3 wt.% were successfully synthesized by heating the mixtures in vacuum at 1650°C for three times, as-synthesized powders exhibit fine particle size (<1 µm) and uniform elemental distribution. MBCTR not only increased the purity of monoborides but resulted in abundant twins and stacking faults in the final powders. This work has proposed a new and low-cost strategy of synthesizing high-purity and fine monoboride powders.

# (ICACC-PB074-2025) Microstructure and properties of $ZrB_2\mathchar`-SiC$ composites fabricated by pressure-less sintering of gel-cast green bodies

V. Sn\*1; A. Mishra1; M. Patel3; S. Dhara2; R. Mitra1

- 1. IIT Kharapur, Metallurgical and Materials Engineering, India
- 2. IIT KGP, School of Medical Science and Technology, India
- 3. DRDO Defence Metallurgical Research Laboratory, India

The ZrB<sub>2</sub>-20 vol.% SiC based composites have been processed by pressure-less sintering of gel-cast green bodies at 2000°C for 2 h in inert atmosphere with intermediate holding at 1250 and 1600°C. A novel approach has been developed by involving the use of egg-white (ovalbumin protein) as an environment-friendly natural binder with sucrose as an additive to reduce viscosity. The composite prepared by gel-casting of a slurry comprising 38 vol.% solid loading, 26 vol.% egg-white, and 4 vol.% sucrose containing 0.3 wt.% polyacrylic acid (PAA) as dispersant has exhibited maximum relative green density » 51% with 7.66±2.6 MPa crushing strength and sintered density » 97% and sintering shrinkage (~21.6%). The average grain sizes of ZrB<sub>2</sub> and SiC are found to be respectively,  $8.12 \pm 2.30$  and  $5.54 \pm 1.53$  µm. Elastic constant, hardness and indentation fracture toughness of the ZrB<sub>2</sub>-SiC composites processed using the optimized slurry have been found as 492 GPa, 14.9 GPa, and 5.1 MPa√m, respectively. While these properties are marginally worsened after thermal shock test by quenching from 1000 °C, a much sharper deterioration is observed on quenching from 1200 °C. The optimized slurry composition and process parameters optimised through this study are suitable for processing much sub-scale sizes (100mm\*100mm tile) for use in high temperature structural applications.

#### (ICACC-PB075-2025) MgNiAlVFe and MgNiAlVTi High Entropy Alloys For NiMH Batteries

- G. Çakmak\*1; F. Piskin1; B. Piskin1; H. YÜCE1
- 1. Mugla Sitki Kocman Universitesi Fen Fakultesi, Turkey

It is becoming more and more important for decarbonization all over the world. Today, fossil fuels are used in many vehicles, especially in the transportation sector. Although many electric vehicles continue to be developed, batteries with high energy density are also needed for these vehicles To meet this high energy need, rechargeable batteries with high energy density come to the fore. As an example of these batteries, Mg-based Nickel Metal hydride batteries come to the fore. These batteries stand out with their environmental compatibility and high charging capacity. An interesting development within the interstitial hydrides relates to AB alloy with prototype MgNi CsCl structure). The "high entropy alloy" concept, which has gained significant attention, has reshaped alloy design by favoring nearly equimolar compositions over traditional base-metal alloys with added elements. These alloys, often called multi-component alloys when non-equimolar, are ideal for creating Mg-based alloys that enhance hydrogen storage, catalytic activity, or anti-corrosion properties, improving the performance of Mg-based anodes in NiMH batteries. This study aims to develop Mg-based high-entropy alloys and rechargeable batteries with high charge-discharge capacity. By using appropriate electrochemical methods, bulk discs with optimal conductivity will be produced, and hydrogen permeability performance tests conducted.

### Thursday, January 30, 2025

### FS1 Bioinspiration/Green Processing & Related Technologies of Advanced Materials

# FS1 -Structure and properties of biological materials and advances in multiscale modeling

Room: Flagler C

Session Chair: Zhaoyong Zou, Wuhan University of Technology

#### 8:30 AM

# (ICACC-FS1-001-2025) Biological ceramic composites: Multiscale structure, mechanical properties, and multifunctionality (Invited)

L. Li<sup>\*1</sup>

1. University of Pennsylvania, Materials Science and Engineering, USA

Due to their high mineral content, many biological structural materials, such as shells, teeth, and bones, can be considered ceramic-based composites. These bioceramic composites, through intricate hierarchical organization of mineral building blocks and small amounts of organic materials, often exhibit remarkable mechanical properties, such as high strength and toughness, despite the inherent brittleness of their mineral components. These material systems can also be tailored to possess non-structural properties and functions, including vision and photonic coloration. Understanding the structure-property relationships of these bioceramic composites holds great promise for developing novel multifunctional materials, especially ceramic-based ones. In this talk, I will present our work in this area using several model systems, including mollusk shells and echinoderms. Specifically, I will explore extrinsic and intrinsic strengthening and toughening mechanisms in bioceramic composites. Additionally, I will introduce a unique damage-tolerant, dual-scale, single-crystalline, low-density microlattice we recently discovered in the calcitic skeletal system of starfish. Biomineralbased optical structures in several model organisms will also be discussed.

#### 9:00 AM

## (ICACC-FS1-002-2025) Order induces toughness in anisotropic colloidal crystal composites (Invited)

#### F. Bouville\*1

1. Imperial College London, Department of Materials, United Kingdom

Nacre, enamel, the dactyl club of the mantis shrimp present enhanced fracture resistance by leveraging near-perfect stacking of building blocks and anisotropic microstructures. Numerous research efforts have focused on manufacturing bioinspired structures based on various building blocks and achieved excellent mechanical response. However, synthetic highly mineralized composites have not yet exhibited highly delocalized damage during fracture propagation. We decided to test whether this delocalized damage can only be triggered in more ordered structure. To this end, we synthesised mono-dispersed colloidal silica rods through a sol-gel process and controlled their assembly into tens-of-millimetre-sized highly packed colloidal crystals. Upon resin infiltration, these crystals formed highly textured crystalline-like composites. Our results demonstrate that highly packed and ordered microstructure enhances mechanical response by delocalizing damage in front of a propagating crack, results that can now be fully predicted using a micromechanical model. When compared with disordered particulate composites made by mixing anisotropic reinforcements, either glass fibre or platelets, our ordered composites present a toughness increase with respect to the matrix toughness 10 times higher than the disordered ones.

#### 9:30 AM

## (ICACC-FS1-003-2025) Unveiling Nature's Secrets: HYPAD-FEM for Advanced Materials Engineering (Invited)

#### D. Restrepo<sup>\*1</sup>

1. The University of Texas at San Antonio, Mechanical Engineering, USA

Uncovering the mechanisms enabling Nature to achieve its outstanding properties is not easy. Computational modeling has become an essential tool to enable the understanding of these mechanisms and create a link between theoretical descriptions and experimental observations. However, the simulations required for such investigations are computationally expensive, and the lack of systematic analysis tools to quantify the impact of different parameters on material behavior further complicates the analysis of biological systems. Sensitivity analysis (SA) allows quantifying how the different parameters defining a biological system and their interaction influence the mechanical behavior. However, current SA methodologies are limited to first-order approximations, and subject to computation errors. To tackle these issues, in this talk, we will introduce a new methodology that enhances traditional finite element formulations with the HYPercomplex-based Automatic Differentiation (HYPAD) method providing highly accurate arbitrary-order computations of sensitivities. HYPAD-FEM provides a more precise understanding of how various parameters impact material behavior. This knowledge is invaluable for understanding new systems, optimizing designs, and advancing the research in bioinspired high-performance materials.

#### 10:20 AM

## (ICACC-FS1-004-2025) A Durable, High Strength Carbon-Negative Enzymatic Structural Materials (Invited)

N. Rahbar\*1

1. Worcester Polytechnic Institute, Civil Engineering, USA

Low energy production of strong, carbon-negative construction materials would be essential in addressing the climate crisis. While incorporating biomaterials reduces carbon emissions, these products are not water-resistant and require a protective layer. Here, we introduce an Enzymatic Structural Material (ESM) that employs a capillary suspension combined with an enzyme mixture to integrate precipitated calcium minerals into a sand and carbon matrix. ESM shows high water stability compared to other biologically inspired construction materials with a mechanical strength close to the compressive strength of structural concrete (26 MPa), making it a promising candidate for construction applications. Importantly, ESM production consumes 8.5 kg of  $CO_2$  per m<sup>3</sup>, unlike traditional concrete production, which emits approximately 400 kg of CO<sub>2</sub> per m<sup>3</sup>, aligning with the need for low-carbon building solutions. Physical characterization of ESM confirms its promise as a structural material for advancing sustainable construction technologies.

#### 10:50 AM

## (ICACC-FS1-005-2025) Nature-inspired hierarchical tough and strong ceramic composites (Invited)

#### W. Zhai\*1

1. National University of Singapore, Mechanical Engineering, Singapore

The development of advanced materials that combine high strength and toughness is essential for many engineering applications, such as aerospace, automotive, and biomedical fields. While traditional ceramics offer excellent strength and thermal stability, they tend to be brittle. To overcome this, we turned to nature for inspiration, where materials like bone and nacre exhibit remarkable toughness and strength due to their composite makeup and hierarchical structures. In this talk, we will first present our approach of creating interpenetrating phase composites by infiltrating 3D-printed ceramic scaffolds with polymers. This forms a continuous, interlocking structure that enhances toughness through mechanisms like crack bridging and energy dissipation. Our second approach focuses

on fabricating polymer composites reinforced with ceramic platelets. Using extrusion-based 3D printing, we align these platelets into concentric cylinder microstructures, creating multiple bio-inspired patterns. This hierarchical design enables tunable, anisotropic mechanical properties and increased toughness. The findings of our research demonstrate the broader potential of nature-inspired design principles for developing advanced engineering materials. These strategies open new possibilities for creating tough, strong composites suitable for demanding environments.

#### 11:20 AM

#### (ICACC-FS1-006-2025) Design of Animal-Skin-Patterns-Inspired Composites by Artificial Intelligence for Multifunctional Materials (Invited)

Z. Qin\*1; M. Masrouri1

1. Syracuse University, Civil and Environmental Engineering, USA

Bioinspired composite materials offer several advantages by mimicking the structure of natural counterparts. However, their complex hierarchical structure, in comparing to the limited number of observations, makes it difficult to directly extract all the structural features and set up its correlation to the material functions in experiments. It is also challenging to vary the structure to optimize the material functions without losing their natural structural characteristics. We applied image-based generative artificial intelligence (GenAI) to design composites inspired by animal skin patterns, leveraging a small dataset to generate diverse configurations composed of rigid and soft material phases that closely emulate natural designs. Our computational simulations investigated the structure-mechanics relationship in these materials, revealing significant variations in mechanical functions and identifying patterns that exhibited superior mechanical properties. We validated these outstanding configurations' performance through tensile tests on specimens produced by a multi-material printer. We showcase GenAI's role in structural augmentation that can yield rational bio-inspired designs, complemented by several educational applications with interactive quizzes for public curiosity.

### FS7 Ceramics for global decarbonization

#### FS7- Alternative Fuels Production

Room: Ballroom 5

Session Chairs: Lyndsey McMillon-Brown, NASA Glenn Research Center; Takashi Makino, National Institute of Advanced Industrial Science and Technology

#### 8:30 AM

#### (ICACC-FS7009-2025) Japan's Fine Ceramics Industry and JFCA Carbon Neutral Vision

S. Tsuchiya\*1; Y. Osugi1

1. Japan Fine Ceramics Association, Japan

Fine ceramics support our society and daily life with their properties and functions. Japanese fine ceramics production amount is increasing and will reach 4 trillion JPY (approximately 27.5 billion USD) within a few years. On the other hand, climate change is an important issue that the international community must work together to address immediately. In line with the Sustainable Development Goals (SDGs) adopted by the United Nations and the Paris Agreement adopted at COP21, Japan Fine Ceramics Association (JFCA) is committed to promoting carbon neutrality in the fine ceramics industry. We have established "JFCA Carbon Neutral Vision" and declared our intention. To promote the realization of a sustainable society, we will work together with our member companies to reduce greenhouse gas emissions and provide new values contributing to the realization of a carbon neutral society the unique features and functions of fine ceramics can lead. JFCA Carbon Neutral Vision are from two perspectives; Reduction of greenhouse gas emissions during the production process, and Contribution to carbon neutrality achieved by new products and new services. JFCA will promote carbon neutral initiatives in collaboration with member companies, government, academia, and other industrial sectors.

#### 8:50 AM

#### (ICACC-FS7010-2025) Concepts for Thermal Energy Storage Using Metal Oxide Redox Primary Heat Exchangers

C. Lewinsohn<sup>\*1</sup>

1. Rational Solutions, LLC, USA

Thermal Energy Storage is a method of temporally shifting use of renewable energy sources, i.e. wind and solar, from periods of excess production to periods of excess demand. Thermal energy can be produced by solar iradiation, nuclear heat, combustion, joule heating, or chemical reaction. Thermal energy can be converted to electrical power, or work, through various cycles such as Rankine and Brayton cycles. Ceramics offer significant potential in use as thermal energy storage due to their high heat capacity and relatively low cost. A conceptual component for reversibly capturing and releasing thermal energy with a primary heat exchanger incorporating a metal-oxide material with significant heat of reaction during reduction and oxidation cycles will be described. Opportunities and challenges associated with using metal-oxide redox primary heat exchangers will be presented.

#### 9:10 AM

### (ICACC-FS7011-2025) Freeze-casting of polysiloxane-derived ceramics for $CO_2$ utilization

K. Rauchenwald\*1; P. Miksovsky2; K. Bica-Schröder2; T. Edtmaier1;

- R. Shirvani<sup>3</sup>; M. Steiger<sup>3</sup>; K. Föttinger<sup>4</sup>; T. Konegger<sup>1</sup>
- 1. Technische Universitat Wien, Institute of Chemical Technologies and Analytics, Austria
- 2. Technische Universitat Wien, Institute of Applied Synthetic Chemistry, Austria
- 3. Technische Universitat Wien, Institute of Chemical, Environmental and Bioscience Engineering, Austria
- 4. Technische Universitat Wien, Institute of Materials Chemistry, Austria

Conversion of CO<sub>2</sub> to fuels via gas phase catalysis or high-value products via heterogeneous organic synthesis or biocatalysis will be crucial to reduce industrial carbon footprints. In all cases, suitable carriers are required for high catalytic performance. A versatile approach is presented combining freeze-casting with polymer-derived ceramics, showcased for various CO<sub>2</sub> utilization technologies. In a first example, microreactors for CO<sub>2</sub> methanation are developed: By depositing 25wt.% Ni on dendritically structured SiOC, CO<sub>2</sub> conversions up to 58% can be reached at 400°C, demonstrating the material's suitability at elevated temperatures. The second example involves SiOC-supported ionic liquids for selective production of limonene carbonate by cycloaddition of supercritical CO<sub>2</sub> to bio-based epoxides, where SiOC outperforms silica-60. Tunable water affinity of SiOC by interrupting the pyrolysis promotes catalytic performance. In a third example, freeze-cast SiOC is evaluated for supporting biosynthetic processes. The macropores are accessible for microorganisms like K. phaffii to form biofilms, providing a promising starting point aiming for heterogeneous whole cell catalysis. Results on freeze-cast SiOCs for a variety of CO2 conversion processes demonstrate that linking in-depth knowledge on chemistry, structuring and conversion of preceramic polymers can create a versatile materials platform for CO<sub>2</sub> utilization.

#### 9:30 AM

### (ICACC-FS7012-2025) Application of $\rm CO_2$ -free Alternatives for Sustainable Glass Production

M. Al Hamdan\*1; S. Wiltzsch2; M. Wahab1; F. Gygas2

- 1. Technische Universitat Bergakademie Freiberg, Institute of Glass Science and Technology, Germany
- 2. Technische Hochschule Nurnberg, Fakultät Werkstofftechnik, Germany

The glass industry is a major contributor to global  $CO_2$  emissions through the use of carbon-based raw materials such as limestone  $(CaCO_3)$  and soda  $(Na_2CO_3)$ . Our current research aims to evaluate the use of available CO<sub>2</sub>-free alternatives, specifically NaOH and CaO, to replace traditional raw materials in glass production. Our research includes selection and testing of these materials to ensure they meet industry standards for glass quality and performance. As part of this research, we are also evaluating the technological viability of these alternative raw materials through laboratory testing and aim to lower the barriers to their use in the glass industry. A major objective of our research is to study the practical applications, problems in industrial glass production. In particular, we consider the Influence of NaOH and CaO, either individually or together, with cullet. From our experiments, we were also able to evaluate the melting behaviour of NaOH and/or CaO-containing batches in terms of glass-forming reactions, quartz solution, and properties of the resulting glass, including glass bubble count, OH content. Some important results of our work will be shown in this presentation.

### <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

# **S1-** Ceramic Matrix Composites (CMCs) Mechanical Behavior and In-situ Characterization

Room: Coquina E Session Chairs: Stefan Schaf

Session Chairs: Stefan Schafföner, University of Bayreuth; Aly Badran, GE Research

#### 8:30 AM

#### (ICACC-S1-048-2025) Proposition of a complete methodology to determine the onset of inter-yarn debonding in a 3D woven ceramic matrix composite material (Invited)

F. Laurin\*1; A. Mavel1; B. Lacombe2; M. Gimat2

- 1. ONERA, DMAS, France
- 2. SAFRAN Ceramics, France

Ceramic matrix composites are interesting candidates for the manufacture of hot parts for civil or military aircraft engines operating at high temperatures. In addition, the use of a 3D woven architecture allows the different layers to be bonded together and limits the propagation of large delamination cracks. However, predicting the onset of inter-yarn debonding for different local 3D stress states remains a scientific challenge for the design of composite parts. Therefore, the objective of this study is to propose a complete methodology to determine the onset of inter-yarn debonding for 3D ceramic woven materials. A 4-point bending device has been developed for CMC L-angles to identify the out-of-plane tensile strength associated with the onset of inter-yarn debonding. In addition, another original experimental setup was developed to apply either unfolding or folding loads to L-angle specimens to validate a stress-based 3D failure criterion for combined out-of-plane tension/compression and shear stresses. Particular attention was paid to the design of the jaws to achieve failure only in the region of interest, especially for folding loads. An original method based on finite element analysis has been proposed to use the data obtained from this type of structural tests to validate a stress-based 3D failure criterion.

#### 9:00 AM

#### (ICACC-S1-049-2025) In-situ CT-Scan Observation and Modeling of Damage in Oxide/Oxide Composites

T. Drouin\*1; F. Laurin2; F. Guillet1; G. Couégnat3

- 1. Commissariat a l'energie atomique et aux energies alternatives Direction des applications militaires Le Ripault, France
- 2. Office National d'Etudes et de Recherches Aerospatiales, France
- 3. Laboratoire des Composites Thermostructuraux, France

Oxide/Oxide composites (Ox/Ox) offer an advantageous balance of mechanical properties and cost for moderate thermo-mechanical applications. However, their tendency to experience damage at low load levels results in highly non-linear behavior, which requires precise understanding of their mechanical behavior and damage mechanisms at the ply level. Our study aims to elucidate the damage scenario in Ox/Ox through in-situ micro-computed tomography (µCT) tests. to achieve this, tensile/compression, bending using compression with pivot device, and tensile/torsion tests are conducted on a quasi-isotropic 2D woven Ox/Ox laminate both at room temperature and up to 800°C. These tests are analyzed using mechanically-regularized global Digital Volume Correlation (DVC) to access global and local displacements and strains, towards a DVC-based identification of constitutive parameters for a damage model at the ply level. Our methodology integrates these tests with nonlinear finite-element simulations in a test/simulation dialogue approach. We present comparisons between numerical results and experimental observations, discuss the validity of DVC for local strain measurement, and address damage scenarios, particularly delamination.

#### 9:20 AM

# (ICACC-S1-050-2025) Effects of interfacial boron nitride layers on the mechanical behaviors of SiC/BN/SiC mini-composite reinforced by Tyranno Fiber<sup>®</sup>

M. Sumino\*1; T. Matsunaga<sup>1</sup>

1. UBE Corporation, Specialty Products Division, Japan

The interfacial layer generally serves to transfer the load from the matrix to the fibers and to protect the fibers from being notched by the propagating cracks. Thus, the interfacial layer plays a key role in the mechanical behaviors of SiC/BN/SiC composites. Nevertheless, there were a few literatures of SiC/BN/SiC composites reinforced by the polycrystallized Tyranno SA Fibers. In this study, a mini-composite fabrication facility was designed and a basic study of fundamental mini-composites was carried out. As a result, it was confirmed that sound mechanical behaviour can be observed as CMC if an appropriate interface coating is applied. In addition, these mechanical behaviours are discussed from the interface point of view using push-out and push-in tests.

#### 9:40 AM

#### (ICACC-S1-051-2025) Effect of Ceramic Inclusions on Deformation Behavior and Energy Absorption Capacity of Composite Metal Foams Used for High Impact Load Mitigation

F. Z. Weldemariam\*1

1. Indian Institute of Technology Delhi, Mechanical Engineering, India

This study investigated the impact of SiC particles on the matrix and reinforcement of a composite metal foam to analyze the strength-to-weight ratio and energy absorption capacity. Al-9Si-4Cu alloy reinforced with the SiC at various weight ratios was utilized as a hard matrix (HM), and the alloy was employed as a soft matrix (SM). The hard reinforcements (HR) were hollow spheres (HS) with diameters ranging from 3 to 6 mm and shell thickness of 0.5 mm fabricated from SiC and stainless steel (SS) using powder metallurgy technique. The soft reinforcement (SR) was the SSHS, which was the same size as the HR and was reinforced to the HM at different volume ratios to create porosity. Besides the high strength-to-ratio obtained in both manufactured foam samples, the SM reinforced with the HR

resulted in a higher energy absorption capacity of 88 MJ/m<sup>3</sup> with compressive strength (CS) 420 MPa and 36% strain, while the HM reinforced with the SR was with 80 MJ/m<sup>3</sup>, CS of 382 MPa and 28% strain. It was observed that the HR embedded in the SM enhanced CS and improved the deformation pattern of the foam, optimizing the primary characteristics of metal foam, such as porosity, density, strain, CS and strength-to-weight ratio. In contrast, earlier crack initiation and fracture resulted in lower strength, strain and damping properties in the HR foam.

#### 10:20 AM

# (ICACC-S1-052-2025) Mechanical testing of ceramic matrix composites: Size effect of strength and the role of sample alignment (Invited)

- S. Flauder<sup>1</sup>; N. Langhof<sup>1</sup>; S. Schafföner<sup>\*1</sup>
- 1. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

Ceramic matrix composites (CMC) overcome the brittleness of monolithic ceramics and combine a damage tolerant material behavior with high thermo-mechanical resistance. This study discusses the strength as a function of the tested sample size of carbon fiber-reinforced silicon carbide composites (C/C-SiC). Consequently, different sample sizes and geometries were tested under bending and tensile loads. The C/C-SiC samples were fabricated by the liquid silicon infiltration (LSI) process with fabric reinforcement. The statistical behavior and the influence of the sample size and testing method on the strength of C/C-SiC was evaluated. A decrease of the bending strength with increased tested specimen size was determined. It was found that the Weibull modulus was not a material constant and the application of Weibull statistics could not properly describe the size effect of strength. Furthermore, a test device for self-alignment and centering of tensile samples was developed to minimize errors in tensile testing. The proper sample alignment was tested prior tensile testing by preloading and evaluation of two alignment criteria determined by optical strain measurement. This method allows to predict valid and invalid failure and increases the validity of testing. C/C-SiC was found to be somewhat less sensitive to misalignment than monolithic ceramics.

#### 10:50 AM

#### (ICACC-S1-053-2025) In-situ observation, characterization and control of the crack formation during manufacturing of non-oxide Ceramic Matrix Composites (CMC) (Invited)

N. Langhof\*1; F. Wich1; M. Moos1; W. Krenkel1; S. Schafföner2

- 1. University of Bayreuth, Ceramic Materials Engineering, Germany
- 2. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

Ceramic matrix composites (CMC) like C/C-SiC are often manufactured including a pyrolysis step which inevitably leads to characteristic shrinkage induced cracks. This work aims at characterizing the formation of pyrolysis crack patterns for carbon fiber reinforced phenolic resins used to produce C/C, C/C-SiC and other (UHT)-CMC materials. Mass loss, expansion and shrinkage of various composites were measured using thermogravimetry and dilatometry. Crack initiation and growth were observed in-situ of a pyrolysis process with µ-scale resolution by using advanced light-microscopic techniques. Fracture toughness of composites was measured along the pyrolysis and the crack patterns were characterized by the measurement of crack width and distance between cracks. µCT was performed on to investigate the spatial orientation of cracks. Interconnections between fiber architecture, fiber volume content, fiber-matrix bonding, crack pattern morphology as well as crack initiation have been found and correlated with the flexural and tensile strength of the derived C/C and C/C-SiC materials. For example, the tensile strengths increase at 90 % from 35 to 55 fiber vol.%. Finally, statistical functions describing the crack patterns were developed enabling accurate modelling of CMC.

#### 11:20 AM

#### (ICACC-S1-054-2025) Mechanical behaviour of towpreg-based oxide-oxide ceramic matrix composites visualised by in-situ X-ray computed microtomography (Invited)

- T. Nelson\*1; J. Binner<sup>2</sup>; I. M. Edmonds<sup>3</sup>
- 1. University of Birmingham, School of Metallurgy and Materials, United Kingdom
- 2. University of Birmingham, Ceramic Science & Engineering, United Kingdom
- 3. Rolls-Royce plc, United Kingdom

Traditional oxide-oxide ceramic matrix composite (ox-ox CMC) manufacture can involve manual slurry infiltration into precut fabric sheets, followed by hand lay-up onto a mould of the required shape. Automated fibre placement (AFP), currently used for production of polymer matrix composites, promises a capability for highly reproducible laminate production of complex geometries using unidirectional towpreg feedstock. However, there is little information regarding the fracture mechanisms and mechanical behaviour of these oxide composites in the open literature. Crack mechanisms during loading have been characterised using in-situ three-point bending tests with simultaneous synchrotron X-ray computed microtomography at ambient conditions and elevated temperature. Image analysis of ex-situ short-beam-shear tests with similar samples identified a cracking mechanism unique to unidirectionally reinforced ox-ox CMCs, and the correlation between inter-ply matrix thickness and interlaminar shear strength.

#### 11:50 AM

#### (ICACC-S1-055-2025) Observation of Temporal Cracking Behavior in SiC/BN/SiC Ceramic Matrix Composites via Acoustic Emission and Digital Image Correlation

H. Gross\*1; T. Jackson2; J. Pierce2; N. Klingbeil1; K. Detwiler3

- 1. Wright State University, Mechanical and Materials Engineering, USA
- 2. University of Dayton Research Institute, USA
- 3. Air Force Research Lab, Materials & Manufacturing Directorate, USA

SiC/BN/SiC ceramic matrix composites (CMCs) are being used in extreme environments, such as the hot sections of turbine engines due to their high heat resistance, relatively low densities, and high fracture toughness. The idea of "load relaxation" while holding a sample in displacement control is noted in literature, but not well explored. Macroscale dogbone samples were tensile-tested with a ramped loading schedule, where samples were loaded to a given percentage of ultimate stress and then held at a fixed displacement for up to an hour. Acoustic emission (AE) was used to monitor events occurring during the test. Digital image correlation (DIC) was used on some samples to be able to visualize strain behavior occurring during displacement holds. Metrics such as normalized stress drop, stress drop rate and AE event rate were explored. Initial results demonstrating use of the techniques with measurements will be presented.

### S3 22th Intl Symp on Solid Oxide Cells Materials Science & Technology

#### S3- Interconnects and coatings

Room: Ballroom 4

Session Chair: Sebastian Molin, Gdansk University of Technology

#### 8:30 AM

#### (ICACC-S3-044-2025) Low-cost Cobalt-free Approach for the Interconnects in Solid Oxide Cells Stacks (Invited)

- Y. Naumovich\*1; L. Ajdys1; M. Lazor1; A. Zurawska1; A. Niemczyk1
- 1. Institute of Power Engineering National Research Institute, Department of Hight Temperature Electrochemical Processes, Poland

H<sub>2</sub>-based energy production and storage are expected to play a sufficient role in a transformation to low-carbon technologies. While state-of-the-art for related technologies, based on solid oxide cells corresponds to the top of the TRL scale, production costs still put serious pressure on the possibility of deployment. Institute of Power Engineering-National Research Institute (IPE-NRI) is developing stacks, both SOFC and SOE, using patented design. Among other features, the IPE-NRI stack is based on the corrugated interconnects, with a thickness of 0.2-0.3 mm (~2 mm per SRU). Such interconnect has to have substantial protection on the air side from oxidation and Cr evaporation. IEN-PIB developed a procedure, based on electrophoretic deposition and reductive sintering, which allows an application 10-20 µm layer of (Mn,Co)<sub>3</sub>O<sub>4</sub> or (Mn,Cu,Fe)<sub>3</sub>O<sub>4</sub> spinels on the preoxidated surface of the steels, like Crofer 22 APU or AISI 430. Protective layers demonstrated sufficient conductivity and negligible diffusivity of the Cr. The migration from Co-based Mn<sub>1.5</sub>Co<sub>1.5</sub>O<sub>4</sub> to (Mn,Cu,Fe)<sub>3</sub>O<sub>4</sub> solid solutions allowed not only exclude scarce cobalt, but also led to the some enhancements in ASR. Current IPE-NRI stacks have an Ohmic part of the ASR ~0.20  $\Omega$  cm<sup>2</sup> below 700 °C with a typical depth of the Cr diffusion in the spinel layer below 7 µm after 1000 h. Studies are supported by UMO-2023/49/B/ST8/03265, NCN, Poland.

#### 9:00 AM

#### (ICACC-S3-045-2025) Evaluation of Electrical Conductivity in Oxide Scale of Ferritic Heat-Resistant Alloy for Solid Oxide Cell Interconnects

T. Mitani\*1; R. A. Budiman2; M. Yamaguchi1; K. Yashiro1; T. Kawada2

- 1. Shimane Daigaku, Faculty of materials for energy, Japan
- 2. Tohoku Daigaku, Graduate School of Environmental Studies, Japan

Interconnect is a crucial component in solid oxide cell for stacking multiple cells to make a cell stack. Typically, Ferritic alloys are used for these interconnects. During operation, these alloys are oxidized under high-temperature redox conditions, forming a resistive oxide layer that may degrade interconnect performance over time. Despite its importance, the relationship between the conductivity of this oxide layer and the environmental factor remains poorly understood. Therefore, in this study, Crofer 22 H was pre-oxidized in air at 1273 K for 50 hours, resulting in the formation of a 10 µm-thick oxide layer. Following this, electrical conductivity measurements were performed controlling the oxygen partial pressure and temperature while measuring the resistance of the oxide layer. The results revealed that the oxide layer exhibited semiconductor-like behavior, with resistance decreasing at high temperature. Notably, no significant changes in resistance were observed as a function of oxygen partial pressure, suggesting minimal influence of oxygen pressure on oxide layer conductivity. In future work, we will investigate how oxygen partial pressure in a reducing atmosphere affects the resistance of the oxide layer, and clarify the relationship between oxygen partial pressure, ionic/electrical defect structure, and conductivity under redox conditions.

#### 9:20 AM

#### (ICACC-S3-046-2025) Enhancing protective performance of MnCo2O4 spinel coating on solid oxide cells interconnects through partial substitution of Mn, Co with Mg, Al, Y

J. Ignaczak\*1; P. Jasinski1; S. Molin2

- 1. Politechnika Gdanska, Department of Functional Materials Engineering, Poland
- 2. Gdansk University of Technology, Department of Functional Materials Engineering, Poland

In Solid Oxide Cells (SOCs) stacks, Cr2O3-forming ferritic stainless steel (FSS) is considered the most suitable material for interconnects due to its thermal expansion coefficient compatibility with other components, high electrical conductivity, and low cost. However, Cr-poisoning caused by Cr2O3 may degrade the SOFC cathode. Protective coatings are employed to mitigate this detrimental effect. The current state-of-the-art protective coating material is the (Mn,Co)3O4 spinel (MCO), which demonstrates high electronic conductivity and low Cr diffusion. Nevertheless, due to the need for further technological improvements and extending the lifespan of fuel cell stacks, alternative materials that can offer enhanced protective properties are being sought. Crucial physico-chemical properties can be optimized by substituting manganese and cobalt with other elements. We have decided to study the modification of MnCo2O4 spinel by the addition of either Mg, Al, Y. We have partially substituted Mn and Co, which results in changes in oxidation kinetics, and has a compatible TEC and possibly retain low Cr evaporation. We will present results concerning materials synthesis, electrophoretic deposition on steels, and subsequent oxidation exposures. Extensive post-mortem characterization of alloys by SEM/TEM microscopy will be also presented.

#### 9:40 AM

#### (ICACC-S3-047-2025) Enhanced Densification of GDC Barrier Layers in Solid Oxide Cells via Physical Vapor Deposition Process

S. Ryu<sup>\*1</sup>; E. Polikarpov<sup>1</sup>; T. Liu<sup>1</sup>; T. Kaspar<sup>1</sup>; L. M. Seymour<sup>1</sup>; S. B. Karki<sup>1</sup>; R. Springer<sup>1</sup>; D. Kim<sup>1</sup>; O. A. Marina<sup>1</sup>

1. Pacific Northwest National Laboratory, USA

Solid oxide cells (SOCs) are advancing in sustainable hydrogen production and energy storage due to their efficiency and high-temperature operation. A critical component is the barrier layer between the yttria-stabilized zirconia (YSZ) electrolyte and La and/or Sr-containing oxygen electrode, preventing chemical interactions at high sintering temperatures. Samaria- or gadoliniadoped ceria (GDC) effectively mitigates cation interdiffusion from the oxygen electrode into the YSZ. Traditionally, GDC barrier is applied using screen printing followed by high-temperature sintering (1250-1350°C), which can be inadequate for full densification and may cause undesirable reactions between Ce, Sm, Gd, and Zr. This study introduces alternative physical vapor deposition techniques, including pulsed laser deposition (PLD), e-beam deposition, and sputtering, for fabricating GDC layer at temperatures below 500°C. These methods produce a thinner, denser GDC layer without high-temperature firing, avoiding interdiffusion issues and maintaining high oxygen ion conductivity. The performance of electrode-supported cells with these thin GDC barriers was tested in electrolysis mode for up to 3,000 hours, followed by SEM/EDS and TEM characterization. These low-temperature deposition techniques offer a cost-effective solution, enhancing SOC performance with reduced energy and time requirements.

#### **S3-** Novel processing

Room: Ballroom 4

Session Chair: Harry Abernathy, National Energy Technology Laboratory

#### 10:20 AM

### (ICACC-S3-048-2025) 3D printing of Monolithic Solid Oxide Cells (Invited)

- V. Esposito\*1; Z. Zhou1; V. K. Nadimpalli2
- 1. Danmarks Tekniske Universitet, Department of Energy Conversion and Storage, Denmark
- 2. Danmarks Tekniske Universitet, Department of Civil and Mechanical Engineering, Denmark

The Solid Oxide Cell (SOC) exemplifies highly efficient electrochemical energy conversion. Nevertheless, traditional manufacturing methods have limited the design of SOC stacks, which have predominantly remained in planar forms with minimal innovation over recent decades. The conventional SOC stack also involves complicated assembly processes, resulting in bulkier designs with greater weight and limiting its flexibility for applications such as transportation and aviation, where its efficiency would be highly advantageous. This work moves beyond the two-dimensional approach to embrace a true 3D structure. We use advanced additive manufacturing technologies to create a monolithic SOC featuring geometrically intricate geometries. This structure optimizes spatial usage, enhances volumeand mass-specific metrics, simplifies manufacturing, and ensures electro-chemo-mechanical stability.

#### 10:50 AM

### (ICACC-S3-049-2025) New horizons in shaping and sintering of solid oxide cells (Invited)

A. Sabato<sup>\*1</sup>; S. Marquez<sup>1</sup>; A. Martos<sup>1</sup>; A. Maria Asensio<sup>1</sup>; N. Kostretsova<sup>1</sup>; I. Babeli<sup>1</sup>; M. Torrell<sup>1</sup>; A. Tarancón<sup>2</sup>

- 1. IREC, Nanoionics and Fuel Cells, Spain
- 2. IREC / ICREA, Spain

Nowadays conventional Solid Oxide Cells (SOC) are mainly based on multilayered functional ceramic materials produced by expensive and long manufacturing processes. Here we present recent results concerning two main manufacturing processes for SOC: 3D printing and Ultrafast High temperature Sintering (UHS). In the first case, 3D printing of Yttria Stabilized Zirconia (YSZ) electrolytes is explored to enhance the performances at cell and stack level, unlocked by complex architectures: corrugated membranes, embedded functionalities, monolithic concepts. The shapes are tailored in order to: i) increase the active area (up to 1.6 times), ii) improve mechanical resistance of the cells, iii) increase the power densities at stack level (2x state of the art), iv) operate at high pressure without the use of a pressure vessel. On the other hand, the implementation of UHS for debinding and sintering thermal treatments, which are especially long in the case of 3D printed components, is investigated. Here we report a fully working cell based on 3D printed 8YSZ electrolytes debinded and sintered by UHS. The electrolytes were fully sintered in <15 min., in coparison with conventional debinding/sintering process, which typically takes around 100 hours. The electrolytes exhibited conductivityof 0.050 S/cm at 900 °C and high densification (>95%). While the full cell based on these electrolytes reached 0.5 mA/cm<sup>2</sup> at 0.7 V at 850°C.

#### 11:20 AM

#### (ICACC-S3-050-2025) Impact of Rapid Sintering Methods on Microstructure and Electrochemical Performance of Solid Oxide Fuel Cells (SOFCs) Materials

J. A. Mena\*<sup>1</sup>; E. M. Sabolsky<sup>1</sup>; K. Sabolsky<sup>1</sup>; S. Waseem<sup>1</sup>; T. Yumak<sup>1</sup>; M. Cavalier<sup>1</sup>; T. Musho<sup>1</sup>

1. West Virginia University, Mechanical, Materials and Aerospace Engineering, USA

Solid-oxide fuel cells (SOFCs) are energy conversion devices capable of producing electrical energy efficiently using hydrogen and various hydrocarbon fuels. To achieve the required porous electrode and dense electrolyte microstructures, these layered ceramics must be thermally processed to temperatures ranging from 1000-1450°C in sequential cycles using electrical resistive kilns. The total processing time, energy consumption, and cost can be extensive and are major barriers for mass production and application of SOEC technology. This work investigated fast heating methods to remove organic binders and densify the active SOFC layers, reducing processing time and energy consumption. The first method evaluated was microwave (MW) heating, achieving accelerated rates through local MW suscepting heat sources near the targeted ceramic. The second method was ultra-fast high-temperature sintering (UHS) using rapid Joule heating of carbon felt surrounding the ceramic sample. Heating rates of >1000 °C/min have been demonstrated for UHS. This work will review both heating technologies, focusing on the effect of input power, heating rate, and processing atmosphere on the final microstructure and electrochemical properties of the electrode and electrolyte materials.

#### 11:40 AM

#### (ICACC-S3-051-2025) Managing Residual Stresses in Co-Sintered Multi-Layer Electrolytes for Solid Oxide Cells

D. J. Ramler<sup>\*1</sup>; Y. Sohn<sup>1</sup>; C. Lenser<sup>1</sup>; O. Guillon<sup>1</sup>; N. H. Menzler<sup>1</sup>

1. Forschungszentrum Julich GmbH, Institute of Energy Materials and Devices IMD-2, Germany

Gadolinium-doped ceria (GDC) is a promising alternative to 8YSZ in solid oxide cells, offering advantages as a fuel electrode. However, interdiffusion between YSZ electrolytes and Ni-GDC electrodes limits its potential. Utilizing a GDC electrolyte in combination with a Ni-GDC electrode is expected to mitigate interdiffusion and enhance performance. In this study, a 3-layer electrolyte was prepared via screen printing. However, co-sintering of half-cells poses challenges due to mismatches in sintering behavior and thermal expansion, leading to stresses that cause cracking or spalling, reducing structural and operational stability of the cell. To address this, the sintering behavior of the half-cell was systematically investigated by thermooptical dilatometry. The NiO-YSZ substrate shrinkage during co-sintering was found to be crucial in achieving dense electrolytes. By leveraging this shrinkage, the co-sintering temperature was reduced to lower residual stresses while maintaining densification. The effect of different substrate pre-sintering temperatures, combined with various co-sintering temperatures, were evaluated in relation to electrolyte microstructure and residual stresses. Additional doping of GDC was intended to enhance sintering activity at lower temperatures. Microstructures were examined via scanning electron microscopy. Residual stresses were analyzed by X-ray diffraction.

### <u>S5 Next-Generation Bioceramics and</u> <u>Biocomposites</u>

### S5- Porous, nanostructured and hybrid bioceramics

### and composites I

Room: Ponce de Leon Session Chair: Thomas Webster, Brown University

#### 8:50 AM

#### (ICACC-S5-012-2025) Additive manufacturing of porous melilite bioceramics from engineered emulsions based on silicone polymers (Invited)

V. Diamanti<sup>1</sup>; A. Zilio<sup>1</sup>; H. Elsayed<sup>1</sup>; E. Bernardo<sup>\*1</sup>

1. University of Padova, Department of Industrial Engineering, Italy

Melilite bioceramics (Ca2XSi2O7, X=Mg<sup>2+</sup>/Zn<sup>2+</sup>) are attractive for the excellent compromise between biological response and mechanical properties. The additive manufacturing of these systems is supported by novel formulations, designed to improve the homogeneity of oxide additives, in a silica-yielding matrix, and the phase purity after firing at 1000-1200 °C, in air. A uniform SiO2/CaO distribution is offered by emulsification: droplets of molten hydrated calcium nitrate or of concentrated calcium nitrate solutions, in water, are dispersed in blends of H44 commercial polysiloxane and photocurable acrylate resin, with the help of surfactants. Vat photopolymerization is adopted for the production of gyroid scaffolds, with enhanced strength-to-density. Direct ink writing (DIW) is employed for water-containing blends, realizing scaffolds with 'spongy' struts, due to enhanced gas evolution, by water evaporation during heat treatment. Photopolymerization, in DIW, is still useful, to consolidate reticulated scaffolds soon after extrusion. The chemistry of melilites is easily tuned, according to the introduction of magnesium nitrate hydrate and/or ZnO nanoparticles as additional components of the blends. Water-containing blends, for DIW, offer a further tuning possibility: B2O3, dissolved in water solution, in fact, yields even more complex solid solutions (Ca<sub>2</sub>Zn<sub>1-y</sub>B<sub>2y</sub>Si<sub>2-y</sub>O<sub>7</sub>).

#### 9:20 AM

### (ICACC-S5-013-2025) Novel Geopolymer-based Scaffolds for Bone Tissue Regenerative Engineering

G. Dal Poggetto\*1; A. Akono1

1. North Carolina State University, USA

Musculoskeletal diseases affect 1 in 2 adults in the United States and result in an annual loss of 5% of the Nation Gross Domestic Product in both direct and indirect costs. An important subset is musculoskeletal trauma that creates a major challenge for restoring full function and appearance. Due to a reliance on titanium-based, polymer-based, and ceramic-based orthopaedic implants, standard tissue engineering methods often result in complications such as infection or bone degeneration due to a mismatch in both geometry and physical properties between the implant and the surrounding natural bone structure. Therefore, there is a gap of knowledge in novel functionally-graded materials for tissue regenerative engineering that are patient-specific, can mitigate bone loss, and promote bone proliferation around the host bone structure. We focus on a new class of materials, geopolymers that are X-ray and alkali-bonded amorphous inorganic polymers, and investigate their biocompatibility. We show that geopolymers are bioinductive. We show that geopolymers are biodegradable using accelerated biodegradation tests. We show that geopolymers are biocompatible using mouse fibroblast cells. Finally, the mechanical properties of geopolymers are shown to be close to that of cortical bone. These results suggest that geopolymer materials can be used to replicate bone tissue behavior and induce bone regeneration.

#### 9:40 AM

# (ICACC-S5-014-2025) Polysilazane-based antimicrobial composite coating incorporating AgNPs-decorated ${\rm SiO}_2$ nanospheres

F. Gattucci\*1; M. Miola1; C. Balagna1

1. Politecnico di Torino, DISAT, Italy

In response to global concerns about the spread of superbugs and viruses, innovative antimicrobial coatings are being developed as potential solutions. One such approach involves synthesizing a composite coating composed of a polymeric ceramic precursor and silica nanospheres decorated with silver nanoparticles (AgNPsnSiO<sub>2</sub>). The synthesis process consists of two main phases: initially, AgNPs-nSiO<sub>2</sub> is produced through a sol-gel process. Subsequently, these AgNP-decorated nSiO<sub>2</sub> nanospheres are integrated into a polymeric matrix to introduce silver as an antibacterial agent. The resulting composite coating is then applied to soda-lime glass substrates using the spin-coating technique. Morphological, compositional, and structural analyses confirmed the successful synthesis of AgNPs on nSiO<sub>2</sub> and allowed for the quantification of their concentration. The antibacterial properties of the AgNPs-nSiO<sub>2</sub> were demonstrated through inhibition tests against Staphylococcus epidermidis. The dispersion of AgNPs-nSiO<sub>2</sub> within a polysilazane ceramic precursor (commercially known as Durazane 1800) was successfully achieved, demonstrating the suitability of nSiO<sub>2</sub> as silver carrier in the polysilazane matrix. The composite coating that was then characterized by its morphology, composition, structure, and antibacterial efficacy.

# S5- Porous, nanostructured and hybrid bioceramics and composites II

Room: Ponce de Leon Session Chair: Francesca Tallia, Imperial College London

#### 10:20 AM

## (ICACC-S5-015-2025) Exploring Biopolymers as Capping Agents for Lanthanide-Based Nanoparticles (Invited)

E. Hemmer<sup> $\star 1$ </sup>

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

The remarkable optomagnetic properties of the lanthanides (Ln) make Ln-based materials ideal for biomedical applications, including diagnostic and therapeutic approaches. Sodium lanthanide fluorides (NaLnF<sub>4</sub>) are our favorite materials, and we developed a microwave-assisted synthetic approach allowing crystalline phase, size, and architectural control in the sub 20 nm realm. Such control is crucial for the understanding of fundamental structure-property relationships and to optimize their optical and magnetic properties. For instance, NaGdF<sub>4</sub> and NaDyF<sub>4</sub> nanoparticles (NPs) are gaining interest as alternative MRI contrast agents, while doping with Ln34 ions adds optical properties. For biomedical applications, dispersibility, chemical and optical stability of the Ln-NPs in aqueous media are key in addition to lack of toxicity, which can be achieved through surface modification. The use of non-toxic biopolymers is of particular interest. For instance, the encapsulation of NaLnF<sub>4</sub> NPs into phytoglycogen-based sub-micron vehicles shows potential for multiplexed imaging. Gum Arabic stands out as capping agent that leads to excellent dispersion and chemical stability as well as minimal toxicity as demonstrated by in vitro and in vivo assays. This presentation will shine a light on NaLnF<sub>4</sub> NPs modified with biopolymers and the suitability of hyperspectral imaging to study their nano-bio interactions.

#### 10:50 AM

### (ICACC-S5-016-2025) Self-assembling, antibacterial hybrid calcium phosphate-based composites

J. P. Czechowska\*1; P. Pantak1; A. Belcarz2; K. Kowalska1; A. Zima1

- 1. Akademia Gorniczo-Hutnicza im Stanisława Staszica w Krakowie, Department of Ceramics and Refractories, Poland
- 2. Uniwersytet Medyczny w Lublinie, Chair and Department of Biochemistry and Biotechnology, Poland

Self-assembling materials have emerged as a groundbreaking solution in tissue engineering, offering innovative strategies to combat bacterial infections. Special attention is given to the hybrid granules. Our research focuses on self-assembling, antibacterial hybrid granules composed of hydroxyapatite, methylcellulose, and/or chitosan. These granules were produced via modified wet-chemical method and enriched with ions or nanoparticles (Cu<sup>2+</sup>, CuONPs). The chemical and phase compositions (XRF, XRD, FT-IR, Raman), compressive strength, thermal properties and microstructure were analyzed. Additionally, their bioactivity in simulated body fluid and antibacterial effectiveness against E. coli and S. aureus were tested. The obtained results are particularly promising as hybrids showed high mechanical strength, biocompatibility and antibacterial properties. Granules may be applied independently or as components of innovative biocomposites. Supported by the programme "Excellence initiative - research university" for the AGH University of Science and Technology and the AGH Faculty of Materials Science and Ceramics (No. 16.16.160.557). This research was funded in whole or in part by National Science Centre, Poland (Project MINIATURA7 No. 2023/07/X/ST11/00705). For the purpose of Open Access, the author has applied a CC-BY public copyright licence to any Author Accepted Manuscript (AAM) version arising from this submission.

### <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

#### **S6- Solid Electrolytes for Batteries II**

Room: Coquina B

Session Chairs: Palani Balaya, National University of Singapore; Donald Dornbusch, NASA Glenn Research Center

#### 8:30 AM

(ICACC-S6-037-2025) Ti-Doped Na3Zr2Si2PO12 Ceramic Electrolytes for Seawater Batteries and Insights into Failure Mechanisms during Na Plating and Stripping (Invited) M. Li<sup>\*1</sup>

1. Oak Ridge National Laboratory, USA

Ceramic solid-state electrolytes are crucial for advancing long duration energy storage technologies, offering enhanced safety and energy density. This study focuses on Ti-doped Na3Zr2Si2PO12 (Ti-NZSP), a NASICON-type ceramic electrolyte, and its performance in seawater batteries. Ti-NZSP shows improved ionic conductivity, critical current density, and structural stability compared to undoped Na3Zr2Si2PO12, making it a promising candidate for solid-state applications. Operando synchrotron X-ray tomography revealed that the primary failure mechanism in Ti-NZSP during sodium plating and stripping is pore filling, leading to dendrite formation and short-circuiting. However, the densely packed microstructure and uniformly distributed pores in Ti-NZSP significantly delay failure, enhancing cycling stability. In seawater batteries, Ti-NZSP demonstrated superior performance in Na | SE | hard carbon cells, achieving higher ionic conductivity and stable cycling under various conditions. The doping enhances the surface stability and reduces porosity, making Ti-NZSP effective in both aqueous and non-aqueous environments. This study highlights

the potential of Ti-doped Na3Zr2Si2PO12 ceramic electrolytes to improve the performance and safety of sodium-ion and seawater batteries by addressing critical failure mechanisms.

#### 9:00 AM

#### (ICACC-S6-038-2025) Nanoscale ion transport enhances conductivity in solid polymer-ceramic lithium electrolytes (Invited)

J. Li<sup>\*1</sup>; G. Polizos<sup>2</sup>

- 1. Argonne National Laboratory, Applied Materials Division, USA
- 2. Oak Ridge National Laboratory, USA

Solid-state batteris (SSBs) are on emerging technology for energy storage with the potential for high energy density and superior safety. Fabricating SSBs especially with ceramic electrolyte remains challenging. From materials processing perspective, polymer electrolyte could be a near-term solution to manufacture SSBs due to their flexibility, roll-to-roll processing and excellent interfacial properties. In this presentation, we establish a correlation among the composite structures, polymer segmental dynamics, and lithium ion (Li+) transport in a ceramic-polymer composite. In addition, this presentation will discuss compatibility of polymer electrolyte with cathodes and fabrication of polymer electrolyte with various solvents and techniques.

#### 9:30 AM

### (ICACC-S6-039-2025) Sodium-Ion Conducting Chlorides with Tantalum as Central Cation (Invited)

K. Motohashi\*1; A. Sakuda1; A. Hayashi1

1. Osaka Metropolitan University, Graduate School of Engineering, Department of Applied Chemistry, Japan

Developing materials with high sodium-ion conductivities is crucial for improving the electrochemical performance of all-solid-state batteries. Chloride solid electrolytes are promising owing to their high conductivity, formability, and good compatibility with positive electrode. Compared to lithium-ion conducting materials, fewer sodium-ion conducting chlorides have been developed. Recently, we have developed NaTaCl<sub>6</sub> solid electrolyte as an end-member of sodium-ion conductors. We report on recent developments in chloride electrolytes based on NaTaCl<sub>6</sub>.

#### **S6- Solid Electrolytes for Batteries III**

Room: Coquina B

Session Chairs: Eric Wachsman, University of Maryland; Olivier Guillon, Forschungszentrum Juelich

#### 10:20 AM

#### (ICACC-S6-040-2025) Pyrochlore-to-garnet: A versatile approach for garnet solid electrolytes with improved microstructure and cycling behavior (Invited)

J. Guo<sup>1</sup>; C. K. Chan<sup>\*1</sup>

1. Arizona State University, Materials Science and Engineering; School for Engineering of Matter, Transport and Energy, USA

Garnet-type Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> (LLZO) is a promising electrolyte for solidstate batteries because of its high electrochemical stability and ionic conductivity. We demonstrate that doped-pyrochlore can serve as starting precursor for LLZO through a reactive sintering approach, a process we call "pyrochlore-to-garnet" (P2G), which provides an alternative way to prepare dense LLZO material with greatly reduced sintering time and different microstructure properties compared to other methods. The P2G method is used to prepare Ta-doped LLZO (LLZTO) with high relative density and ionic conductivity >0.5 mS/cm, comparable to LLZTO prepared by solid-state reaction (SSR), but achieved using only 2 h sintering at 1100 °C. Galvanostatic Li stripping/plating measurements show that P2G LLZTO can withstand higher critical current densities than those seen in SSR LLZTO, but with less Li deposition along the grain boundaries. The improved cycling behavior in P2G LLZTO could be from the smaller grain sizes, more homogenous current density at the interfaces, and different grain boundary properties. The P2G method is also applied to prepare other kinds of doped garnets, including mixed conductors. This work shows the P2G method is a promising and versatile alternate method for the synthesis and processing of many kinds of garnet solid-electrolyte materials.

#### 10:50 AM

## (ICACC-S6-041-2025) Toward suppression of crystal structure changes upon electrochemical ion intercalation (Invited)

K. Kawai\*<sup>1</sup>

1. Waseda University, Japan

Electrochemical energy storage based in intercalation chemistry leads to high energy efficiency and long cycle life as established by lithium-ion batteries. Electrochemical ion intercalation is accompanied by solid-state redox reactions of host structures, leading to changes in an ionic radius of redox species and its bonding character. Ion-ion, ion-host, and host-host interactions also vary in various ways upon ion intercalation. These changes usually result in large volume change, and then performance degradation such as cracking of electrode materials and delamination of solid-solidinterfaces. Therefore, electrode materials that show small structure changes during charge/discharge are required to improve cycle performance of energy storage devices. This presentation focuses on crystal structure changes upon electrochemical ion intercalation. General models of structure changes are discussed. Then, electrode materials that show small volume changes enough to improve cycle performance will be introduced with a main focus on our research findings. The first one is an open-tunnel Mo<sub>3</sub>Nb<sub>2</sub>O<sub>14</sub> bronze phase that exhibits long-term cycling in aqueous proton batteries owing to near-zero volume change. The second one is Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene that maintain interfacial contact with solid-state electrolytes because of its negligible changes in interlayer distance upon (de)lithiation.

#### 11:20 AM

## (ICACC-S6-042-2025) Strategies for the Low-Temperature Synthesis of Garnet-Type Lithium-Ion Conductor

K. Onoue\*1; S. Mori2; A. Nasu1; H. Kobayashi1; M. Matsui1

1. Hokkaido Daigaku, Faculty of Science, Japan

2. Osaka Koritsu Daigaku, Japan

Garnet-type lithium-ion conductors have attracted great attention as solid electrolytes for oxide-based all-solid-state batteries. Among these solid electrolytes, cubic  $Li_{6.5}La_3Zr_{1.5}Nb_{0.5}O_{12}$  (LLZNO), in which the Zr site of tetragonal Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> is substituted with Nb, has a high ionic conductivity (3×10<sup>-4</sup> S/cm). A major challenge in the design of all-solid-state batteries with the garnet is the difficulty in forming a good interface between the cathode active material and the solid electrolyte. High temperature sintering is necessary to obtain a good interface. This sintering process, however, causes a high-resistive layer to hinder the fast ion transportation at the interface. To reduce the sintering temperature, a synthesis of fine particles that shows high sintering properties at low temperatures has been reported. In a previous report, fine garnet particles can be achieved by a preparation of transition metal composite oxide as a precursor. We consider that transition metal reactions are the bottleneck for low-temperature synthesis. In this study, we explored the low-temperature formation pathways of LLZNO utilizing unstable amorphous starting materials so that spontaneous reactions between transition metal oxides can be promoted to produce LLZNO at a lower temperature without the preparation of transition metal composite oxide.

#### 11:40 AM

#### (ICACC-S6-043-2025) Investigating Multi-Cation Doping in Garnet Solid-State Electrolytes - Insights into Ionic-Electronic Conductivity

- A. Cuper<sup>3</sup>; K. Pachulska<sup>1</sup>; P. Michalski<sup>1</sup>; M. Winkowska-Struzik<sup>2</sup>; M. Struzik<sup>\*1</sup>
- 1. Politechnika Warszawska, Faculty of Physics, Poland
- 2. Uniwersytet Warszawski, Faculty of Chemistry, Poland
- 3. Politechnika Warszawska, Centre for Advanced Materials and Technologies, Poland

Solid-state electrolytes based on lithium garnet frameworks, such as Li7La3Zr2O12 (LLZO), offer potential for improving the safety and performance of next-generation lithium-ion batteries. However, despite the promise of higher energy and power densities, their practical superiority over liquid electrolyte systems remains unproven. This gap may be due to incompatibilities between current battery electrode designs and solid electrolytes. A potential solution lies in composite electrodes that incorporate LLZO-based materials modified to conduct both lithium ions and electrons, enhancing charge transfer between the solid electrolyte and active electrode materials. In this study, we explore the effects of doping LLZO with variable valence cations. Specifically, Ta/Nb cations are substituted at the Zr-site, while Pr/Ni/Co cations are introduced at the La-site, aiming to induce and adjust mixed ionic-electronic conductivity and improve overall conductivity. We use X-ray diffraction (XRD) to study crystal structure and Raman spectroscopy to identify local structural changes. Additionally, impedance spectroscopy and direct current (DC) measurements provide detailed insight into the electrical transport properties crucial for battery performance. This research was funded by the National Science Centre, UMO-2019/33/B/ST5/02134.

### S10 Integrated computational-experimental modeling ad design of ceramics and composites

# S10- Modeling mechanical performance of advanced ceramics

Room: Coquina G Session Chair: Gerard Vignoles, University Bordeaux

#### 8:30 AM

#### (ICACC-S10-008-2025) Biphasic modeling of Ceramic Matrix Composites: applications, effectiveness, and perspectives (Invited)

A. Airoldi<sup>\*1</sup>; A. Caporale<sup>1</sup>; E. Novembre<sup>1</sup>; M. Riva<sup>1</sup>; M. De Stefano Fumo<sup>2</sup>; L. Cavalli<sup>3</sup>; D. Sciti<sup>4</sup>

- 1. Politecnico di Milano, Dept. of Aerospace Science and Technology, Italy
- 2. Centro Italiano Ricerche Aerospaziali, Italy
- 3. Petroceramics S.p.A., Italy
- 4. Consiglio Nazionale delle Ricerche, ISSMC, Italy

The fast development of Ceramic Matrix Composites (CMCs) and Ultra High-Temperature CMCs (UHTCMCs) unlocked a new generation of hot structures for hypersonic aircraft and spacecraft applications. Biphasic modelling approaches offer a computationally efficient method to capture both the complex damage modes in such materials. In this work, three implementations of this technique are outlined. First Carbon/Carbon (C/C) specimens are modelled, showing the possibility of capturing the complex response of quasi-random lamination sequences including the development of delaminations and the interactions with in-plane damage, which cannot be captured with more conventional techniques. In a second case, the approach is used to model the non-linear response and failure of LSI-produced C/SiC laminates, capturing failures in tensile specimens and the significant bending-to-tensile strength ratio

of laminates with different lay-ups. Finally, biphasic modelling is effectively used to capture the non-linear behaviour of a ZrB<sub>2</sub>-based UHTCMC, by successfully introducing into the material model the thermal residual stresses, generated during the sintering process. This last implementation opens the possibility of modelling some effects of manufacturing processes, which for CMCs is strongly linked to the final geometry of the components, as well as to their mechanical performances.

#### 9:00 AM

#### (ICACC-S10-009-2025) Multiscale Modeling of Ceramic Matrix Composites: Progress and Challenges (Invited)

G. Couégnat\*1

1. Laboratoire des Composites Thermostructuraux, France

This presentation examines recent advances and persistent challenges in multiscale modeling of Ceramic Matrix Composites (CMCs), emphasizing the complex relationship between constituent materials and macroscopic properties. Key challenges addressed include: (i) modeling intricate CMC architectures, (ii) incorporating stochastic variability, (iii) resolving scale separation issues, and (iv) integrating chemo-mechanical couplings. We discuss the evolution of numerical models at micro- and mesoscales, from simplified geometric representations to high-fidelity, image-based digital twins. Micromechanical models are explored, focusing on damage and failure mechanisms at the fiber-matrix interface and within the matrix, while accounting for nonlinear material behavior and environmental effects such as oxidation and matrix self-healing. Strategies for bridging the scale gap between micromechanical and macroscopic continuum models are presented, including finite element homogenization techniques and multiscale stochastic computational frameworks. These approaches are validated through in-situ mechanical testing. The presentation concludes by addressing current limitations and future research directions, with emphasis on overcoming scale separation issues and enhancing the accuracy and predictive capabilities of CMC modeling.

#### 9:30 AM

#### (ICACC-S10-010-2025) New image segmentation strategy to characterize failure modes of struts in uniaxial compression of ceramic foam (Invited)

- V. Deshpande\*1; R. Piat1
- 1. University of Applied Sciences, Darmstadt, Mathematics and Natural Sciences, Germany

The work investigates the failure modes of the struts in a ceramic foam subjected to uniaxial compression. The foam material is manufactured using the direct foaming method and has polydisperse pores homogeneously distributed in the microstructure. The effective stress-strain curve and the material's macroscopic strength differ significantly from the Gibson-Ashby model's predictions. This difference is investigated in this work by studying the failure mode of each strut and how it affects the macroscopic failure of the material. An image segmentation algorithm based on skeletonization is developed that uses novel pruning strategies to isolate the struts in the 3D image of the microstructure. A pruning strategy based on cross-sectional area overcomes the hairy-skeleton problem common to skeletonization algorithms. Pruning based on a physics-based significance measure identifies the struts that cause the macroscopic failure. The stress states in the struts are determined by a finite element simulation to identify their failure modes. This leads to a correlation between orientation distribution and the failure modes of the struts. The energy dissipated by the failure mode of each strut as the loading is increased shows that there are two dominant failure modes that are different from the bending failure reported in the Gibson-Ashby model.

# S10- Modeling mechanical and thermal performance of advanced ceramics

#### Room: Coquina G

Session Chair: Alessandro Airoldi, Politecnico di Milano

#### 10:20 AM

### (ICACC-S10-011-2025) Mechanical Stability of Bonded Dissimilar Materials (Invited)

E. Hernandez\*1; S. G. Hirsch1; B. Butler1; P. Moy1

1. US Army Combat Capabilities Development Command, Army Research Laboratory, USA

Technological advances have demonstrated the need for advanced materials that can perform at increasingly extreme environments. It is generally understood that to achieve the desired performances, different material classes will be required (e.g., ceramic coated metals). This is especially true in applications where mechanical stability is required at extreme temperatures; where ultra-high temperature ceramics (UHTC) are used as thermal barriers, while the metallic constituent contributes the overall toughness. Unfortunately, when bonding dissimilar materials, differences in material properties (e.g., thermal expansion) result in mechanically unstable interfaces. Typically, these instabilities can be mitigated by bonding techniques like brazing. However, this leads to the formation of complex intermetallics along the bonded interface, which could result in weak bonds. Hence, understanding the structural stability of the interfaces formed when bonding dissimilar materials is critical. Therefore, a finite-element thermo-micromechanics model was developed to explore the mechanical stability of bonded SiC/Ti64. The mechanical state under processing conditions is analyze, and methods to stabilize the bonds are explored.

#### 10:50 AM

#### (ICACC-S10-012-2025) 3D fiber reinforcements for CMCs: Modelling of mechanical characteristics using NASA's Multiscale Analysis Tool (NASMAT) and Finite Element Analysis

M. R. Welsh\*1; F. Jung1; T. Gries1

1. RWTH Aachen University, Institut für Textiltechnik, Germany

Compared to metallic turbine materials, oxide ceramics have a higher oxidation stability and temperature resistance. However, in order to make these materials suitable for turbine applications, it is necessary to reinforce the ceramics with complex continuous fiber reinforcements, thereby significantly increasing the damage tolerance of the composite. The reinforcement architecture applied poses a major challenge for the production of the CMC using colloidal manufacturing routes. Therefore, a novel 3D-braided reinforcement architecture was developed at RWTH Aachen University's Institut für Textiltechnik to reduce the filtering effect of dense textiles and allow the production of ceramic composites using a pressure slip casting route. To evaluate the performance of the braided structure, a micromechanical model using the NASA Multiscale Analysis Tool (NASMAT) will be created, which can predict the equivalent properties of the composite structure and perform progressive damage modeling. These equivalent properties and damage accumulation can be coupled with an FEM model at the component level to obtain an overall structural response under load.

#### 11:10 AM

# (ICACC-S10-013-2025) An image-based technique to compute effective properties of ceramic matrix composites preforms and its impact on modeling their infiltration by TG-CVI

R. Bechara\*'; G. L. Vignoles'; G. Mangeon'; B. Dubroca'; T. Nguyen-Bui'; C. Descamps $^1$ 

1. Laboratoire des Composites Thermostructuraux, France

The manufacturing of Ceramic-Matrix Composites (CMC) relies on the Chemical Vapor Infiltration (CVI) process. Thermal-Gradient variations of CVI (or TG-CVI, among which MW-CVI) are promising candidates for the preparation of better CMCs; however, they are difficult to monitor and control. Multi-physics and multiscale modeling are considered as potential solutions to overcome these challenges. Here, we present such a modeling suite. It breaks down as follows: (1) Image based identification of fiber content in a SEM micrograph of a CMC (2) homogenization of thermal, gas transfer and electro-magnetic properties at different phase contents, (3) correlation of obtained results via Machine Learning techniques, (4) construction of a reactor-scale model for the CVI process and (5) injection of the effective properties in this model. The key findings highlight the effectiveness of non-periodic boundary conditions, the non-linear relationship between effective properties and phase content, the advantage of using well-trained machine learning techniques and the improvement of simulation results with the inclusion of these correlations. This work has been funded by Horizon 2020 (CEM-WAVE, 958170), the Aquitaine Region (IMPPECC, 2023-24915310), CEA and Safran.

#### 11:30 AM

#### (ICACC-S10-014-2025) Insights from Molecular Dynamics, Finite Elements and Machine Learning into the elastic behavior of pyrolytic carbons (Invited)

F. Polewczyk<sup>2</sup>; J. Leyssale<sup>4</sup>; P. Lafourcade<sup>3</sup>; C. Denoual<sup>3</sup>; N. Pineau<sup>3</sup>; P. Aurel<sup>4</sup>; S. Jouannigot<sup>4</sup>; G. Couégnat<sup>5</sup>; G. L. Vignoles<sup>\*1</sup>

- 1. Universite de Bordeaux, LCTS Lab. for ThermoStructural Composites, France
- 2. Universite de Bordeaux, ISM Inst. for Molecular Sciences, France
- 3. Commissariat a l'energie atomique et aux energies alternatives Siege administratif, DIF, France
- 4. Centre National de la Recherche Scientifique, ISM Institute for Molecular Sciences, France
- 5. Centre National de la Recherche Scientifique, LCTS Lab. des Composites ThermoStructuraux, France

Pyrolytic carbons are used in several high-tech applications nuclear energy, ceramic-matrix composites, electrodes, etc ... ; they have a great versatility of multi-scale structural/textural organization, which greatly impacts their mechanical properties. Modeling tools are developed to address the structure-elasticity relationships. Nanoscale modeling has been made possible thanks to an original method allowing the production of hundreds of polygranular molecular models in 12.4nm edge size cubes starting from experimental data acquired with XRD and HRTEM chained to efficient MD simulations. A supervised learning algorithm applied to the raw simulation results data set shows that elastic constants can be accurately predicted using only 3 experimentally accessible descriptors. Their evolution with temperature has also been followed, showing a moderate decrease, as for graphite. We also show how softening occurs in an indentation / compression situation, thanks to a multiscale approach mixing MD and finite element simulations. CEA and DGA are acknowledged for their financial support to F.P.'s PhD.

### S11 Advanced Materials and Innovative Processing Ideas for Production Root Technologies

# S11- Future-oriented techniques for coating, forming, and shaping materials

Room: Coquina C

Session Chair: Chisung Ahn, Korea Institute of Industrial Technology

#### 8:30 AM

### (ICACC-S11-001-2025) Ultra-fast Boriding as a Green and Efficient Surface Treatment Process for Harsh Service Conditions (Invited)

A. Erdemir\*1

1. Texas A&M University, Department of Mechanical Engineering, USA

Boriding is an effective surface treatment process for the creation of thick and hard boride layers on ferrous materials. Currently, it is done using an energy- and carbon-intensive powder pack boriding process. In this talk, an ultra-fast electrochemical boriding technique will be introduced together with its effectiveness in boriding not only ferrous but also a wide range of refractory metals and their alloys. In this technique, boriding is done in a borax-based molten salt electrolyte at temperatures from 850 to 1000°C. Structural, chemical, and mechanical characterization of the boride layers confirms that they are structurally dense, highly stochiometric, and uniformly thick. Depending on the alloy type, the mechanical hardness of the resultant boride layers may range from 25 GPa to 45 GPa. Some of the alloys such as rhenium-tungsten exhibit duplex layers with a graded composition and microstructure with hardness values as high as 43 GPa.

#### 9:00 AM

# (ICACC-S11-002-2025) A study on the development of Zr-Cu based multi-component alloys for the nanocomposite coatings and their properties

H. Yoon<sup>1</sup>; B. Choi<sup>1</sup>; K. An<sup>1</sup>; K. Moon<sup>\*1</sup>

1. KITECH, Republic of Korea

While modern industries are becoming more sophisticated, diversified, and globalized, they requires the development of smart materials have multi-functionality, high mechanical properties, and extreme durability. Also they could be prepared environmentally friendly and energy efficiently. In particular, there is an urgent needs to develop a novel coating materials capable of stably maintaining microstructures and mechanical properties in various external environments, unlike conventional coating materials whose properties and structures are easily changed by the some harsh environments. To get this kinds of objects, the coating material with multi-components are essential. So, it is necessary to develop a coating layer composed of various components those could be formed various phases and more complex structures. In this study, various single alloy materials with various compositions based on the amorphous composition of Zr-Cu have been tried to be prepared by powder metallurgy methods such as atomization, mechanical alloying, and Spark Plasma Sintering (SPS). The properties of as-prepared nanocomposite coatings will be summarized in this present.

#### 9:20 AM

#### (ICACC-S11-003-2025) Development of MXene-reinforeced ceramic matrix composite with low temperature self-healing property by cold sintering process (Invited) *WITHDRAWN*

- S. T. Nguyen\*1; A. Okawa2; T. Nakayama3; H. Suematsu4
- 1. National Institute of Technology, Kushiro College, Department of Creative Engineering, Japan
- 2. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials, Japan
- 3. Nagaoka University of Technology, Japan
- 4. Nagaoka University of Technology, Extreme Energy-Density Research Institute, Japan

MXenes are two dimensional (2D) materials of metal carbides or nitrides that has many potential applications, therefore they have been widely used as fillers to improve the properties of composites. However, due to their relative ease oxidation at elevating temperature, there have been few studies on fabrication of MXene-reinforced ceramic matrix composite (CMC). In this work, we present a method to synthesize MXene CMC by cold sintering process. Firstly, delaminated 2D MXene flakes was synthesized by in-situ HF generating etching method, then the as-received MXenes flakes were dispersed into ZnO matrix, cold-pressed to become pellets and sintered at 250 degree celcius for one to four hours. The self-healing property of the sintered products then investigated with Vickers indenter followed by heat treatment. XRD analysis and SEM observation can be used to evaluate the phase change in the composite and the crack dissappearance, both caused by the oxidation of MXene in the matrix.

# S11- Fundamental materials: mining, particles, bulk, and functional materials and precursors I

Room: Coquina C

Session Chair: Ayahisa Okawa, Tohoku University

#### 10:20 AM

# (ICACC-S11-004-2025) Synthesis of novel oxides and their oxygen content tuning under high oxygen partial pressures (Invited)

H. Suematsu\*1; Y. Noa1; Z. Feng1; T. Do1; T. Nakayama1

1. Nagaoka University of Technology, Extreme Energy-Density Research Institute, Japan

Various superconductive phases have been discovered by utilizing high pressure synthesis appratus. We have developed an oxygen content tuning method by introducing oxidizing agents including KClO<sub>3</sub>, KClO<sub>4</sub>, Ag<sub>2</sub>O or AgO with the samples in the high pressure synthesis capsule. By using this method, even Au could be oxidized to synthesize a novel Au-Sr-Ca-Cu-O cuprate. Powders of Au, SrO<sub>2</sub>, SrCuO<sub>2</sub>, Ca<sub>2</sub>CuO<sub>3</sub> and CuO were mixed. The mixture and Ag<sub>2</sub>O powders were compacted in a gold capsule separated by a gold sheet. A cubic anvil type press was used for the high pressure synthesis at 5.5 GPa and 1150-1100 °C for 3 hours. Lattice images showed a layered structure similar to CuSr<sub>2</sub>CaCu<sub>3</sub>O<sub>9</sub>. From EDS data, Au was detected and was identified as Au<sup>3+</sup> by XPS. These results indicated that Au was successfully oxidized to form a novel (Au,Cu) Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>9</sub> superconductive phase.

#### 10:50 AM

#### (ICACC-S11-005-2025) Carbon fiber-reinforced thermoplastic synthesized by the hypercrosslinking polyether ether ketone with laminated structures (Invited)

T. Yamamoto<sup>\*1</sup>; T. Nakamoto<sup>1</sup>; Y. Ota<sup>1</sup>

1. Nagoya Daigaku, Chemical Systems Engineering, Japan

Thermoplastic resins were used as matrix to synthesize carbon fiber-reinforced thermoplastic (CFRTP) for recycling it easily. In this study, a CFRTP with excellent mechanical properties and heat resistance was synthesized using a polyether ether ketone (PEEK) as a matrix resin. The PEEK resin was modified to form crosslinked structures through Friedel–Crafts reaction alkylation. The cross-linked PEEK resin was partially used as a matrix resin, and the mechanical properties of the CFRTP were enhanced. From this result, a technique was developed to enhance CFRTP using polypropylene (PP) and nylon (PA6) to make laminate structures, wherein a PP colloid was prepared using a surfactant and adsorbed onto carbon fibers (CFs) using an electrodeposition system. The interfacial adhesion between the thermoplastic and the CF was enhanced by the adsorption of PP colloids, which improved the mechanical properties of the CFRTP. The bending strength of the laminated structure of the CFRTP was enhanced as the layer thicknesses of the PP and PA6 became thinner.

#### 11:20 AM

# (ICACC-S11-006-2025) Characterization of Philippine Clay and Diatomite for Potential Ceramic Robocasting Applications

P. Labandero<sup>1</sup>; J. Talondong<sup>1</sup>; R. V. Virtudazo<sup>1</sup>; L. I. Cabalo<sup>1</sup>; E. d. Magdaluyo<sup>\*2</sup>

- 1. Mindanao State University-Iligan Institute of Technology, Department of Materials and Resources Engineering & Technology (DMRET), Philippines
- 2. University of the Philippines Diliman, Department of Mining, Metallurgical and Materials Engineering, Philippines

Additive manufacturing has revolutionized production technique, particularly in crafting intricate ceramic designs for specific applications. Ceramic robocasting, a key subset, involves extruding viscous ceramic mixtures with precise rheological properties. Despite extensive research, the use of locally sourced ceramics is underexplored. This study explores the potential of Talakag clay and Kapatagan diatomite from Mindanao Island, Philippines, for ceramic robocasting. The raw materials were mechanically processed and subjected to rheological and morphological characterization to determine their suitability. Test pellets were fired at 900 °C to assess dimensional stability. Talakag clay demonstrated shear-thinning and thixotropic behaviors essential for effective robocasting. Eight ceramic mixtures were developed, blending clay and diatomite with feldspar and carboxymethyl cellulose (CMC) to improve homogeneity and printability. The extrudability and printability were tested using manual piston extrusion and 3D printing. Mixtures with 60% solid loading and 1 to 1.5 wt% CMC binder showed excellent robocasting potential. Fired samples were analyzed for shrinkage, bulk density, porosity, and water absorption according to ASTM standards. The results reveal promising characteristics, opening new possibilities for advanced manufacturing and innovative applications across industries

#### 11:40 AM

#### (ICACC-S11-007-2025) Influence of Al ions eluted from coal ash particles in chemical structures controlling of silicate network during solidification process

- T. Sangu\*1; Y. Xin1; K. Kato1; Y. Xu1; T. Shirai1
- 1. Nagoya Institute of Technology, Advanced Ceramics Research Center, Japan

Coal ash(CA), as an industrial waste which disposed by landfill causes serious environmental issues. In recent years, efforts are made to recycle CA as inorganic materials because it contains ceramic resources such as quartz and mullite. Our group succeeded in fabricating a novel solidified body by mixing surface activated CA with low-concentrated alkali solution, whose process is driven via condensation reaction of Si and Al ions eluted from CA and proposed as new alternative construction materials. Also, the amount of silicate ions eluted from only CA is insufficient considering from the viewpoint of long-term stability, so silicate solution is used to ensure the high-concentrated silicate ions. Herein, we prepared silicate solution with different structure ( $Q0\sim Q4$  as different coordination state of Si) and investigated the effect of Q ratio on the solidification behavior and the chemical structure of silicate network formed on CA surface/interface. With assistance of ICP-OES, NMR, FT-IR, the Al ion elution behavior and changes in chemical structure of silicate network during reaction process were evaluated in detail, whose results will be discussed in correlation with the reactivity between silicate ions with different structure and Al ions, and the physical properties of solidified bodies such as drying dynamics and compressive strength.

### <u>S13 Development & Applications of Adv</u> <u>Ceramics & Composites for Nuclear Fission/</u> <u>Fusion Energy Sys</u>

# S13- SiC material technologies for core structures of light water reactors and advanced reactors III

Room: Coquina D

Session Chair: Dong Liu, University of Oxford

#### 8:30 AM

#### (ICACC-S13-019-2025) Development of a Multilayer Silicon Carbide Composite for Accident-Tolerant Fuel Cladding (Invited)

F. Mohammadi<sup>\*1</sup>; J. Halfinger<sup>1</sup>; J. Neiderer<sup>1</sup>; T. Daspit<sup>2</sup>; X. Li<sup>2</sup>; Q. Zhang<sup>3</sup>; D. Liu<sup>4</sup>

- 1. Ceramic Tubular Products, LLC, USA
- 2. University of Virginia, USA
- 3. University of Bristol, United Kingdom
- 4. University of Oxford, United Kingdom

Silicon carbide (SiC) materials have been considered for accident-tolerant fuel applications due to their excellent thermal properties, creep resistance, low neutron absorption, and lack of explosive hydrogen production in the event of a loss of coolant accident. A multilayer SiC fiber composite cladding was developed using a polymer infiltration and pyrolysis (PIP) process. In this design, the inner monolithic SiC layer provides a hermetically sealed barrier to contain fission gases, while the overwrapped SiC fiber composite provides protection against thermal shock and fracture. Additionally, a chemical vapor deposited β-SiC outer layer is applied as an environmental barrier coating to provide further protection against corrosion. The multilayer SiC tubes demonstrated an elastic modulus of 300-340 GPa and withstood a maximum internal pressure of 30 MPa in hoop tensile tests. X-ray computed tomography of SiC c-ring compression test revealed a correlation between the maximum fracture load and tangential crack propagation within the ceramic matrix composite (CMC). Radial crack propagation through the inner SiC monolithic layer occurred at a lower load, only after CMC failure, indicating that the CMC overlap effectively protects the inner monolithic SiC layer. This paper presents the design, manufacturing process, and mechanical performance of the multilayer SiC cladding.

#### 9:00 AM

#### (ICACC-S13-020-2025) Advancements in Joining SiC/SiC Ceramic Matrix Composites via Embedded Wire CVD

S. Harrison\*1; J. Vervlied1; J. Pegna1

1. Free Form Fibers, USA

Mechanical properties and joint integrity, including hermiticity, of Embedded Wire Chemical Vapor Deposition (EWCVD) formed SiC fiber/SiC Matrix (SiC/SiC) ceramic matrix composites (CMC) joints were developed under Department of Energy (DOE) support. Monolithic SiC and SIC/SiC CMC structures joined using the unique properties of the Laser CVD formed SiC fibers (LCVD), and architecture of the LCVD SIC non-woven mattes, will be discussed.

#### 9:20 AM

# (ICACC-S13-021-2025) Multiscale Modeling of Silicon Carbide Cladding

G. Singh\*<sup>1</sup>; F. Xu<sup>1</sup>; T. Yao<sup>1</sup>; J. Yu<sup>1</sup>; P. Xu<sup>1</sup>

1. Idaho National Laboratory, USA

SiC composites are complex materials which make their modeling and analysis challenging. In this work, multiscale modeling of SiC composite is performed for light water reactor cladding applications. The modeling involves a modular approach of developing models at different length scales, with the properties evaluated at lower scale serving as an input to higher scale models. The details of this modeling approach will be presented along with the verification, validation and demonstration cases.

#### 9:40 AM

#### (ICACC-S13-022-2025) Fabrication Uniformity and Length Scaling of SiC/SiC Cladding for Commercial Nuclear Reactors

S. Oswald\*<sup>1</sup>; R. Haefelfinger<sup>1</sup>; D. Kuebler<sup>1</sup>; S. Gonderman<sup>1</sup>; C. Deck<sup>1</sup>;

L. Borowski<sup>1</sup>; A. Giles<sup>1</sup>; C. Jones<sup>1</sup>; J. Unangst<sup>1</sup>; D. Frazer<sup>1</sup>; J. Quan<sup>1</sup>; J. Gazza<sup>1</sup>

1. General Atomics Electromagnetic Systems Group, USA

GA-EMS is developing full length (12+ foot) engineered silicon carbide composite (SiC/SiC) cladding (SiGA®) for commercial nuclear reactors. SiC's unique properties offer significant performance and safety benefits yet present manufacturing challenges for scaling in length and quantity. The long aspect ratio and material hardness require specialized fabrication equipment and machining practices to meet performance and geometry requirements with good inter- and intra-batch uniformity. Inner diameter (ID) and outer diameter (OD) machining processes have been developed for controlling cladding geometry and surface roughness - integral for good mechanical strength, leak rate, heat transfer, and pellet-cladding interaction. On shorter tubes, ID and OD tolerances meeting specification (+/-0.01 mm) are achieved with high yield. OD machining equipment modified for 12+ foot lengths has been demonstrated with diameter accuracy equivalent to 1-foot tubes. Recent fabrication and characterization of SiC/SiC tubes made in GA-EMS's 10-meter-tall chemical vapor infiltration (CVI) furnace shows deposition rate and grain size uniformity throughout the coating region. Currently, full sealing capability is being demonstrated on 12-foot SiGA® tubes to support a lead test rod irradiation campaign of SiGA® ATF cladding in the late 2020's.

#### **S13- Ceramics and composites in nuclear fusion, blanket structural and functional materials** Room: Coquina D

Session Chair: David Sprouster, Brookhaven National Laboratory

#### 10:20 AM

# (ICACC-S13-023-2025) Fabrication of accident-tolerant hybrid ceramic breeder for fusion applications (Invited)

K. Mukai\*1; M. Kusaba1

1. Kaku Yugo Kagaku Kenkyujo, Japan

Nuclear fusion is a low-carbon energy source, in which solid breeding blanket contains Li-containing ceramics and Be-intermetallics as tritium breeder and neutron multiplier, respectively. Water-cooled solid breeding blanket has a potential risk of hydrogen generation and explosion caused by chemical reactions of the metallic Be compound with steam in a loss-of-coolant accident. Hybrid ceramics containing both Li and Be is a multifunctional material for the breeding and multiplication, which can significantly reduce hydrogen generation in the severe accident. Previous study reported their successful fabrication of Li-Be-O ceramic; however, its melting point is low for the application. In this study, based on computational predictions, Li-Be-X-O hybrid ceramics are synthesized and characterized. Stable structures with four elements were predicted by using CSPML (crystal structure prediction with machine learning-based element substitution) pretrained with stable structures in the Materials project database and then investigated by density functional theory (DFT) simulations. Thereafter, Li-Be-X-O samples were synthesized via a solid state route. Successful synthesis of the hybrid ceramics was confirmed by powder X-ray diffraction. In a steam exposure test, the synthesized hybrid ceramic shows a good chemical stability in a humid atmosphere at elevated temperatures.

#### 10:50 AM

# (ICACC-S13-024-2025) Compositionally-complex rare earth oxides for fusion applications (Invited)

- T. Davey\*1; H. M. Gardner2; D. M. Nguyen2; J. Wade-Zhu2; S. Middleburgh1
- 1. Bangor University, Nuclear Futures Institute, United Kingdom
- 2. UKAEA, Materials Division, United Kingdom

In fusion reactors, hydrogen isotopes act as the fuel, but diffuse rapidly in steel structural materials having serious safety and economic implications. As such, permeation barrier coatings are necessary. Individual rare earth oxides have shown some degree of success, but demonstrate inadequate adhesion and property continuation across layers. To counter this, and to withstand irradiation damage, amorphous coatings have been investigated, but exhibit undesirable crystallisation and grain growth under temperature and irradiation exposure. For this work, an alternative strategy is taken where a disordered or heavily-distorted structure is used instead: a compositionally-complex rare-earth oxide (CCREO). Compositionally-complex materials have shown improved stability, particularly at high-temperatures and under irradiation. This work begins exploration of potential CCREO systems specifically targeting an application as a thermally- and irradiation-stable hydrogen permeation barrier. Density functional theory (DFT) calculations are used to model an array of compositionally-complex oxide combinations containing yttrium, erbium, and holmium.

#### 11:20 AM

#### (ICACC-S13-025-2025) Lithium-Based Tritium Breeder Pellets by Volume-controlled Spark Plasma Sintering with Promising Microstructure

- S. K. Sharma\*1; C. N. Taylor3; K. Yan1; J. Lian2
- 1. Rensselaer Polytechnic Institute, Department Of Mechanical, Aerospace, And Nuclear Engineering, USA
- 2. Rensselaer Polytechnic Institute, USA
- 3. Idaho National Laboratory, USA

Multifunctional ceramic breeder materials are required for fusion nuclear reactors, which are recognized as one of the most promising renewable energy sources to achieve net-zero carbon emissions. Potential tritium breeder materials, available in either liquid or solid forms, each present unique advantages and challenges. Among the solid breeder materials, Li2TiO3, Li2ZrO3, Li4SiO4, and Li8PbO6 are under consideration, and the key features of the promising ceramic breed materials include effective tritium release behavior, high lithium density, optimal pore volume with 10-15% porosity for tritium extraction, excellent thermo-mechanical characteristics (such as low thermal expansion, high thermal conductivity, and mechanical strength), high melting points, low reactivity with water, and low neutron activation. In this work, we have developed nanocrystalline porous solid breeder materials, like Li2TiO3 with controlled porosities of 14% and 20% are manufactured by volume-controlled spark plasma sintering (SPS). An optimized 3D interconnected pore structure has been engineered featuring a combination of micronsized and nano-sized pores within a nanocrystalline matrix. The SPS-densified ceramic breeder pellets with controlled pore structures also display enhanced thermal and mechanical properties.

#### 11:40 AM

# (ICACC-S13-026-2025) Laser assisted joining of SiC/SiC for nuclear applications

- M. Ferraris\*3; M. De Maddis2; C. Lorrette1
- 1. Commissariat a l'energie atomique et aux energies alternatives Siege administratif, France
- 2. Politecnico di Torino, DIGEP, Italy
- 3. Politecnico di Torino, DISAT, Italy

Several technologies and materials have been proposed for joining of SiC/SiC components for nuclear reactors, both fusion and fission, and more recently for new small modular reactors. Laser assisted joining seems to give promising results as a fast, pressure-less, localized heating joining technology suitable for SiC/SiC operating in a nuclear (and other) environment. The present work reports on preliminary results on laser assisted joining of SiC/SiC; several joining materials have been used to join SiC/SiC by a diode laser (LDF 4000-40, Laserline GmbH) operating in the infrared (1020-1060 nm). Morphology, micro-structure and mechanical properties of laser joined SiC/SiC tubes joined to a SiC/SiC end-plug will be discussed, together with new steps to improve and extend this technology.

### <u>S15 9th International Symposium on</u> <u>Additive Manufacturing and 3-D Printing</u> <u>Technologies</u>

#### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies-

#### **Emerging Applications**

Room: Coquina A

Session Chairs: Marcelo Farfan, University of South Florida; Lisa Biasetto, University of Padova

#### 8:30 AM

#### (ICACC-S15-020-2025) Design and Thermal Characterization of 3D-Printed Hybrid Cooling System for Battery Thermal Management Systems (Invited)

Y. Zheng\*<sup>1</sup>; A. S. Almansour<sup>2</sup>; M. C. Halbig<sup>2</sup>; M. Singh<sup>4</sup>; M. Ranaiefar<sup>2</sup>; Z. J. Tuchfeld<sup>3</sup>

- 1. Northeastern University, Mechanical and Industrial Engineering, USA
- 2. NASA Glenn Research Center, USA
- 3. NASA, LMC, USA
- 4. Ohio Aerospace Institute, USA

The development and integration of lithium-ion batteries into aerospace and ground transportation systems has attracted global interest due to their high energy storage density and extended service life. However, these batteries are quite sensitive to temperature fluctuations and generate heat during operation which impacts their safety and performance. This study presents design, 3D printing, fabrication of phase-change composite material, and thermal characterization of a hybrid cooling system tailored for a cylindrical (18650 type) and a pouch-type Li-ion cell analogues. The system integrates both passive and active cooling mechanisms to enhance thermal management efficiency for a battery pack. A novel design approach is employed, leveraging advanced 3D printing techniques to create a highly customized and efficient cooling hexagonal structure. The hybrid cooling system combines thermally conductive phasechange material with embedded water-cooling pathways, optimized through computational simulations. The effectiveness of the designs is validated via experimental testing, demonstrating significant improvements in temperature regulation and overall cooling performance. The test results indicate that the hybrid cooling system offers a promising solution for maintaining optimal operating temperatures in high-performance battery packs in various applications.

#### 9:00 AM

#### (ICACC-S15-021-2025) Revolutionizing Inductors, Transformers, and Power Modules: Additive Manufacturing of Alumina Ceramics for Enhanced Performance and Design Flexibility

N. Leak\*1

1. Stony Brook University College of Engineering and Applied Sciences, Electrical Engineering, USA

This paper provides a comprehensive review of the current state of innovative applications of additive manufacturing (AM) techniques for the production of advanced ceramic materials, particularly alumina, in the context of inductors, transformers, and power module development. We highlight the potential of AM to revolutionize the design and manufacturing processes of these critical electrical components, offering unprecedented flexibility in geometry, reduced lead times, and enhanced performance. The paper delves into the various AM methods suitable for alumina, such as direct ink writing, lithography-based ceramic manufacturing, and powder bed fusion, discussing their advantages and limitations. We also present case studies demonstrating the successful integration of additively manufactured alumina components in power electronics applications, showcasing improved thermal management, reduced weight, and increased power density. Additionally, we address the challenges and future research directions in this emerging field, aiming to inspire further innovation and adoption of AM in the power electronics industry.

#### 9:20 AM

### (ICACC-S15-022-2025) Polysiloxane-BaTiO<sub>3</sub> Piezoelectric Composite with Advanced Structural and Thermal Performance

H. Zhao\*1; Y. Li1

1. Dartmouth College, Engineering, USA

Piezoelectric materials, which can convert mechanical energy to electrical energy, are extensively used in various applications. Among these, piezoelectric composites merge the advantages of piezoelectric ceramics and polymers, while overcoming their individual limitations. However, maintaining stable performance in high-temperature environments remains a significant challenge due to the poor structural integrity and thermal stability of conventional polymer matrices at elevated temperatures. To address this issue, we have developed a new piezoelectric composite by employing a preceramic polymer (PCP) matrix. PCPs are silicone-based polymers that undergo a unique polymer-to-ceramic phase transition upon heating. Our results show that this novel composite can withstand temperatures up to 500°C without structural damage, maintain a 30 MPa compressive load, and endure up to 20% strain. Additionally, the piezoelectric performance of this composite remains consistent even after multiple thermal cycles. Moreover, this composite can be manufactured into arbitrary geometries using 3D printing, meeting diverse design requirements for various applications. This innovative material opens up possibilities for using piezoelectric composites in high-temperature environments for sensing, energy harvesting, and actuation.

### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies-Direct Writing

Room: Coquina A

Session Chairs: Yi Zheng, Northeastern University; Nicholas Leak, Stony Brook University College of Engineering and Applied Sciences

#### 10:20 AM

#### (ICACC-S15-024-2025) $\rm Ti_3C_2T_x$ MX enes as Multifunctional Additive for Direct Ink Writing

M. Scholl<sup>\*1</sup>; S. Barg<sup>1</sup>

1. Universitat Augsburg Mathematisch-Naturwissenschaftlich-Technische Fakultat, Institute of Materials Research Management, Germany

MXenes are a family of 2D materials showing a wide range of functional properties such as high electrical and thermal conductivities, mechanical strength, EMI shielding and catalytic properties for certain chemical reactions. Their effective incorporation into ceramic matrixes can open new opportunities to develop materials with enhanced performance and functionalities for applications beyond ambient conditions. MXenes high aspect ratio, aqueous dispersion stability, and tunable surface chemistry, further make them well-suited for colloidal processing, including 3D printing. Here, we investigate the possibilities to develop printable MXenebased ceramic structures. By designing efficient MXene-based formulations, we show it is possible to create colloidal inks with ideal rheological properties for printing ceramic structures via extrusion-based 3D printing, i.e., direct ink writing, DIW. We use a Bayesian optimization approach, to find suitable composition and processing parameters efficiently, achieving good printing results within a few optimization cycles. We further elucidate the challenges and opportunities for their consolidation using novel pressureless sintering methods. The results open-up exciting opportunities to print functional MXene-based ceramics for potential use in a myriad of applications requiring functional and structural properties.

#### 10:40 AM

#### (ICACC-S15-025-2025) Direct Ink Write of Porous Carbon Fiber-Loaded Silicon Nitride

- A. Bai\*1; J. P. Youngblood2; R. Trice2
- 1. Purdue University, MSE, USA
- 2. Purdue University, Department of Materials Engineering, USA

Vehicles that fly at hypersonic speeds need RF windows to protect sensitive equipment that guides the aircraft. These forward-facing windows are subject to temperature extremes, and as such, require ceramic-based solutions. Silicon nitride, with its low dielectric constant, is a candidate material for this application. In the work reported here, the effect of different sintering aids and/or the addition of carbon fibers on densification was studied. SEM microstructural studies and mechanical properties were used to quantify differences as a result of composition changes.

#### 11:00 AM

#### (ICACC-S15-026-2025) Development of tunable porous alumina monolith using hollow microspheres via extrusion-based 3D printing

S. Hossein<sup>1</sup>; M. Jonsson<sup>2</sup>; F. Akhtar\*<sup>1</sup>

- 1. Lulea University of Technology, Division of Materials Science, Sweden
- 2. Nouryon Pulp and Performance AB, Sweden

Hierarchical cellular ceramics have attracted considerable interest due to their versatility and unique physico-mechanical effectiveness for advanced applications. Tailorable alumina foams with low shrinkage were fabricated through an innovative combination of 3D printing and sacrificial templating with a low environmental footprint. The viscoelastic pastes were formulated using the aqueous-based solution of binder, dispersant, and plasticizer with different volumes of  $\alpha$ -alumina and lightweight hollow microspheres (HMs) as a template. The solid-to-liquid ratio increased 53–80 vol% with the inclusion of HMs for printable rheology. Cellular architectures of alumina were structured through a material extrusion-based technique and then thermally treated at 1200 °C. Finally, the alumina monoliths achieved a ~55–93 % porosity with three different types of adjustable pores, produced by combining 3D printing, template burning, and inter-particle voids. The HMs generated spherical pores (7–47 µm) in the printing struts with reduced CO<sub>2</sub> emissions compared to conventional sacrificial porogens during the burnout process.

#### 11:20 AM

#### (ICACC-S15-027-2025) Corona-Enabled Electrostatic Printing (CEP) for Manufacturing of Printable Electronics

M. Farfan<sup>\*1</sup>; D. Murphy<sup>1</sup>; W. Mao<sup>1</sup>; A. Kumar<sup>1</sup>; Z. Weng<sup>1</sup>; A. Thor<sup>1</sup>

1. University of South Florida, Mechanical Engineering, USA

Printable electronics is a growing field that enables the placement of flexible sensors in unconventional locations. One key application is vapor detection, which facilitates the monitoring of position, health, and leaks. These sensors are chip-less, incorporating biodegradability into their design. This expectation of disposability necessitates a design suited for mass production. We present a low-cost, simultaneous printing method using powder with high selectivity (such as graphene and titanium oxide) to create sensors through Corona Electrostatic Printing (CEP). CEP involves placing printable powder between two parallel plates. When the top plate is polarized by corona discharge, the powder beneath it is attracted to the top plate. Upon contact, the powder repels back down and repeats in an oscillating motion. By placing a masked film between the plates, the powder self-assembles into a patterned circuit. This self-assembly process eliminates the need for polymer binders, a novel feature, as curing these binders would increase production time and reduce the sensitivity of the powder circuit. A Roll-to-Roll (R2R) machine has been designed to incorporate CEP for the mass production of sensors, enabling the simultaneous creation of four sensors. Achieving simultaneous printing is crucial for meeting market demand for disposable sensors, as it ensures that supply can keep pace with demand.

#### 11:40 AM

# (ICACC-S15-028-2025) Multi-material component fabrication via co-extrusion additive manufacturing for various applications

L. Biasetto\*1; V. Gastaldi2; H. Elsayed2; G. Franchin2

- 1. Universita degli Studi di Padova Dipartimento di Ingegneria Industriale, Industrial Engineering, Italy
- 2. University of Padova, Industrial Engineering, Italy

Co-extrusion of multi-material structures presents both challenges and opportunities. For ceramics and metals, developing highly loaded pastes is critical for maintaining smooth, homogeneous flow during printing. Proper control of de-binding and sintering is essential to avoid phase separation, cracks, and thermal stresses. Co-axial 3D printing has gained attention for producing unique structural and functional properties in ceramics and ceramic-metal combinations. For instance, Al2O3-GNP (Graphene Nanoplatelets) core-shell structures have been developed using Direct Ink Writing (DIW) to optimize thermal performance. Similarly, Al<sub>2</sub>O<sub>3</sub>-graphite-Al<sub>2</sub>O<sub>3</sub> structures have been robocasted to improve fracture toughness, incorporating a porous interlayer to guide crack propagation, achieving a toughness of 9 MPa $\cdot$ m<sup>0.5</sup> and a bending strength of 200 MPa. This study explores various core-shell combinations for specific applications, such as 316L-CaTiSiO<sub>5</sub> bio-scaffolds with enhanced strain energy density, 316L-Al<sub>2</sub>O<sub>3</sub> cellular structures that improve fracture resistance while preserving ceramic strength, and Cu-Al<sub>2</sub>O<sub>3</sub> structures for electrical applications. The development of inks, co-extrusion setups, and de-binding and sintering processes are examined for their impact on the structural and functional properties of the final components.

### **<u>S16 Geopolymers Inorganic Polymers and</u>** <u>Sustainable Construction Materials</u>

# S16- Sustainable construction materials and waste materials

Room: Ballroom 1-2

Session Chair: Isabella Lancellotti, University of Modena and Reggio Emilia

#### 8:30 AM

# (ICACC-S16-016-2025) Revalorization of Coal Mine Tailings for the Development of Geopolymer Composites (Invited)

P. Mokhtari\*<sup>1</sup>; J. Lin<sup>1</sup>; P. Numkiatsakul<sup>1</sup>; W. M. Kriven<sup>2</sup>

- 1. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA
- 2. University of Illinois at Urbana-Champaign, USA

Revalorizing coal mine tailings, the small waste mineral particles from coal ore processing, offers a significant opportunity to address environmental and industrial challenges. These tailings, often disposed of in ponds, pose ecological risks due to reactive minerals like oxides and sulfides, which can contaminate water sources. Annually, over 180 million tons of this hazardous waste are dumped into water bodies, exceeding the amount landfilled in the U.S. Our study aims to create mine tailing-based geopolymer composites (MTGCs) by combining coal mine tailings with alkali solutions. The U.S. generates around 450 million metric tons of tailings annually from mineral deposits like copper, iron, lead, zinc, and coal, with about 70% suitable for revalorization. This revalorization for industrial uses-such as construction materials, pigments, and additives-reduces CO2 emissions and is cost-effective. Our results show that substituting 50 wt.% of metakaolin with valorized mine tailings does not compromise the composite geopolymer's mechanical properties, proving it feasible to reduce metakaolin usage by 50 wt.% using this waste material as a precursor.

#### 9:00 AM

# (ICACC-S16-017-2025) Environmental aspect of alkali activated products and geotechnical materials (Invited)

M. Pavlin\*<sup>1</sup>; K. Fifer Bizjak<sup>1</sup>; V. Ducman<sup>1</sup>

1. Zavod za Gradbenistvo Slovenije, Slovenia

Compliance with technical regulations is essential for the use of building products and materials in the construction sector. However, compliance with regulations on harmful substances is just as important. In Europe, this was underlined once again by the revised Construction Products Regulation (CPR), which was adopted in April 2024. Nevertheless, environmental compatibility is not regulated uniformly in Europe or worldwide. The definition of hazardous substances and their limit values is the responsibility of the individual countries. Particular attention must be paid to alkali-activated materials (AAMs), where alkaline components added to the mixture can be released into the leachate if they are not completely consumed during alkali activation. This can lead to higher dissolution of certain elements or lower binding efficiency due to the partially amorphous microstructure of the AAMs. A suitable mixture design is crucial to control these aspects. This issue is also relevant for soil stabilization processes, where highly alkaline media such as cement, lime or alkaline activators are often used and where the requirements for allowable limits are also more stringent. In this work, the results of leaching tests on AAMs and soils stabilized with various additives are presented and discussed.

#### 9:30 AM

#### (ICACC-S16-018-2025) Durability of geopolymer mortars from feldspar waste: Nitric and sulfuric acids resistance, phase evolution and microstructure (Invited)

A. Nana<sup>1</sup>; S. Tome\*<sup>4</sup>; E. Kamseu<sup>2</sup>; C. Leonelli<sup>3</sup>

- 1. Universite de Dschang, Chemistry, Cameroon
- 2. MIPROMALO, Research, Cameroon
- 3. University of Modena and Reggio Emilia, Department of Engineering Enzo Ferrari, Italy
- 4. Leibniz University of Hannover, Institute of Mineralogy, Germany

The incongruent dissolution of fine mineral feldspathic particles in alkaline solution develops different N-A-S-H phases and polysialate geopolymers. This binder can be used to produce geopolymer mortars with interesting performances. In this investigation, the behavior of feldspar-based geopolymer mortars under nitric and sulfuric acid attack as well as seawater attack provides an understanding of their degradation mechanisms. Geopolymer mortars were cast using feldspar quarry waste (pegmatite) altered with 20-30 wt% of calcined clay and mixed with river sand, then, activated in the alkaline medium. Physico-mechanical, microstructural and structural characterizations were carried out on geopolymer specimens. From the results, the appearance of samples showed a degradation with the time of exposure and the type of solution used from seawater to sulfuric acid. The comprehensive strength showed the lost after 90 days to seawater, nitric and sulfuric acids attack which decreased from 58.6 MPa to 30.8, 10.8 and 7.9 MPa, respectively. Similarly, significant deterioration of microstructure was observed after immersion in acid solutions, which is more pronounced in sulfuric acid compared to nitric acid.

#### 10:20 AM

#### (ICACC-S16-019-2025) Evaluation of the pozzolanic reactivity of two clays from Côte d'Ivoire for the substitution of clinker in cement

A. N. Kouame\*<sup>3</sup>; W. M. Manouan<sup>1</sup>; L. P. Kouakou<sup>3</sup>; B. H. Goure Doubi<sup>2</sup>; N. Meite<sup>3</sup>

- 1. University of Man, Faculty of Science and Technology, Côte d'Ivoire
- 2. Universite Peleforo Gon Coulibaly, Mathematics, Physics and Chemistry, Côte d'Ivoire
- 3. Universite Felix Houphouet-Boigny, Laboratory of Constitution and Reaction of Matter, Côte d'Ivoire

This study is a contribution to the valorization of clays as natural pozzolans for the substitution of clinker in cement. Two clays, ME1 and ME2, calcined at 710°C, were used in this study. Chemical analysis of the raw samples by ICP\_AES revealed that they are mainly composed of three oxides, silica, alumina and iron. The crystalline phases highlighted by X-ray diffraction showed the presence of quartz, kaolinite and iron compounds in the raw samples and only quartz and hematite in the calcined samples following the dehydroxylation of kaolinite and goethite. Laser particle size tests showed a spread distribution of 3 populations centered at approximately 2, 10 and 39  $\mu$ m for the raw samples and a single population centered at 39.23 and 133 µm for ME1\_710°C and ME2\_710°C, respectively. The results of the pozzolanic activity carried out by the saturated lime test showed a significant reactivity for calcined samples with a Ca(OH)2 consumption capacity of more than 80% after 7 days compared to about 48% for raw samples. Evaluation of the remaining amounts of Ca2+ and OH- ions showed good pozzolanic reactivity of the calcined samples.

#### S16- Use of waste materials to make geopolymers

Room: Ballroom 1-2

Session Chair: Cengiz Bagci, Hitit University

#### 10:40 AM

# (ICACC-S16-020-2025) Egg derived porous plasma modified clay composite for wastewater remediation

G. Mbafou Fondjo<sup>\*1</sup>; E. Acayanka<sup>1</sup>; F. T. Boyom<sup>1</sup>; J. Tarkwa<sup>1</sup>;

G. Y. Kamgang<sup>1</sup>; S. Laminsi<sup>1</sup>

1. Universite de Yaounde I, Départment of Inorganic Chemistry, Cameroon

This study focuses on the development of adsorbents from kaolinite and eggshells by calcination and glidarc plasma methods for the application in the removal of dyes in aqueous solutions. The adsorbent was prepared by mixing kaolinite and eggshells with a mass ratio 3:1 (3 kaolinite for 1 eggshells). The latter was then calcined at 800 °C and treated by the sliding of plasma process (ESC-800/PL). The resulting materials were characterized by pH measurement at zero charge's point (pHZPC), Fourier Transformed Infrared spectroscopy, X-ray diffraction, thermogravimetric analysis, nitrogen physisorption. The preparation gives porous platelet agglomerates resulting from the transformation of kaolinite, thereby increasing their internal specific surface area and capacity to retain pollutants. This granular distribution is kept stable by partial pozzolanic reactions avoiding deagglomeration. The specific surface area and total pore volume increased from 14 m2.g-1 to 89 m2. g-1 and 0.049 cm3. g-1 to 0.061 cm3. g-1 respectively leading to an enhanced removal efficiency of Fast Green (FG) and Orange G (OG) dyes from polluted water. At 298 K, the maximum adsorption capacity values were 32.34 and 14.78 mg.g-1 for OG and FG respectively. The experimental data were successfully adjusted to pseudo-first-order kinetic and Liu isotherm model.

#### 11:00 AM

#### (ICACC-S16-021-2025) Enhancing the Value of Spent Zn-C Batteries, steel slag, and Construction & Demolition Waste via Geopolymer Composites

H. A. Colorado L.\*1

1. Universidad de Antioquia, Colombia

There is a significant risk of pollution due to the excessive consumption of energy and materials that need to be reused, recycled, or reduced. New environmentally friendly geopolymer binders have been developed using metakaolin, construction and demolition waste, steel slag, and battery waste powders as base materials. The microstructure, mechanical properties, and gamma shielding of the geopolymer composites was studied. The findings showed that these wastes into the inorganic cement is a good solution for building and irradiation shielding applications.

#### 11:30 AM

### (ICACC-S16-022-2025) Mild alkali activation employed for sustainable upcycling of glassy and volcanic residues

E. De Rienzo<sup>1</sup>; F. Carollo<sup>3</sup>; A. D'Angelo<sup>2</sup>; L. Barbieri<sup>1</sup>; E. Bernardo<sup>3</sup>;

- M. Catauro<sup>2</sup>; C. Leonelli<sup>1</sup>; I. Lancellotti<sup>\*1</sup>
- 1. University of Modena and Reggio Emilia, Department of Engineering Enzo Ferrari, Italy
- 2. Universita degli Studi della Campania Luigi Vanvitelli, Department of Engineering, Italy
- 3. Universita degli Studi di Padova, Department of Industrial Engineering, Italy

Alkali activation of aluminosilicates (A/S) represents a material- and energy-efficient strategy for producing alternatives to traditional ceramic materials for the construction sector. It involves the dissolution of A/S in alkali solutions, resulting in a solid 3-D network with high mechanical performance. The process avoids  $CO_2$  emissions associated with high-temperature consolidation and, depending on the starting material, calcination, and is suitable for up-cycling of A/S-rich residue that is otherwise difficult to reutilize, such as waste glass (WG) from electrical equipment (fluorescent lamps, photovoltaic panels), or tailings from volcanic rock quarries (VT). The study employs WG of various grain size as the main component of the material's matrix, using VT as a fine matrix supplement or coarse aggregate, and explores the conditions for effective activation in dilute alkali solutions (3 molar or less). The products' activation degree was evaluated by XRD, SEM, FTIR, and TG/DTA, and their properties of integrity under environmental stress, mechanical strength, metal leaching in water, and antimicrobial activity were tested. The properties of the successfully activated formulations were related to matrix grain size and consolidation temperature. Fundings: PRIN 2022 PNRR project #P2022S4TK2 GLASS-based TREAtments for Sustainable Upcycling of inorganic RESidues (GLASS\_Trea.S.U.Res).

### **S18 Ultra-High Temperature Ceramics**

#### **S18-** Compositionally Complex UHTCs II

Room: Coquina H

Session Chairs: Zhe Cheng, Colorado State University; Yue Zhou, Missouri University of Science & Technology

#### 8:30 AM

#### (ICACC-S18-040-2025) Synthesis, Processing, and Characterization of Multi-component High-Temperature Ceramics (Invited)

Z. Cheng $^{*1}$ 

1. Colorado State University, Mechanical Engineering, USA

Multi-component high-temperature ceramics, from fine powders to bulk materials, including selected carbides (e.g., (Hf,Ta)C), borides (e.g., (Hf1-xZrx)B2)), nitrides (e.g., (Nb1/3Ta1/3Ti1/3)N), carbonitrides (e.g., (Hf0.2Ta0.2Zr0.2Nb0.2V)C1-xN, are synthesized and processed using different techniques. The obtained ceramics are characterized for their composition, microstructure, as well as physical-chemical properties such as thermal oxidation resistance, mechanical hardness, fracture toughness, and electrical resistivity. Common features across different systems will be identified, while the differences and challenges, both in terms of experimental implementation and theoretical explanation, will be highlighted. Finally, future directions for future research for these multi-component high-temperature ceramics will also be discussed.

#### 9:00 AM

#### (ICACC-S18-041-2025) Accelerated discovery of oxidationresistant ultra-high temperature ceramics via data driven methodology

K. Wang\*1; M. Sevem1; Y. Yan1; S. T. Misture2

- 1. Alfred University, USA
- 2. Alfred University, MSE, USA

Machine learning (ML) methods have been successfully applied to predict the properties of novel materials. However, the application of ML to ultrahigh temperature ceramics (UHTCs) remains limited due to serious data scarcity and quality issues. In this study, we trained an ML model on high-temperature oxidation resistance data of compositionally complex diborides (CCBs)-SiC composites collected through high-throughput experiments (HTEs). The uniform experimental conditions of HTEs facilitated the generation of a high-quality dataset for ML training. We performed high-temperature oxidation tests on materials synthesized using different methods, including spark plasma sintering (SPS) of monolithic diboride powders and reactive SPS using transition metal and boron powders. The results of these oxidation tests were used to train machine learning algorithms, providing a predictive framework for oxidation resistance based on transition metal compositions. Artificial Neural Network (ANN) and Kernel Logistic Regression (KLR) models outperformed other ML models, with the KLR model rapidly identifying optimal compositions with exceptional oxidation resistance. This novel data-driven approach can significantly accelerate the discovery of high-temperature ceramic compositions, improving efficiency in future research.

#### 9:20 AM

### (ICACC-S18-042-2025) Interdiffusion in the ZrB2 – HfB2 system

Y. Zhou\*1; W. Fahrenholtz1; G. Hilmas1

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

The interdiffusion of Zr and Hf in the ZrB2 - HfB2 system was studied using diffusion couples. ZrB2 and HfB2 powders were synthesized by boro-carbothermal reduction. The materials used for synthesis were commercial ZrO2 or HfO2 along with B4C and carbon black. The synthesized powders were densified by spark plasma sintering. After fabrication of bulk ceramics, specimens were sectioned and polished. Polished surfaces of ZrB2 and HfB2 ceramics were used to make diffusion couples that were annealed at temperatures ranging from 2000°C to 2200°C for different times. The morphologies and elemental concentrations near the ZrB2 - HfB2 interfaces were characterized using scanning electron microscopy, transmission electron microscopy, and energy dispersive spectroscopy. Interdiffusion flux profiles were constructed based on the EDS line scans, and the interdiffusion coefficients were calculated. Finally, Arrhenius plots were constructed for each element and the corresponding activation energies were calculated.

#### 9:40 AM

#### (ICACC-S18-043-2025) Thermodynamics, Phase Equilibria, Microstructure and Properties of Arc-melted Ternary Borides

I. Savkliyildiz<sup>1</sup>; A. Celik<sup>1</sup>; Z. Ayguzer<sup>1</sup>; J. Ligda<sup>2</sup>; D. J. Magagnosc<sup>2</sup>; K. D. Behler<sup>2</sup>; R. Haber<sup>1</sup>; E. Akdogan<sup>\*1</sup>

- 1. Rutgers The State University of New Jersey, Materials Science & Engineering, USA
- 2. DEVCOM-Army Research Lab, Ceramics and Transparent Materials Branch, USA

Transition metal diborides, also known as ultra-high-temperature ceramics (UHTC), are a class of materials known for their outstanding high melting temperature, high hardness, high electrical and thermal conductivity, chemical stability, good thermal shock resistance, and excellent corrosion resistance. In this study, we investigated the thermodynamics, phase equilibria, microstructure and mechanical properties of ZrB<sub>2</sub>-TiB<sub>2</sub>-HfB<sub>2</sub> (ZTH-B<sub>2</sub>) containing 10% excess B over the temperature range 3500 to RT under 1 atm. Firstly, extensive thermodynamic modeling by using Thermocalc<sup>TM</sup>, which is based on the CALPHAD method, was accomplished. Secondly, experimental work based on arc melting was carried out. Characterization studies included XRD, Raman spectroscopy, SEM and EDS, TEM as well as nano- and macro-indentation (Vickers). We will show that high temperature phase equilibrium in the ZTH-B<sub>2</sub> is obeyed even under nonequilibrium conditions at temperatures above 1700 °C. We will also show that precipitation strengthening with ZrB<sub>12</sub> can indeed be accomplished in the ZTH-B<sub>2</sub> by the judicious use of excess boron. Moreover, a detailed account will be provided regarding the matrix-precipitate interface. Relevant mechanical properties will be reported. A comparison of the ZTH-B<sub>2</sub> microstructure as processed with arc melting and spark plasma sintering will also be provided.

#### 10:20 AM

# (ICACC-S18-044-2025) Effect of the transition metal segregation on the properties of $(Hf,Ti,Zr)B_2-(Hf,Ti,Zr)C$ Dual Phase Ceramics

- S. Filipovic\*1; W. Fahrenholtz2; G. Hilmas2; N. Obradovic3; S. Curtarolo4
- 1. Missouri University of Science & Technology, Materials Research Center, USA
- 2. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA
- 3. Institute of technical sciences of SASA, Materials, Serbia
- 4. Duke University, Materials Science, Electrical Engineering and Physics, USA

Dual phase mid entropy ceramics are attractive due to potential synergistic effects of the constituents on mechanical properties and thermal stability. The co-synthesis method was used to obtain boride and carbide constituents by boro/carbothermal reduction of mixtures of oxides and appropriate amounts of carbon black and B<sub>4</sub>C. Solid solution formation and densification of the reacted powders were done at 1900 °C or 1950 °C utilizing two-step spark plasma sintering. Chemical compositions were measured using energy dispersive spectroscopy. Based on the transition metal distribution in the dual phase ceramic, individual mid entropy boride and carbide ceramics were produced using the same conditions. The final microstructures had submicron grains due to the pinning effect of the two phases, while grain sizes of the individual mid entropy carbides and borides were higher than the two-phase ceramics. Vickers hardness values for dual phase ceramics were higher than values calculated using a volumetric rule mixtures from individual components. Thermal and electrical properties were also higher values than calculated using volumetric rule mixtures of individual components. Thermal conductivity of the optimized dual phase ceramic produced at 1950 °C displayed an increase of ~15% compared to the constituent phases.

### <u>FS1 Bioinspiration/Green Processing &</u> <u>Related Technologies of Advanced Materials</u>

# FS1- Aqueous synthesis and green processing of advanced materials

Room: Flagler C Session Chair: Florian Bouville, ETH Zürich

#### 1:30 PM

## (ICACC-FS1-007-2025) Nanocluster induced crystallization: in situ visualization and 3D reconstruction (Invited)

Z. Zou\*1; Z. Fu2

- 1. Wuhan University of Technology, China
- 2. Wuhan University of Technology, State Key Lab of Advanced Technology for Materials Synthesis and Processing, China

Revealing the crystallization mechanism of inorganic materials modulated by organic molecules has broad implications in biomineralization, crystallography, and materials science. However, directly visualizing the participation of organic molecules in the inorganic materials crystallization process remains a significant challenge. Here, we introduce carboxyl-functionalized gold nanoclusters (AuNCs) as an alternative to polymers for investigating CaCO3 crystallization via the transient "AuNCs-induced liquid precursor" phase, similar to "polymer-induced liquid precursor". Exploiting the ultrasmall size, high density and spontaneous fluorescence properties of AuNCs, this approach enables direct in situ observation of AuNCs-containing liquid precursor formation and dynamic association/dissociation using light microscopy. The occlusion and 3D spatial distribution of AuNCs within CaCO3 throughout the crystallization process can be visualized using confocal fluorescence microscopy and transmission electron microscopy, demonstrating

preferential adsorption on specific lattice planes of CaCO3. This study significantly advances our understanding of the roles of biomacromolecules during biomineralization and provides a promising tool for investigating crystallization mechanisms.

#### 2:00 PM

## (ICACC-FS1-008-2025) Creating biomorphic strontium sulfate ceramics through polysaccharide incorporation (Invited)

- V. Merk\*1; C. Detwiler Gray2; A. Coronel-Zegarra1; D. Raja Somu1;
- A. Martin<sup>1</sup>; J. Walker<sup>3</sup>
- 1. Florida Atlantic University, Chemistry & Biochemistry, Ocean & Mechanical Engineering, USA
- 2. Florida Atlantic University, Chemistry and Biochemistry, USA
- 3. Diamond Light Source Ltd, 114 Hard X-ray Nanoprobe, United Kingdom

Living organisms sculpt complex mineral architectures by incorporating biomacromolecules into the inorganic lattice. This study focuses on the crystallization of strontium sulfate (celestine, SrSO<sub>4</sub>) in the presence of water-soluble charged polysaccharides, such as heparin, hyaluronan, chitosan, and pectin. We studied the degree of polysaccharide incorporation into SrSO<sub>4</sub> and how it affects the final properties of the organo-inorganic composites. As shown by electron microscopy, the mineral shapes formed under the influence of sugars deviate significantly from the equilibrium morphology. We further investigated how biomolecules are involved in modulating and controlling ceramic morphology and nanostructure by inhibiting crystal growth in specific directions using synchrotron-based scanning nanofocus X-ray diffraction, Transmission Electron Microscopy and Raman spectro-microscopy. This multimodal microscopic investigation sheds light on how physically entrapped polysaccharides affect the mesoscale crystal architecture and coherence length. Transferring biological construction principles to synthetic crystal growth and design can offer an avenue for engineering biomorphic ceramics under ambient conditions. Acknowledgements: VM is indebted to funding from the National Science Foundation (DMR-2137663). CDG thanks the Microscopy Society of America for an Undergraduate Research Fellowship.

#### 2:30 PM

# (ICACC-FS1-009-2025) Photocatalytic substrates by organic-free direct ink writing and cold consolidation of aqueous suspensions of waste glass (Invited)

S. Paolo<sup>2</sup>; A. Ourgessa<sup>2</sup>; J. Kraxner<sup>2</sup>; H. Elsayed<sup>1</sup>; D. Galusek<sup>2</sup>; E. Bernardo<sup>\*1</sup>

- 1. University of Padova, Department of Industrial Engineering, Italy
- Trencianska Univerzita Alexandra Dubceka v Trencine Centre for Functional and Surface Functionalized Glass, Slovakia

A key requirement direct ink writing 3D printing is the pseudoplasticity of pastes. The transition from a low viscosity state (at high shear rates) to a high viscosity (at low shear rates), favours ejection from nozzles and shape preservation, respectively. A fundamental example of fully inorganic inks is provided by geopolymer-yielding slurries, from the suspension of metakaolin in concentrated aqueous solutions of alkali hydroxides and silicates. The pseodoplastic behaviour is determined by the progression of polymerization reactions. The present paper aims at offering strategies for an even more sustainable processing. Fine glass powders (<70 µm, recovered from pharmaceutical containers or fibre insulators or deriving from the melting of inorganic waste) undergo a quite particular interaction with diluted alkaline solutions: slurries show progressive hardening by condensation reactions involving just hydrated layers, on the surface of glass powders, formed upon disruption of glass network operated by OH<sup>-</sup> ions. These reactions imply the regeneration of Si-O-Si and Si-O-Al bonds, as strong and durable bridges between adjacent particles. Slurries in the early stages of reaction may be used as pseudoplastic pastes, for the manufacturing of reticulated constructs. These products are directly usable, as catalytic supports, just after drying at 40-80 °C.

#### 3:20 PM

#### (ICACC-FS1-010-2025) In situ photoluminescence spectroscopy for monitoring phase evolution under pressure at room temperature (Invited)

C. Packard\*1

1. University of Southern California, Mork Family Department of Chemical Engineering & Material Science, USA

Pressure-induced phase transformation presents an interesting parallel to thermally driven transition, but it is more difficult to study because the confinement that generates the pressure limits the access of characterization probes. Synchrotron x-ray diffraction and Raman spectroscopy are frequently used for phase identification, monitoring pressure, and identifying the onset of transformation. This talk contrasts the information gathered from those techniques with that generated from in situ photoluminescence spectroscopy using the phase transition in a rare earth orthophosphate ceramic as a case study. Photoluminescence spectroscopy is uniquely sensitive to the local bonding environment of a structure, is widely available, and produces data with high signal-to-noise. We find that direct excitation photoluminescence spectroscopy detects the xenotime-monazite phase transition onset and end pressure in TbPO4 consistent with synchrotron x-ray diffraction results, while also showing more subtle changes in certain band intensity ratios that can be connected to stress history. Using various characterization modalities provides a richer understanding of the structural distortions experienced during and after pressure-induced phase transition.

#### 3:50 PM

# (ICACC-FS1-011-2025) Grain-refinement fabrication of ceramics by ultra-high-pressure low-temperature sintering

W. Ji\*1

1. Wuhan University of Technology, China

Zirconium carbide (ZrC) with an ultra-high melting point is applicable for severe environments. However, it is difficult to fabricate high-performance ZrC and its application scope is limited. In the study, fully dense ZrC with refined grains and high boundary dislocation density was fabricated under the conditions of 15 GPa and 1400°C. The fabricated ZrC showed excellent plasma corrosion resistance and mechanical properties, including the hardness of 23.76 GPa and the elastic modulus of 410.31 GPa. The grain size was 64.6% smaller than that of raw powder. Compared with the control specimen sintered above 1900°C under 200 MPa, the ultra-high pressure sintered ZrC realized 3 orders of magnitude higher dislocation density and 74.1% smaller grain size.

#### 4:10 PM

#### (ICACC-FS1-012-2025) Microwave synthesis of nano-Hydroxyapatite from decarbonized eggshells: A sustainable and eco-friendly approach (Invited)

M. M. Mahmoud\*1

1. Abdullah Al Salem University, Materials Science and Engineering, Kuwait

Microwave (MW) synthesis of hydroxyapatite (HAp) from decarbonized eggshells was investigated. The decarbonization was done at ambient conditions to diminish the environmental impact of  $CO_2$  emissions released when eggshells were either calcined or directly treated with acids. To turn eggshells into  $Ca(OH)_2$  and store  $CO_2$  as  $Na_2CO_3$  by-product, eggshell decarbonization was done using NaOH. Before being exposed to MW irradiation at 2.45 GHz frequency for 5 minutes using 800 Watts, the generated  $Ca(OH)_2$  was combined with  $NH_4H_2PO_4$  reagent at pH~11. Using XRD and the Scherrer equation, the produced nano-HAp was characterized to have a crystal size of ~ 28 nm. SEM/EDS, FTIR, and TEM were used to analyze the elongated rod-like nano-HAp crystals. A sustainable and eco-friendly method of producing potential bioceramics like

nano-HAp was achieved. Furthermore, eggshell decarbonization simultaneously provides the capacity to store  $CO_2$  as a highly valuable  $Na_2CO_3$  which is necessary in many industrial sectors.

### FS5 High Voltage Materials for Advanced High Power Electrical Applications

### FS5- High Voltage Materials for Advanced High Power Electrical Applications I

#### Room: Coquina H

Session Chairs: Maricela Lizcano, NASA Glenn Research Center; Kristina Vailonis, NASA Glenn Research Center

#### 1:30 PM

#### (ICACC-FS5001-2025) Field Emission from 3D Graphene as a Cathode Prepared by Chemical Vapor Deposition and Cold Rolling (Invited)

N. Hernandez\*<sup>1</sup>; R. Piovesan Azumbuja<sup>1</sup>; M. Cahay<sup>1</sup>; J. Ludwick<sup>2</sup>; T. Back<sup>2</sup>; A. Raut<sup>3</sup>; M. Marzana<sup>3</sup>; V. Kondapalli<sup>3</sup>; Q. Fang<sup>4</sup>; V. Shanov<sup>4</sup>

- 1. University of Cincinnati, Electrical and Computer Engineering, USA
- 2. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
- 3. University of Cincinnati, Mechanical and Materials Engineering, USA
- 4. University of Cincinnati, Chemical and Environmental Engineering, USA

A new architecture of 3-Dimensional Graphene (3DG) has been achieved by Dr. Shanov's group at the University of Cincinnati through Chemical Vapor Deposition (CVD) and cold rolling. The performed comprehensive materials characterization of 3DG revealed micro-motion of the graphene flakes from their random orientations into a stacked and aligned structure along with the extrusion of bulk material into the structural pores which acted as stress-relief spaces. The obtained new bulk morphology significantly enhanced its properties causing an increase in 3DG density, strength and electrical conductivity. Field Emission (FE) from this novel material, initiated either from the surface of the sheet or from its edge, has been explored and reported here. For a given distance between the tip of the cathode and the anode, it was found that the FE current from the edge of a single sheet of cold rolled 3DG-based cathode can be increased by over one order of magnitude when rolling the 3DG sheet in the shape of a cylinder with several turns. A FE current in the order of 4.5 mA was measured from a 3 mm diameter cold rolled 3DG cylinder with 6 turns at a bias of 2400 V for a separation of 0.5 mm between the tip of the cylindrical cathode and the anode.

#### 2:00 PM

#### (ICACC-FS5002-2025) Automated Materials Discovery with Machine Learning for the Optimization of Aerospace-grade Electrical Insulation

D. Santiago\*1; J. Stuckner1; M. Lizcano1; M. Kelly1

1. NASA Glenn Research Center, USA

Developing new aerospace materials with multi-functionality can be a time consuming and complex process. There is a growing trend to combine laboratory automation with machine learning to modernize materials processing methodology and reduce discovery time with little human interaction. Benefits of a fully automated material processing lab have recently been demonstrated with a NASA-developed machine learning tool on candidate aerospace electrical insulation for high altitude, high power (> 10 MW) electrified aircraft propulsion systems. This presentation will give an overview of our findings from coupling automated materials processing with machine learning to optimize the development of thermally conductive electrical insulation for next generation electrified propulsion systems.

#### 2:20 PM

#### (ICACC-FS5003-2025) Manufacturing and Characterization of Multilayer Graphene-Copper Wires

R. A. Paddock\*1; M. Tehani2; M. Cullinan1

- 1. The University of Texas at Austin, Walker Department of Mechanical Engineering, USA
- 2. University of California San Diego, Structural and Materials Engineering, USA

Copper's high electrical and thermal conductivity are why this material is used for various industrial products. However, challenges related to the material's weight and performance in extreme environments limit copper's usage in aerospace applications. Adding multilayer graphene (MLG) to a copper substrate using chemical vapor deposition (CVD) improves this conductor's performance in high-temperature applications, while not significantly contributing weight to the final product. This graphene-copper composite begins as a singular foil that is then consolidated into a wire through repeated annealing and roller drawing reductions. A reference wire made from the same copper foil without graphene is compared to the composite sample to highlight the benefits of graphene during the cross-sectional consolidation and resulting electrical conductivity tests. This research correlates the composite's resulting material properties to the microstructure and creation process. Based on the resulting data, recommendations are given on how to reduce void defects and improve the quality and performance of the graphene-copper composite wires.

#### 2:40 PM

#### (ICACC-FS5004-2025) Graphene-Based Composite Conductors for Aerospace Applications

Y. Bekele<sup>\*1</sup>

1. University of Texas, Walker Department of Mechanical Engineering, USA

This thesis explores the utilization of copper-graphene composite conductors as an alternative to traditional copper conductors for aerospace applications. Previous studies have indicated that coppergraphene composites can achieve higher electrical conductivity compared to traditional copper conductors with a relatively low graphene loading. In this paper, the feasibility of achieving higher graphene loadings is investigated by transferring high-quality graphene onto thin copper films and annealing of these thin films under various conditions to maximize conductivity. Additionally, different graphene transfer methods is explored to ensure that the transferred graphene on the copper film achieves a high coverage and is defect-free. Lastly, the electrical properties of the composite are investigated and compared to those of a pure copper conductor and a reference sample.

#### FS5- High Voltage Materials for Advanced High Power Electrical Applications II

Room: Coquina H

Session Chairs: Diana Santiago, NASA Glenn Research Center; Rachel Paddock, The University of Texas at Austin

#### 3:20 PM

## (ICACC-FS5005-2025) Novel Power Transmission Solutions for Megawatt Scale Electric Aircraft

M. Lizcano<sup>\*1</sup>; D. Santiago<sup>1</sup>

1. NASA Glenn Research Center, USA

NASA's goal for sustained and green aviation has inspired the development of novel power transmission materials for extreme environments, including electrical insulation. As an increasing number of public and private entities set their sights towards electrified flight in transportation, the demand for power will continue increasing to megawatt levels for high altitude flight. High voltage (≥ 300 V) is utilized to reduce electrical wiring conductor weight. The resulting consequences of high voltage are vulnerabilities to partial discharge from high electric fields. Although transmission lines to propulsors are more easily addressed through gas insulation system or thicker insulation, these power transmission lines are relatively short, approximately a 100 ft in length. The distributed power to other electrical systems is more difficult to manage with thicker insulation. The need for novel lightweight electrical insulation solutions becomes obvious when considering that high altitude flight aircraft can have 100's of miles of wiring within a single aircraft and are not yet fully electric. In this talk, advances in novel electrical insulation materials and structures solutions at NASA Glenn Research Center with be discussed providing a path to achieving high power high altitude all electric aircraft.

#### 3:40 PM

#### (ICACC-FS5006-2025) Interfacial fracture toughness of GaN film on diamond substrate for application in ultra-high power RF devices

D. Liu\*1

1. University of Oxford, Engineering Science, United Kingdom

GaN thin film (~800nm) integrated to polycrystalline diamond (~100µm) is a novel microwave transistor material with significantly improved heat dissipation capability. GaN, Ga2O3 and Diamond are also high voltage power electronics materials where heterogenous integration is essential. Therefore, a mechanically stable interface is the key for extended device life and reliability. In this work, the interfacial toughness of three generations of GaN-on-Diamond materials has been measured by in situ cantilever bending and ex situ nano-indentation induced buckling methods. For the latter, four models including Evan&Hutchinson, Marshall&Evans, Hutchinson&Suo and a two-step approach have been used and their suitability on this ceramic/rigid-substrate system are discussed. The interfacial toughness, G<sub>1</sub>, was 0.7, 0.9 and 0.6 J/m<sup>2</sup>, respectively, for the three materials. Postmortem imaging of the fracture interface indicates that those with better heat spreading capability and smoother fracture surfaces were less tough due to the lack of active toughening mechanisms. Nevertheless, the interfacial toughness in all three materials is in a similar range as most other commercial material systems.

#### 4:00 PM

#### (ICACC-FS5007-2025) Space Charge Analysis Capabilities for the Evaluation of High Voltage Insulation Materials (Invited)

K. Vailonis<sup>\*1</sup>; T. Benyo<sup>1</sup>

1. NASA Glenn Research Center, USA

Materials development is crucial for the advancement of electric aviation. Current research focusing on novel multifunctional materials is underway to solve the needs for aerospace systems; however, additional testing of these materials to understand their failure modes is equally critical. This project will utilize pulsed electroacoustic (PEA) instrumentation to investigate space charge accumulation of multifunctional composites and other insulation materials critical to robust high power transmission systems. Evaluating the space charge phenomena in dielectric materials will provide unique and fundamentally necessary data to determine the feasibility and lifetime of any high voltage insulation system. When electrical charge is injected into a solid dielectric, charge can accumulate and become trapped, leading to the failure of the insulation via breakdown or arcing events. This study will discuss the pulsed electroacoustic methodology and its use on evaluating various dielectric polymer and composite films.

#### 4:30 PM

# (ICACC-FS5008-2025) Reactive Exfoliation of Hexagonal Boron Nitride by Aluminum and Titanium Nitrides (Invited)

C. Brady\*1

1. NASA, USA

Hexagonal Boron Nitride (hBN) has become a material of interest in aerospace applications due to its favorable properties such as high in-plane thermal conductivity, electrical resistivity, and stability in a range of thermal and chemical environments. Exfoliation of hBN platelets yields 2-dimensional sheets with nano-scale thicknesses, or Boron Nitride Nano-Sheets (BNNS). Such engineered particles may be used to impart useful dielectric and thermal management properties to electrical insulation materials, for example. Researchers at NASA Glenn Research Center have previously demonstrated chemical exfoliation by metal halide and metal-organic intercalation and subsequent thermal processing to produce BNNS with remaining intercalant reaction products. This work investigates the reactive exfoliation of hBN by intercalated metal species, specifically by nitriding of aluminum and titanium. Commercially available hBN particles were intercalated, heat treated in a tube furnace under forming gas atmosphere to temperatures ranging from 600-1450°C, and the exfoliated products analyzed by X-ray diffraction. The reaction pathways and phase evolution as a function of exfoliation temperature are elucidated herein.

#### 5:00 PM

#### (ICACC-FS5009-2025) Electrical insulation at high-temperatures: A case study for reactively grown AlN thin films

N. Salvadores Farran\*<sup>5</sup>; T. Wojcik<sup>1</sup>; C. Jerg<sup>2</sup>; A. Gies<sup>2</sup>; J. Ramm<sup>2</sup>; S. Kolozsvári<sup>6</sup>; P. Polcik<sup>6</sup>; J. Fleig<sup>3</sup>; T. M. Huber<sup>3</sup>; H. Riedl<sup>4</sup>

- 1. Technische Universitat Wien, Institute of Material Science and Technology/E308, Austria
- 2. OC Oerlikon Balzers AG, Liechtenstein
- 3. Technische Universitat Wien, Chemical Technologies and Analytics, Austria
- 4. TU Wien, Institute of Materials Science and Technology, Austria
- 5. Christian Doppler Laboratory for Surface Engineering of
- high-performance Components, TU Wien, Austria, Austria
- 6. Plansee Composite Materials GmbH, Lechbruck am See, Germany, Germany

Aluminum nitride-based ceramics are renowned for their insulating properties and high thermal conductivity. Their range of applications is vast, whether as structural components or thin films. As the electrical conductivity is highly depended on the temperature, the mobility of charge carriers at elevated temperatures causes distinct challenges for insulating thin film materials. Therefore, in this study the growth of insulating AlN thin films via PVD and their electrical insulation up to 750 °C is in focus. For the growth various reactive PVD routes have been explored, including magnetron sputtering (DCMS), high-power pulsed magnetron sputtering (HIPIMS), and pulsed magnetron sputtering (PMS). For all depositions a 3" Al target was used in mixed Ar/N2 atmospheres. Phase formation has been examined using XRD, while the deposition rate and film morphology were investigated through SEM and TEM. The insulating behavior of the coatings was analyzed using in-situ impedance spectroscopy across a temperature range from RT to 750°C utilizing differently sized Ti/Pt lithography pads. The electrical properties are closely related to the morphology of the film, with the densest HIPIMS grown films exhibiting the highest electrical resistance over temperature. Nevertheless, the influence of impurities, such as O2, plays a significant role in reducing the insulating properties of the films.

### <u>S1 Mechanical Behavior and Performance of</u> <u>Ceramics & Composites</u>

#### **S1-** Ceramic Matrix Composites (CMCs)

# Thermomechanical Performance and Environmental Effects

Room: Coquina E

Session Chairs: Yuanxin Zhou, GE Aviation; Craig Smith, NASA Glenn Research Center

#### 1:30 PM

# (ICACC-S1-056-2025) Environmental effects on the interlaminar shear behavior and bearing failure of oxide/oxide ceramic matrix composites (Invited)

K. Sanghvi<sup>1</sup>; J. Lambros\*1

1. University of Illinois Urbana-Champaign, Aerospace Engineering, USA

Oxide/oxide ceramic matrix composites, known for their thermal and environmental stability, are increasingly employed in critical applications where their mechanical performance under various environmental conditions is necessitated. This study investigates the impact of environmental factors - specifically heat treatment, thermal shock, and humidity exposure - on the interlaminar shear behavior and bearing failure of these composites. The interlaminar shear strength and delamination behavior were evaluated using Short Beam Shear (SBS) tests while bearing failure was examined through Half-Hole Pin-Bearing experiments. Both experiments were performed on samples in their as-received state as well as those subjected to one or more of the three environmental conditioning types listed above. Postmortem analysis, including optical and SEM microscopy as well as X-ray tomography, was employed to characterize damage and observe microstructural changes following environmental conditioning. Additionally, Stereo-Digital Image Correlation (3D-DIC) was utilized to measure full-field displacement (both in-plane and out-of-plane) and in-plane strain fields during loading. The findings reveal that environmental conditioning significantly influences, both positively and negatively depending on the conditioning type, the mechanical behavior of the composite samples.

#### 2:00 PM

#### (ICACC-S1-057-2025) High Temperature Mechanical Properties and Damage Mechanisms of Unidirectional SiC/SiC Composites under Tensile Loading

C. Brockman\*<sup>2</sup>; A. S. Almansour<sup>1</sup>; R. K. Goldberg<sup>1</sup>; J. D. Kiser<sup>1</sup>; P. Sarin<sup>2</sup>

- 1. NASA Glenn Research Center, Ceramic and Polymer Composites Branch, USA
- 2. Oklahoma State University, Materials Science and Engineering, USA

Silicon carbide (SiC) based ceramic matrix composites (CMCs) are of interest for high-temperature structural applications, including use in turbine engine components. To understand the damage mechanisms and predict the durability of these systems, in-depth knowledge of their behavior at ambient and high temperatures is necessary. A method to conduct tensile testing of SiC/SiC minicomposites at elevated temperatures to investigate their thermomechanical behavior will be presented. Results from mechanical testing and nondestructive techniques will be presented. Temperature dependence of specimen mechanical properties including elastic moduli, ultimate tensile strength, crack density, and AE-based onset of matrix cracking will be presented and discussed. Understanding surface strain distribution of materials at elevated temperatures could be very useful. Progress on experimental studies coupling AE and digital image correlation (DIC) using a lamp furnace with line-of-sight access to the sample in the hot zone will be discussed.

#### 2:20 PM (ICACC-S1-058-2025) Stress evolution during oxidation of SiC fibers

I. Duan\*1; M. Begley1; F. W. Zok1

1. University of California Santa Barbara, Materials, USA

Stresses in growing oxide scales accelerate the degradation in properties of SiC fibers in SiC/SiC composites. Stress evolution is heavily influenced by the nonlinear creep behavior of silica, and while closed-form stress solutions have been developed for flat substrates, corresponding solutions for cylindrical substrates currently require numerical methods. In the present work, finite element results are used to inform key simplifications regarding the oxidation process and the nature of the stress: coupled ordinary differential equations are then derived for hoop and axial stresses throughout the oxide scale as a function of oxidation time. The predicted stresses match well with those calculated through finite element simulations. The analytical expressions provide insight into the interplay between various material and environmental parameters, and paves the way for predicting critical events such as scale cracking and stress rupture at elevated temperatures.

#### 2:40 PM

# (ICACC-S1-059-2025) Rupture behavior of an orthogonal 3-D woven amorphous SiC fiber/SiC/YSi<sub>2</sub>-Si based matrix composite at elevated temperature in air

Y. Ikarashi\*1; S. Kanazawa2; S. Fukuhara1; T. Watanabe1; Y. Asakura1;

T. Aoki3; T. Matsumoto4; T. Ogasawara4

- 1. IHI Corporation, Japan
- 2. IHI Americas Inc., USA
- 3. Japan Aerospace Exploration Agency, Advanced Composite Research Center, Institute of Aeronautical Technology, Japan
- 4. Tokyo University of Agriculture and Technology, Japan

This study examined the effect of temperature on stress-rupture mechanisms of an orthogonal 3D woven amorphous SiC fiber/SiC/ YSi<sub>2</sub>-Si based matrix composite. Constant load tensile (stress-rupture) testing was conducted at 973 and 1373 K in air. The matrix crack density after stress-rupture testing was evaluated using a digital microscope. To reveal rupture mechanism, microscopic observation after stress-rupture testing was conducted using scanning electron microscope. Stress-rupture testing result showed that the lifetime decreased with decreasing test temperature. The matrix crack density was obviously lower at 1373 K compared to 973 K. The crack sealing by oxide (glass) on several surface cracks were also observed. As the test temperature increase, the oxidation rate of SiC increase. One possible reason for longer lifetime under constant tensile loading at 1373 K is that the crack sealing by glass could have inhibited the fiber/matrix interface oxidation within the internal crack. To attempt crack sealing, the specimen was subjected to constant tensile load at 1373 K for 20 hr. Subsequently, stress-rupture testing at 973 K was conducted until specimen rupture. The lifetime and microscopic observation results of this specimen were compared with that of stress-rupture testing at 973 K (non-sealing specimen).

#### 3:20 PM

# (ICACC-S1-060-2025) In situ measurement of elastic and total strains during ambient and high temperature deformation of a nuclear graphite composite (Invited)

D. Liu\*1

1. University of Oxford, Engineering Science, United Kingdom

Nuclear-grade graphite is a quasi-brittle ceramic-like composite material that is critically important as structural component for current and future fission reactors worldwide. It is imperative to understand its deformation and fracture behaviors under conditions relevant to service. In situ neutron diffraction and synchrotron X-ray diffraction, combined with image correlation analysis of 2D optical and 3D X-ray tomography datasets, have been used to investigate the relationship between elastic lattice strain and total strain during deformation of Gilsocarbon (IM1-24) polygranular nuclear grade graphite composite. The specimens were flat-end Brazilian discs under diametral loading, such that a compressive-tensile biaxial stress state was developed in the central region. The X-ray study was at ambient temperature, and the neutron diffraction was conducted at temperatures from ambient to 850°C. When under compression, there is a temperature-insensitive linear relationship between the total strain and the lattice strain that is measured perpendicular to the graphite basal planes. However, when under tensile stress, there is saturation in tensile lattice strain which is attributed to microcracking in the graphite microstructure. Improved resistance to microcracking and damage tolerance at elevated temperatures explains the increase in tensile strength.

#### 3:50 PM

#### (ICACC-S1-061-2025) Testing and Evaluation of SiC/SiC Interlaminar Tensile Strength at Both Room Temperature and Elevated Temperature

Y. Zhou\*1; K. Maxwell1

1. GE Aviation, Engineering Material System, USA

In this study, flatwise tenile test, L brack flex test, flex ILT test and Brazilian disc compression test have been carried out on SiC/SiC CMC to characterize materials's interlaminar tensile strength (ILT). Amount these mothod, flex ILT and Brazilian disc compression can be used at high temperature. However, due to samples geometry differences, ILT value from different method various. Volume normalization was used to bridge ILT value of different testing method.

#### 4:10 PM

# (ICACC-S1-062-2025) Oxidation behavior of unidirectional ceramic minicomposites

S. Kanazawa\*1; P. Maxwell2; S. Fukuhara3; F. W. Zok2

- 1. IHI Americas Inc., USA
- 2. University of California Santa Barbara, USA
- 3. IHI Corporation, Japan

Oxidative degradation of SiC/SiC composites has been attributed to deterioration of fiber coatings due to internal oxidation. However, the effects of compositional and geometrical heterogeneity on oxidation behavior remain poorly understood. In this study, we investigated the oxidation behavior of unidirectional SiC/SiC minicomposites with matrix cracks of varying widths at 1000 °C in both dry and wet air. In regions with wider crack openings (>  $1.5 \mu m$ ), the BN coatings were heavily degraded, leading to either fiber adhesion to the matrix via oxides in dry air or to the formation of gaps between the fiber and matrix in wet air. Conversely, in regions with narrower crack openings (< 0.2 µm), the matrix cracks were filled with oxides while the BN coatings remained intact. The extent of coating loss, taken as the distance from the matrix crack plane to the intact BN, was found to depend on the distance from the sample surface. The experimental observations were used to devise an internal oxidation model that accounts for the effects of crack opening width and the distance from the specimen surface.

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#### 4:30 PM

#### (ICACC-S1-063-2025) Thermal strain measurement of an orthogonal 3D woven SiC fiber/SiC composite under rapid radiant heating using an infrared lamp

N. Sugawara\*1; y. sone1; T. Ogasawara1; R. Inoue2; T. Aoki3; Y. Kitamura4; H. Sato4

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- 2. Tokyo University of Science, Japan
- 3. Japan Aerospace Exploration Agency (JAXA), Japan
- 4. IHI Corporation, Japan

Turbine blades and vanes in gas turbine engines, which are considered for applying SiC-fiber reinforced SiC matrix (SiC-f/SiC) composites, are subjected to thermal stresses due to the temperature gradient in the components. However, there are few reports on material evaluation tests under the condition of a temperature gradient in the specimen thickness direction, and the effects of thermal gradient have not been elucidated in detail. The objective of this study is to establish an experimental method for evaluating the mechanical behavior of SiC-f/SiC composites under temperature gradients in the specimen thickness direction, and to elucidate the thermal response, damage and fracture behavior. As a temperature gradient testing, a local rapid radiant heating test method using an infrared lamp was examined. The surface temperature and strain distribution at high temperatures were, respectively, measured using a thermography camera, and digital image correlation method (DIC method) under UV light. As a result, it was confirmed that DIC method was effective to measure the strain distributions of the SiC-f/SiC composites at 1300°C. The measured strain distributions was corresponded to the fabric structure.

#### 4:50 PM

### (ICACC-S1-064-2025) Stress-Induced Erosion of Oxide/Oxide Ceramic Matrix Composites in Combustion Environments

F. Mirza\*1

1. University of Akron, Mechanical Engineering, USA

This research examines stress-induced erosion in oxide/oxide ceramic matrix composites under various thermo-mechanical erosive conditions. The experiments include erosion-only, erosion-fatigue, and erosion-creep tests, with impacts from both single and double-sided erosion. Microscopic analysis conducted after each test evaluates erosion patterns. Residual strength tests post-erosion indicate limited reduction in material strength due to stress-induced erosion. However, the erosion process itself visibly undermines material integrity, as evidenced by crack initiation at the bases of erosion craters. Keywords: High-temperature, Stress-induced erosion, Fatigue, Creep, Burner-rig.

#### 5:10 PM

#### (ICACC-S1-065-2025) Experimental Characterization and Modeling of Ablation Behavior of Ceramic Matrix Composites under Hydrogen Combustion Conditions

F. Faysal\*<sup>1</sup>; C. Varela<sup>1</sup>; M. Tonarely<sup>1</sup>; D. Barnhard<sup>2</sup>; C. Maitti<sup>1</sup>; K. Ahmed<sup>1</sup>; Q. Yang<sup>2</sup>; J. Gou<sup>1</sup>

- 1. University of Central Florida, Mechanical and Aerospace Engineering, USA
- 2. University of Miami, Mechanical and Aerospace Engineering, USA

Ceramic matrix composites (CMCs) are known for their endurance in high temperatures. This study investigated the thermo-mechanical performance of the silicon carbide nitride (SiCN) reinforced with yttria-stabilized zirconia (YSZ) fiber for hydrogen-fueled gas turbine engines. To explore its thermal stability at high temperatures, a hydrogen torch test was used to expose the CMC to a high heat flux under hydrogen combustion conditions. In addition, the inner wall of a hydrogen combustion chamber was lined with the CMC to study its application as a protective layer. The composite surface could withstand a temperature of 1,400C for 10 minutes during the torch test. High temperature hydrogen flame also caused the formation of  $SiO_2$  as confirmed from the SEM and XRD measurements. The CMC liner was subjected to hydrogen flame of about 680C at 1 atm pressure and the layer was successful in maintaining 185C at the combustion chamber wall. Analytical and numerical modeling were employed to understand heat conduction process in the CMC. Results generated from numerical model agreed with the experimental data. The results suggest a feasible prospect for the CMC to be used in high temperature application maintaining both its thermal and mechanical stability.

#### 5:30 PM

## (ICACC-S1-066-2025) SiC Ceramics in Extreme Conditions of Wear: Effect of Nitride Reinforcement

N. V. Dorkar<sup>1</sup>; B. Kumar<sup>\*1</sup>

1. Indian Institute of Technology Roorkee, Metallurgical and Materials Engineering, India

While SiC ceramics are considered for wear resistance components, a limited understanding of the effect of composition on wear behaviour in extreme humidity and temperature conditions restricts applicability. The present work exhibits the feasibility of obtaining a wide range in sliding friction and erosive wear resistance of SiC ceramics with nitride (0 to 10 vol%) h-BN and ZrN) reinforcement in extreme conditions of humidity (20% to 90% RH) and temperature (RT to 500°C). A reduction of ~15-50% in COF and ~36-76% in wear rate is observed with h-BN addition, while a reduction of ~20-40% in COF and ~29-79% in wear rate is observed with ZrN addition. Material removal mechanism changed from fracture to hydroxylative and oxidative wear for h-BN reinforcement with varying sliding conditions. In contrast, oxidative wear is dominant for ZrN reinforcement irrespective of sliding conditions. Further, the erosive wear rate of SiC ceramics increased with an increase in impingement angle irrespective of reinforcement. However, reinforcement (h-BN or ZrN) addition of up to 4vol% led to a significant enhancement in resistance to erosive wear. The temperature-dependent erosive wear resistance is explained with the feasibility of protective oxide layer formation.

### S3 22th Intl Symp on Solid Oxide Cells Materials Science & Technology

#### S3- Proton conducting ceramic cells

Room: Ballroom 4

Session Chair: Remi Costa, German Aerospace Center, DLR, Institute of Engineering Thermodynamics

#### 1:30 PM

# (ICACC-S3-052-2025) Protonic Ceramic Membranes: up-scaling and application to E-Fuels synthesis (Invited)

J. Dailly\*1; D. Schmider1; P. Blanck2; O. Deutschmann2

- 1. European Institute for Energy Research, Germany
- 2. Karlsruher Institut fur Technologie Institut fur Technische Chemie und Polymerchemie, Germany

Using a multi-step manufacturing wet chemical route, hydrogen electrode supported samples up to 50 cm2 have been achieved. The H<sub>2</sub> electrode substrate is firstly manufactured by tape-casting from a slurry containing NiO and BaCe<sub>1-x-Y</sub>Zr<sub>x</sub>Y<sub>y</sub>O<sub>3-δ</sub> (BCZY). The BCZY-based electrolyte is coated by screen-printing, and the bilayer assembly is co-sintered at a temperature around 1300°C to limit the effect of shrinkage and diffusion. The last electrode layer is also coated by screen-printing and fired at a lower temperature to keep its structure and ensure a good bonding with the membrane. The final microstructure results in a thin (below 10 µm) and dense membrane, whereas the electrodes remain porous to ease the gas diffusion. To enhance the activity, catalysts are either infiltrated or directly

incorporated in the electrode layer(s). The multi-layered assemblies are tested in adapted laboratory-scale reactors. The gas produced are analyzed using mass spectrometry and the electrochemical behavior of the samples is analyzed by impedance spectroscopy. Finally, the microstructure of the layers is observed and compared before and after electrochemical measurements. Here, EIFER's main achievements for the manufacture of large multi-layered assemblies and the synthesis of hydrogen derivatives will be discussed.

#### 2:00 PM

#### (ICACC-S3-053-2025) Advancing P-SOEC Technology: Scientific Insights and Engineering Strategies for Enhanced 5x5 Cell Testing

S. Koomson\*1; Z. Zhao1; J. Y. Gomez1; W. Wu1; D. Ding1

1. Idaho National Lab, Hydrogen and electrochemistry, USA

The urgent demand for sustainable energy conversion and storage technologies has driven recent progress in solid oxide electrolysis cells (SOECs). Proton-conducting solid oxide electrolysis cells (P-SOECs) offer promise for efficient hydrogen production through water electrolysis. However, the road to achieving optimal performance and durability is not an easy one. In this study, we comprehensively investigate P-SOEC technology, combining scientific insights and engineering strategies. Our research focuses on 5x5 cell testing, i.e., cell design, experimental setup, and operational conditions. By coupling engineering modifications and experimental data, we uncover fundamental electrochemical processes within the cell that address cell performance, durability, and degradation. Key findings highlight performance-limiting factors, such as electrode polarization losses, ohmic loss, and gas diffusion limitations. We propose engineering approaches to enhance cell performance and long-term stability for practical applications, including improved sealing, cell size optimization, and improved experimental setup designs. By bridging the gap between scientific understanding and practical engineering solutions, this work provides a roadmap for advancing P-SOEC technology and supports the broader goal of developing efficient, sustainable hydrogen production systems.

#### 2:20 PM

#### (ICACC-S3-054-2025) Advancing Intermediate-Temperature Protonic Ceramic Electrolysis Cells for Efficient Green Hydrogen Production at Idaho National Laboratory

F. Liu\*'; W. Wu'; Z. Zhao'; H. Li'; W. Wang'; Y. Zhang'; Q. Sun'; Z. Wang'; D. Ding'

1. Idaho National Laboratory, Energy & Environmental Science and Technology, USA

The pursuit of sustainable and efficient methods for green hydrogen production is crucial for advancing renewable energy technologies. Protonic ceramic electrolysis cells (PCECs) represent a promising intermediate-temperature electrolysis solution, operating between 350-600°C. This temperature range leverages the advantages of both low- and high-temperature electrolysis, offering benefits such as high energy efficiency, cost-effective catalysts, material compatibility, and long-term operational stability. Despite their potential, PCECs are still an emerging technology facing significant challenges, particularly concerning Faradaic efficiency (FE). This efficiency is affected by various factors, including operating conditions, cell manufacturing processes, and single-cell device compositions. In this presentation, we will focus on advancing PCEC technology at Idaho National Laboratory (INL) by developing novel ceramic compositions, optimizing operating conditions, and designing innovative cell structures to enhance FE and electrolysis durability. We will also offer detailed insights into our precise testing methods and FE evaluation for hydrogen production-a critical yet often overlooked aspect of current research. Our goal is to contribute to the development of more efficient and reliable PCECs for sustainable hydrogen energy solutions.

#### 2:40 PM

# (ICACC-S3-055-2025) Robust and Highly Conductive Protonic Ceramics against High Concentration of Steam & $\rm CO_2$

S. Chen<sup>1</sup>; H. Tian<sup>1</sup>; W. Li<sup>1</sup>; Q. Li<sup>1</sup>; X. Liu<sup>\*1</sup>

1. West Virginia University, Mechanical & Aerospace Engineering, USA

Proton-conducting ceramics have gained significant attention as a viable solution in CO<sub>2</sub>-rich environments. These advanced materials demonstrate exceptional performance across various industrial applications, including power generation, steam reforming of natural gas, and coal or biomass gasification, where  $CO_2$  concentrations range from 3% to as high as 50%, posing a serious challenge to protonic ceramics. Their robust performance as electrolytes or membranes under extreme conditions, combined with low energy requirements and simplified architectures, distinguishes them from conventional approaches. Current research is centered on improving conductivity, optimizing microstructural properties, and enhancing durability to address the demands of these harsh operational environments. In this study, we synthesized BNHCYb0.1 (BaNb $_{0.05}$ Hf $_{0.1}$ Ce $_{0.6}$ Yb $_{0.25}$ O $_{3-\delta}$ ) and BNHCYb0.2  $(BaNb_{\scriptscriptstyle 0.05}Hf_{\scriptscriptstyle 0.2}Ce_{\scriptscriptstyle 0.5}Yb_{\scriptscriptstyle 0.25}O_{\scriptscriptstyle 3-\delta}).$  BNHCYb0.1 exhibited a conductivity of 0.0128 S cm<sup>-1</sup> at 600°C in a 3% CO<sub>2</sub>, 5% H<sub>2</sub>, and 92% N<sub>2</sub> (3% H<sub>2</sub>O) atmosphere, maintaining stability for over 1000 hours. BNHCYb0.2 achieved a conductivity of 0.0139 S cm<sup>-1</sup> under similar conditions with 10% H<sub>2</sub>O, maintaining stability for over 1500 hours. These results outperform the well-known BZY20 (BaZr<sub>0.8</sub>Y<sub>0.2</sub>O<sub>3-δ</sub>), demonstrating superior conductivity and long-term stability.

#### 3:20 PM

## (ICACC-S3-056-2025) Advanced Ceramic Oxides for Proton Conducting Cells

A. D. Dyrli<sup>\*1</sup>; L. Jøsang<sup>1</sup>

1. Ceramic Powder Technology AS, Norway

Technologies for energy cconversion has been investigated over the years. As manufacturer of advanced ceramic oxides, Cerpotech has been involved in development of materials for several of the fuel cell and electrolyzer technologies such as solid oxide cells (SOC) and proton conducting cells (PCC). The potential for the Protonic ceramic cells (PCC) within a variety of applications for electrochemical energy conversion such as hydrogen production, electrochemical synthesis as well as power generation, has resulted in increased interest in proton conducting materials. Development has been ongoing worldwide for some time, however a lot of challenges remain in the development of PCCs for industrial scale manufacturing processes including raw materials. Various compositions of barium cerates and barium zirconares have been prepared by use of spray pyrolysis and powder properties characterized. Powders with variations in composition such as ratio of zirconia versus cerium and addition of ytterbium have been made and challenges in manufacturing and storage of powders investigated. Post treatment of teh powders to remove organics and carbonates has been evaluated. Spray pyrolysis give very fine powders and have potential for scalable large volume manufacturing of a broad range of compositions. Focus for further development of protocols will depend on results of postprocessing and functionality.

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#### 3:40 PM

#### (ICACC-S3-057-2025) Assembly of proton ceramic electrolysis cell (PCECs) single repeating unit for ultrapure hydrogen production

F. Da Prato\*1; S. Anelli2; A. Moranti5; D. Ferrero1; M. Marasi3; A. Donazzi3;

G. Massobrio<sup>4</sup>; M. Lauldi<sup>4</sup>; M. Santarelli<sup>1</sup>; F. Smeacetto<sup>6</sup>

- 1. Politecnico di Torino, Energy Department DENERG, Italy
- 2. Politecnico di Torino, DISAT, Italy
- 3. Politecnico di Milano, Department of Energy, Italy
- 4. Hydrogen Team of HyAccelerator -SNAM, Italy
- 5. Politecnico di Torino, Italy
- 6. Politecnico di Torino, Applied Science and Technology, Italy

PCECs provide key advantages over solid oxide electrolysis cell (SOECs), including lower activation energies, reduced operating temperatures (400-600°C), simpler gas separation, and no fuel dilution at the electrode. Reliable sealants are essential for scaling up to commercial stacks to ensure electrical separation and gas tightness. Glass-based materials are promising candidates, with additive manufacturing techniques like robocasting enhancing their effectiveness through uniform deposition. Glass pastes are prepared and their formulations optimized to achieve the correct printability and shape fidelity for the extrusion process. Furthermore, robocasting printing parameters are studied to obtain the required thickness and width of the sealing profiles. The chemical and thermo-mechanical compatibility of different glass-based systems with a PCEC halfcell composed of BaZr<sub>0.625</sub>Ce<sub>0.2</sub>Y<sub>0.175</sub>O<sub>3-d</sub> (BZCY622)/NiO-BZCY622 and a metallic interconnect made of ferritic stainless steel AISI441 are assessed in both dry and humidified air. The post-mortem characterization (FESEM and XRD) results on the joined samples are presented and discussed. Finally, an initial SRU is assembled using a complete button cell composed of Ba<sub>0.5</sub>La<sub>0.5</sub>CoO<sub>3-d</sub> (BLC)-BZCY622/ BZCY622/NiO-BZCY622 and then electrochemically tested to assess the impact of each element on overall performance.

#### 4:00 PM

# (ICACC-S3-058-2025) High-performance PCFCs with dense BZYb20 electrolytes fabricated through Ba-diffusion sintering

- A. Sharma\*<sup>1</sup>; K. Watanabe<sup>1</sup>; H. Shimada<sup>1</sup>; Y. Yamaguchi<sup>1</sup>; K. Nomura<sup>1</sup>;
- Y. Mizutani<sup>1</sup>; M. Momai<sup>1</sup>; H. Sumi<sup>1</sup>; M. Fujioka<sup>1</sup>
- 1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Protonic ceramic fuel cells (PCFCs) operate efficiently at intermediate temperatures below 600°C. BaZr<sub>0.8</sub>Yb<sub>0.2</sub>O<sub>3-8</sub> (BZYb20) is a chemically stable proton-conducting perovskite, but its poor sinterability at low temperatures leads to high porosity and grain boundaries, reducing ionic conductivity and electrochemical performance. Our research shows that adding 2 wt% excess BaCO<sub>3</sub> to a NiO-BZYb20 anode effectively enhances the BZYb20 sinterability at lower temperatures by promoting Ba and Ni diffusion, forming a transient BaNiO<sub>3</sub> phase in the electrolyte that aids densification. In this study, we optimized BaCO<sub>3</sub> content and sintered a half-cell containing 6 wt% excess BaCO<sub>3</sub> in the NiO-BZYb20 anode at 1500°C for 7 hours. This process yielded a dense electrolyte with a 5 µm grain size on a porous anode. The resulting PCFC with 10 µm thick BZYb20 electrolyte achieved a peak power density of 0.8 Wcm  $^2$  at 600°C, with  $R_{\Omega}$  = 0.26  $\Omega cm^2$ and  $R_p = 0.06 \ \Omega \text{cm}^2$ , outperforming the 0.49 W cm<sup>-2</sup> of a cell without BaCO<sub>3</sub> ( $R_{\Omega} = 0.31 \ \Omega \text{cm}^2$  and  $R_p = 0.2 \ \Omega \text{cm}^2$ ). The enhanced performance is due to the reduction in R<sub>p</sub>, results from the maintained stoichiometry facilitated by Ba diffusion. This diffusion lowers the activation energy and increases the reaction rate at the triple-phase boundaries. Although R<sub>o</sub> is still high and can be further reduced by decreasing the electrolyte thickness, improving overall performance.

#### 4:20 PM

## (ICACC-S3-059-2025) Experimental and model investigation of $BaZr_{0.625}Ce_{0.2}Y_{0.175}O_{3.6}$ based proton conductive ceramic cells

M. Marasi<sup>\*1</sup>; A. Cammarata<sup>1</sup>; P. Colbertaldo<sup>1</sup>; G. Massobrio<sup>2</sup>; M. Lauldi<sup>2</sup>; S. Campanari<sup>1</sup>; A. Donazzi<sup>1</sup>

- 1. Politecnico di Milano, Department of Energy, Italy
- 2. SNAM, Italy

Protonic ceramic electrolysis cells (PCECs) are a promising technology for hydrogen production from steam and electricity based on proton-conducting perovskites. In these materials, the protonic conduction mechanism requires smaller activation energy than oxide ion conduction, allowing PCECs to operate at lower temperature than conventional solid oxide electrolysis cells. This leads to enhanced mechanical and chemical stability, reduced costs, and improved performance. However, electrolytes based on proton-conducting perovskites, such as the Ba(Ce, Zr, Y)-based ones, exhibit competitive electron-hole conduction alongside proton conduction, which impairs the PCEC's performance. In this study, we characterize a novel proton-conducting electrolyte with the composition  $BaZr_{0.625}Ce_{0.2}Y_{0.175}O_{3-\delta}$  (BZCY62). Conductivity experiments were performed with EIS between 400 and 600°C, varying O<sub>2</sub> (21 to 2%), H<sub>2</sub>O (30% to 0%) and H<sub>2</sub> molar fractions. Electrolyte- and electrode-supported button cells were fabricated via the solid state reactive sintering method, and were tested in electrolysis between 500 and 600°C with up to 50/50 H<sub>2</sub>O/air feed. A physical model was also developed to predict the partial conductivity of the charge carriers within the electrolyte, and the performance of the complete PCEC. Strong consistency is found comparing the model predictions and the experimental results.

#### 4:40 PM

### (ICACC-S3-060-2025) Additive manufacturing and integration of protonic ceramic electrolysis cells

S. Anelli\*1; D. Ferrero2; M. Santarelli2; F. Smeacetto1

- 1. Politecnico di Torino, DISAT, Italy
- 2. Politecnico di Torino, DENERG, Italy

Protonic ceramic electrolysis cells (PCECs) can produce pure and dry H<sub>2</sub> at considerably lower temperature ranges compared to other high-temperature electrolyzers (400-650 °C). These cells feature electrolytes composed of Ba(Ce, Zr)<sub>1-v</sub> $Y_vO_{3-\delta}$  perovskites, which are challenging to integrate into practical systems. In particular, the chemical expansion and contraction of the Ba-based perovskite in hydrated conditions during operation can lead to system failure. For these reasons, the compatibility of these materials with other stack components (e.g., glass sealant and metallic interconnects) is critical. In this study, PCECs are manufactured using digital light processing (DLP). The utilization of DLP effectively enhances cell performance by modifying the electrolyte design and increasing the active area. Furthermore, the tightness of the joined interfaces can be improved through 3D printing, which increases roughness and interlocking between the electrolyte and the glass sealant. The glass sealant is deposited via robocasting to ensure reproducible deposition. The compatibility between the cell materials and the sealant is investigated after aging under relevant conditions. The cells are electrochemically characterized using current-polarization curves and impedance spectroscopy. Post-mortem characterization of the measured cells and joined samples is presented and discussed.

### <u>S5 Next-Generation Bioceramics and</u> <u>Biocomposites</u>

# S5- Bioceramics and composites for implants and medical devices I

#### Room: Ponce de Leon

Session Chairs: Eva Hemmer, University of Ottawa; Aneta Zima, Akademia Gorniczo-Hutnicza im Stanisława Staszica w Krakowie

#### 1:30 PM

#### (ICACC-S5-017-2025) Eliminating Implant Infections: 30,000 Nanotextured Implants in Humans with No Failures and Still Counting (Invited)

T. Webster\*1

1. Brown University, USA

Implant infection is rising with the U.S. Centers for Disease Control predicting one person every three seconds will die from a bacteria infection by 2050. Nanomedicine is the use of nanomaterials to improve disease prevention, detection, and treatment which has resulted in hundreds of FDA approved medical products. This presentation will provide an over 25 year journey of commercializing nano orthopedic implants now in over 30,000 patients to date showing no signs of failure, including no infection. Current orthopedic implants face a failure rate of 5 - 10% and sometimes as high as 60% for bone cancer patients. Further, Artificial Intelligence (AI) has revolutionized numerous industries to date. However, its use in nanomedicine has remained few and far between. One area that AI has significantly improved nanomedicine is through implantable sensors. This talk will present research in which implantable sensors, using AI, can learn from patient's response to implants and predict future outcomes. In vitro and in vivo experiments will be provided that demonstrate how AI can be used towards our advantage in nanomedicine, especially implantable sensors. Lastly, this talk will summarize recent advances in nanomedicine to both help human health and save the environment.

#### 2:00 PM

# (ICACC-S5-019-2025) Synthesis and Robocasting of Tri-calcium phosphate, hydroxyapatite and Wollastonite based bio ceramic composite

G. Rajan\*1; M. V. Sudandaradoss1

1. Anna University, Ceramic Technology, India

The "GREEN PRINT HEALTH" project is a pioneering initiative that utilizes waste bio-materials like sugarcane bagasse to synthesize hydroxyapatite (HA) for bone tissue engineering (BTE). This approach not only reduces waste but offers a sustainable solution for bone reconstruction, aligning with the growing demand for eco-friendly practices in healthcare. The project synthesizes HA through a combination of tri-calcium phosphate (TCP) and wollastonite (WS), key components in bio-material fabrication. Using robocasting, the composite is shaped into grafts, with the process optimized for minimal volatilization, induced porosity, and whisker incorporation to enhance properties. Material characterization is conducted using SEM, EDAX, and X-ray diffraction (XRD) to analyze structure and composition. The emphasis on in vitro studies shows promising results for bone regeneration, indicating potential for clinical applications. By integrating materials science with healthcare, the project aims to create sustainable, low-cost bone replacement materials, addressing environmental concerns and making bone reconstruction more accessible, especially for trauma, neoplasms, or aging cases.

#### 2:20 PM

### (ICACC-S5-020-2025) Machine Learning Guided Biohybrid Interfaces and Materials Design for Oral Health (Invited)

#### C. Tamerler<sup>\*1</sup>

1. University of Kansas, Mechanical Eng & BioEngineering, USA

Oral diseases remain among the most common noncommunicable diseases. The combined complexity and prevalence of dental diseases requires well engineered and effective interventions to optimize patient outcomes. Our particular focus has been on exploring biomimetic approaches that can impart the key biological activity toward prevention of dental and oral diseases to restoring oral health. Here, we will discuss our approach for next generation materials that are composed of peptides, peptide-mimetics, and peptide-polymer hybrids. Using machine learning approaches, we classify bioactive and antimicrobial peptides and enrich sequence domains for effective activity search with targeted and/or enhanced properties. By incorporating multi-pronged strategy to repair and protect exposed dentin and collagen, we combined different peptide, peptide-mimetic and peptide-polymer hybrid to treat different lesion types. Our peptide design and engineering approach targeting biohybrid interfaces provides an alternative delivery strategy to deploy peptides on the sites and increases their availability and preserving their efficacy.

#### 2:50 PM

## (ICACC-S5-021-2025) Zinc oxide-reinforced baghdadite-zirconia ceramic composite for dental applications

J. Jimenez<sup>1</sup>; R. Raguindin<sup>1</sup>; E. d. Magdaluyo\*<sup>1</sup>

1. University of the Philippines, Philippines

This study explores the enhancement of zirconia-based dental restorative materials by incorporating varying amounts of baghdadite and zinc oxide (ZnO) nanoparticles. Baghdadite was synthesized via solid-state sintering and combined with zirconia at concentrations of 0%, 5%, and 10%. ZnO nanoparticles (0.6% by weight) were added to improve antimicrobial activity. The crystal structure, surface morphology, antibacterial properties, and cell viability of the composite were analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), agar plate method, and trypan blue exclusion assay, respectively. Bovine serum albumin (BSA) was used to assess protein absorption. Results showed that higher baghdadite concentrations increased protein adhesion, while ZnO-reinforced composites exhibited strong antimicrobial activity, especially against Staphylococcus aureus. The trypan blue exclusion assay indicated 83.71% cell viability, suggesting good support for cell growth. Overall, the incorporation of baghdadite and ZnO nanoparticles enhances zirconia's bioactivity, antimicrobial properties, and biocompatibility, making it a promising dental restorative material.

### <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

#### **S6- Sodium and Potassium Storage Systems**

Room: Coquina B

Session Chairs: Chunmei Ban, University of Colorado, Boulder; Palani Balaya, National University of Singapore

#### 1:30 PM

# (ICACC-S6-044-2025) Recent developments in Na-based pseudocapacitive materials (Invited)

A. Zambotti<sup>1</sup>; B. Dunn\*<sup>2</sup>; Q. Nguyen<sup>1</sup>; Q. Wei<sup>3</sup>; Y. Luo<sup>1</sup>

- 1. University of California Los Angeles, Materials Science, USA
- 2. UCLA, Materials Science and Engineering, USA
- 3. Xiamen University College of Materials, China

The increased interest in sodium ion batteries (SIBs) has led to an active effort in identifying a new generation of electrode materials. Electrode materials exhibiting pseudocapacitive properties have attracted considerable attention because of the prospect of achieving high energy density at high rates of charge and discharge. Although a number of Li<sup>+</sup> electrode materials have been shown to possess pseudocapacitive properties, there are relatively few Na<sup>+</sup> electrode systems which display pseudocapacitive signatures. This presentation reviews our recent findings involving crystalline and amorphous TiO<sub>2</sub> and VO<sub>2</sub> and their function as anodes and cathodes for sodium ion batteries. Crystalline VO<sub>2</sub>(B) and especially anatase TiO<sub>2</sub> exhibit excellent Na<sup>+</sup> capacities at relatively high rates when prepared in nanoscale forms. Interestingly, their amorphous counterparts exhibit higher sodium capacity despite having a disordered structure that occurs in the as-prepared material or is induced by the sodiation process. These results indicate that short-range structure of electrode materials is an important consideration in designing redox-active electrode materials.

#### 2:00 PM

#### (ICACC-S6-046-2025) Improvements in the Electrochemical Performance of Magnesium Batteries through Advanced Membrane Materials and a Chloride-Free Electrolyte (Invited)

M. Ng\*1; W. Ren4; W. Tang2; J. Jeevarajan3; Y. Yao5

- 1. Underwriters Laboratories Inc, UL Research Institutes | Electrochemical Safety, USA
- 2. Underwriters Laboratories Inc, Electrochemical Safety Research Institute, USA
- 3. UL Resarch Institutes, Electrochemical Safety Research Institute (ESRI), USA
- 4. University of Houston System, Department of Chemical and Biomolecular Engineering, USA
- 5. University of Houston, Department of Electrical and Computer Engineering and Texas Center for Superconductivity at the University of Houston (TcSUH), USA

Magnesium batteries are being developed for their potentially higher energy density, faster-charging capability, and improved safety as compared to lithium-ion batteries due to their resistance to dendrite deposition. However, magnesium batteries encounter technical challenges, such as strong interactions of  $Mg^{2+}$  with nucleophiles in the electrolyte solution and the shuttle effect caused by conventional separator membrane materials, leading to sluggish cycling stability. This research outlines our recent advancements in scaling up the synthesis of a boron cluster-based electrolyte known as magnesium alkoxyl fluorinated borates  $(MgC_{12}H_{30}O_6)(B_2C_{24}H_8O_8F_{48})$ , (MBF). This chloride-free electrolyte has demonstrated high conductivity across a wide temperature range, enhancing reaction kinetics. Additionally, the investigation of selective membranes that can conduct magnesium ions while effectively blocking soluble organic compounds is promising. This part of the research aims to balance the selectivity and conductivity in magnesium-Nafion membranes. It also explores fluorine-free, non-Nafion-based selective membranes, resulting in improved cycling stability of magnesium-organic cells equipped with these membranes.

#### **S6-** Multivalent Redox Batteries

Room: Coquina B

Session Chair: Mahalingam Balasubramanian, Oak Ridge National Lab

#### 3:20 PM

#### (ICACC-S6-047-2025) Computationally-guided design of aqueous electrolytes for rechargeable iron batteries (Invited) B. Narayanan<sup>\*1</sup>

1. University of Louisville, Mechanical Engineering, USA

Rechargeable aqueous iron batteries (AIBs) offer sustainable solution for storing electrical energy from intermittent renewable energy sources at the grid-scale owing to the earth-abundance of iron. Unfortunately, longstanding challenges related to (a) parasitic hydrogen evolution on metallic iron electrode (during charging), and (b) accumulation of electrochemically inert Fe<sub>3</sub>O<sub>4</sub> (during discharging) have thwarted progress in AIBs. These challenges stem from a dearth of atomic-scale understanding of solvation chemistry, ion-transport, and electrochemical reactions at electrode/ electrolyte interfaces. Here, we employ a combination of density functional theory calculations, classical molecular dynamics simulations, and operando X-ray characterization to advance fundamental electrochemistry in AIBs. Specifically, we find that (a) sulfate ions promote reversible Fe(OH)<sub>2</sub>/FeOOH conversion (limiting Fe<sub>3</sub>O<sub>4</sub> formation) under low-alkaline conditions by tuning the strength of the hydrogen bond network in water, and (b) silicate anion additives hamper kinetics of Fe<sub>3</sub>O<sub>4</sub> formation by screening interaction between Fe(OH)<sub>2</sub> and hydroxyl ions, as well as suppress hydrogen evolution by impairing energetics of water dissociation and hydroxyl de-sorption on iron surfaces. These findings will be discussed in the context of accelerating development of green, sustainable, and low-cost battery systems for grid storage.

#### 3:50 PM

#### (ICACC-S6-048-2025) Design Strategies for High Voltage Spinel Cathode Materials to Enable Reversible Mg-Ion Intercalation (Invited)

B. Key\*<sup>1</sup>

1. Argonne National Laboratory, Electrochemical Energy Storage, USA

Reversible Mg2+ insertion into metal oxides is key to developing high-energy-density Mg-ion batteries. While Mg-ion batteries with soft anions like S<sup>2-</sup> and Se<sup>2-</sup> have been achieved, their low insertion potentials prevent them from reaching energy densities required to compete with lithium-ion batteries. This highlights the need for an oxide-based cathode capable of operating at higher potentials. The sluggish diffusion of Mg2+ in oxides, caused by strong electrostatic interactions between Mg2+ and oxide anions, is believed to limit the development of such cathodes. Modifying the oxide lattice to create less stable  $Mg^{2+}$ – $O^{2-}$  coordinations may address the issue. Theoretical and experimental findings suggest spinel oxides as promising cathode candidates due to their capacity, insertion potential, and cation mobility. However, single redox metal spinels like MgCr2O4 and MgMn2O4 have shown inadequate reversible Mg-ion intercalation. Therefore, new solid-solution oxide spinels were developed by combining metals like Mn3+ for redox stability and Cr3+ for structural stabilization. By managing defects, such as antisite inversion, and correlating structural changes with redox activity, electrochemical performance improved. These advances enable the design of oxide cathode materials with key attributes of Li-ion batteries, marking a milestone in the pursuit of high-energy Mg-ion batteries.

#### 4:20 PM

#### (ICACC-S6-051-2025) Sodium solid electrolytes- design & technology aspects See page 210 for abstract

### S10 Integrated computational-experimental modeling ad design of ceramics and composites

### S10- Modeling ablation and impact of advanced

#### ceramics

Room: Coquina G

Session Chair: Efrain Hernandez, University of Michigan

#### 1:30 PM

#### (ICACC-S10-015-2025) Lifetime Prediction and Uncertainty Quantification in Self-healing Thermal Barrier Coatings

S. Anusuya Ponnusami\*<br/>'; A. Kumthekar²; J. Krishnasamy²; S. van der Zwaag²; S. Turteltaub²

- 1. City, University of London, Engineering, United Kingdom
- 2. Technische Universiteit Delft Faculteit Luchtvaart- en
- Ruimtevaarttechniek, Netherlands

Thermal barrier coatings (TBCs) are widely used in jet engines operating at high temperatures to protect the underlying structural components from oxidation and degradation. Upon prolonged thermal cycling, microcracks evolve, eventually leading to detrimental failure of the TBC. To delay such failure, a self-healing (SH) TBC system has been designed based on encapsulated healing particles dispersed in the coating. Engineered interactions between the microcracks and the particles lead to crack healing. A multiphysics micromechanical framework that incorporates a cohesive-zonebased crack healing model was developed to estimate the lifetime of SH-TBC. Nonetheless, this deterministic model does not account for the uncertainties associated with the microstructural design variables. For this, a data-driven surrogate model based on a Polynomial Chaos Expansion was developed. The training data comprise FE simulations of the SH-TBC involving variables such as the interface amplitude, growth rate of the thermally grown oxide layer, diameter, volume fraction and mean distance of healing particles. The trained surrogate model allows to establish the statistical characteristics of the TBC lifetime as well as the sensitivity indices of the input variables, a crucial insight critical for the design of a robust SH-TBC system.

#### 2:00 PM

#### (ICACC-S10-016-2025) Deep Learning Approaches for Predicting the Ablation Performance of Ceramic Matrix Composites in the Hydrogen Torch Test

J. Deb\*1; F. Faysal1; J. Gou1

1. University of Central Florida, Mechanical and Aerospace Engineering, USA

In the recent years, hydrogen and biofuels have been investigated as substitute fuels for contemporary gas turbines to lessen these environmental effects. Forecasting ultra-high-temperature CMCs' ablation capability in the hydrogen torch test is essential to comprehend their resilience under challenging thermal conditions of hydrogen combustion engines. Although finite element modeling is still a useful tool for predicting the fundamental mechanics and thermal behavior of CMCs under the hydrogen torch testing, other methods are required due to its inability to accurately represent complicated chemical processes and ablation behaviors. By forecasting CMC performance under high-temperature hydrogen torch test settings, incorporating nonlinear interactions, and learning directly from experimental data, data-driven machine-learning models provide a strong and adaptable solution. This study has developed a deep artificial neural network (DANN) model with two hidden layers having rectified linear unit activation function to predict the ablation performance of CMCs in the hydrogen torch test. A good agreement between the DANN model's predictions and experimental torch data having R<sup>2</sup> score of 0.9671, RMSE of 16.45, an MAE of 14.07, and a MAPE of 3.92% confirmed the acceptability of the developed neural network model in this study.

#### 2:20 PM

#### (ICACC-S10-017-2025) Shock Response of Boron Carbide Using a Machine Learned Interatomic Potential: Influence of Orientation and Polytype

K. Ghaffari\*1; S. Bavdekar3; D. Spearot2; G. Subhash2

- 1. University of Florida, Material Science and Engineering, USA
- 2. University of Florida, Mechanical and Aerospace Engineering, USA
- 3. Illinois State University, Mechanical Engineering, USA

The high strain-rate behavior of boron carbide  $(B_4C)$  is of great interest due to its unique combination of high hardness and low density, making it ideal for protective applications. Available computational studies of B<sub>4</sub>C shock are often limited to the most prevalent polytype ( $B_{11}C_{p}CBC$ ) and one crystallographic orientation for simplicity; thus, the influence of these factors on high strain-rate behavior remains unknown. In this work, we conduct large-scale nonequilibrium molecular dynamics simulations to investigate the shock behavior of  $B_4C$  as a function of two variables: (1) polytype and (2) chain orientation relative to the impact surface. Specifically, the four most prevalent polytypes, including a boron-rich structure, are subjected to shock in five different orientations where the 3-atom chain is 0°, 30°, 45°, 60°, and 90° offset from the direction of shock wave propagation. Results indicate a strong dependence on both polytype and chain-orientation angle, with only the 0° orientation resulting in periodic shear-band formation behind the plastic shock front. The insight gained from this study can assist in understanding the complex deformation mechanisms that evolve during the shock and/or ballistic loading of boron carbide.

# S10- Modeling tribology and vibration performance of advanced ceramics

#### Room: Coquina G

Session Chair: Sathiskumar Anusuya Ponnusami, City, University of London

#### 3:20 PM

# (ICACC-S10-018-2025) CT based approach for the machining simulation of porous silicon carbide

S. Unseld\*1; R. Goller1; D. Koch2

- 1. Technische Hochschule Augsburg, Mechanical Engineering, Germany
- 2. Universitat Augsburg Institut fur Materials Resource Management, Germany

The machining of silicon carbide (SiC) such as porous recrystallized silicon carbide (10% porosity), R-SiC for short, still poses a challenge. Due to its hardness, high strength and brittle fracture behavior, small depth of cut at microscale are necessary. The seemingly random crack development between pore structures in the material lead to complex machining mechanisms that are not yet fully understood. To gain an in-depth understanding of how these materials react under mechanical stresses during machining, simulations are necessary. These, however, are not yet fully established in literature. In this presentation the machining simulation of R-SiC will be presented as an example material using a CT based at pore size level. Material models for machining, mesh-discretization methods (mesh-based and particle-based), representative volumes of interest and the validation of the simulation for R-SiC will be discussed. Not only the right material models, but also the right meshing strategies are necessary to handle both computational time and numerical instabilities in this highly discontinuous numerical process. Thus, a specialized meshing algorithm is also presented to allow the generation of both mesh- and particle-based porous geometries of ceramics directly from CT data.

#### 3:40 PM

#### (ICACC-S10-019-2025) Analysis of Wear Behavior of Crosslinked Polymer Brush via Coarse-grained Molecular Dynamics Simulations

Y. Hara\*1; C. Suzuki1; Y. Su2; S. Fukushima1; Y. Ootani1; N. Ozawa2; M. Kubo1

- 1. Institute for Materials Research, Tohoku University, Japan
- 2. Tohoku University, New Industry Creation Hatchery Center, Japan

To achieve a carbon-neutral society, reduction of friction loss is crucial. Concentrated polymer brushes (CPBs) have attracted much attention as a promising coating material on ceramic substrate surfaces due to their excellent tribological properties, such as high compressive resistance and low friction coefficients. However, improvement of the wear resistance is demanded for practical use. Although experimental approaches have shown that cross-linking enhances CPB wear resistance, molecular-level mechanisms remain unclear. In this study, we used coarse-grained molecular dynamics simulations to elucidate the mechanism why the cross-linking prevents breakage of polymer chains towards the further improvement of wear resistance. We performed the sliding simulations for CPBs with three different degrees of cross-linking in which a rigid slider was rubbed against the CPB surface. The simulations revealed that polymer chain bond breaking occurred less frequently in crosslinked CPBs than in non-cross-linked CPBs. Breakpoint distribution analysis showed that bond breaking most often occurred at the front of the slider, where the slider and brushes were contacted. It also showed that the cross-linker suppressed bond breaking near brush surfaces. These insights provide valuable information for improving CPB wear resistance.

#### 4:00 PM

#### (ICACC-S10-020-2025) Tribochemical Reactions of Amorphous Films Derived from Molybdenum Dithiocarbamate Revealed by Neural Network Molecular Dynamics Simulation

C. Suzuki\*1; Y. Hara1; Y. Su2; S. Fukushima1; Y. Ootani1; N. Ozawa2; M. Kubo1

- 1. Tohoku University, Institute for Materials Research, Japan
- 2. Tohoku University, New Industry Creation Hatchery Center, Japan

Minimizing friction losses is essential for energy saving. Molybdenum dithiocarbamate (MoDTC) has been utilized as an effective lubricant additive to reduce friction of ceramics. MoDTC forms molybdenum disulfide (MoS<sub>2</sub>) film, which reduces friction force, on sliding interface due to tribochemical reaction. However, the mechanism underlying the formation of MoS<sub>2</sub> film remains unclear due to the difficulty of the in situ observation of sliding interface. For the development of superior lubricant additive, it is essential to reveal the mechanism. In this study, we investigated the mechanism of MoS<sub>2</sub> film formation using neural network molecular dynamics (NNMD) simulation. In our previous study, we clarified that chemical reaction of MoDTC forms amorphous compound consisting of Mo, S, and O atoms at the sliding interface of iron. In this study, we focused on the share induced reactions of MoDTCderived amorphous compound of the sliding interface of iron. The simulations show that the amorphous compound transformed to two dimensional MoS<sub>2</sub> crystal due to sliding and the frictional forces on the sliding interfaces decreased. The MD simulations with various temperature showed that the number of MoS<sub>2</sub> crystal layer increases as the temperature increases. In the presentation, we will discuss the detailed mechanism of MoS<sub>2</sub> film formation.

#### 4:20 PM

## (ICACC-S10-021-2025) Physics-Informed Machine Learning for Defect Characterization of Isotropic and Anisotropic Materials

M. P. MacIsaac<sup>\*1</sup>; A. Beck<sup>2</sup>; W. Eum<sup>3</sup>; C. Tran<sup>3</sup>; M. Stormant<sup>3</sup>; G. Subhash<sup>1</sup>; J. Harley<sup>3</sup>

- 1. University of Florida, Mechanical & Aerospace Engineering, USA
- 2. University of Florida, Physics, USA
- 3. University of Florida, Department of Electrical and Computer Engineering, USA

Machine learning has greatly increased our understanding of materials. However, most ML models lack physical interpretability, limiting insights into the underlying causes for a model's predictions. This interpretability is especially crucial when characterizing materials and identifying defects to improve material processing. To address this, we have developed a non-destructive, physics-informed machine learning (PIML) framework for defect characterization. Our model uses ultrasonic wavefield measurements collected via a laser doppler vibrometer, which scans material specimens where an ultrasonic wavefield is generated by a piezoelectric transducer. The PIML algorithm is guided by known wave physics, where the 2-D wave equation is embedded in the loss function, hence linking model predictions to a physical basis. Specifically, our PIML approach decomposes the collected wavefield into a series of modes, allowing subtle material nuances e.g., defects, to be associated with particular mode(s). We have demonstrated the efficacy of our PIML methodology by characterizing both isotropic and anisotropic materials, including identification of mode(s) corresponding to known defects.

# S10- Modeling advanced ceramics for electrical applications

#### Room: Coquina G

Session Chair: Stefan Adams, National University of Singapore

#### 4:40 PM

#### (ICACC-S10-022-2025) Oxygen vacancy formation energetics in MgO-based high entropy oxides from DFT and experimental validation (Invited)

- O. Opetubo<sup>1</sup>; T. Shen<sup>1</sup>; R. Bordia<sup>1</sup>; D. Aidhy<sup>\*1</sup>
- 1. Clemson University, Materials Science and Engineering, USA

In contrast to single or double cation based oxides, high entropy oxides (HEOs) consist of equi- or near equimolar concentation of multiple cations randomly distributed on a crystal lattice. The random distribution causes a wide diversity of nearest-neigbor environments around oxygen atoms. Consequently, a range of bonding environments and oxygen vacancy formation energies are observed. We investigate oxygen vacancy formation energies in Mg(ZnCoNiCu)O-based HEO using density functional theory (DFT). We find that vacancy formation energy trends are controlled by cation valence charge. We explicitly determine the effect of all cations on formation energies. Experimentally, a series of binary, ternary, quaternary and quinary HEOs are synthesized using a simple and scalable polymeric steric entrapment method. By annealing in inert environment, oxygen vacancies are analyzed by XPS and TGA. The experimental obseravtions agree with our DFT calcilations. This understanding contributes to oxygen vacancy transport useful in microstructure evolution and electrochemical applications.

#### 5:10 PM

#### (ICACC-S10-023-2025) AI-Driven Computational Design and Synthesis of Electrochemical Energy Storage Materials (Invited) J. Liu<sup>\*1</sup>

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Electrochemical energy storage materials with complex compositions and multi-scale structures present challenges in process control. Many theoretically predicted materials are difficult to synthesize experimentally, slowing progress in the fast-evolving battery industry. By integrating computational methods, automated experiments, and AI models, we aim to create an intelligent ceramic materials design platform, shifting from traditional "trial-and-error" approaches to advanced, data-driven methods. This talk highlights recent advancements in computational electrochemistry and AI technologies for electrochemical energy storage materials, with a focus on designing and synthesizing next-generation lithium-ion battery materials and electrocatalysts. Using gradient approximation methods, we've developed key battery materials like Li-rich cathode oxides and solid-state electrolytes. Additionally, we've advanced AI algorithms for material structure design and automated solid-phase synthesis, including mixing, pressing, and sintering. Our integrated platform enhances synergy between computational design, synthesis, and characterization, enabling the successful development of high-entropy lithium-rich cathode materials and highly active catalysts for hydrogen and oxygen evolution, ultimately leading to high-performance electrochemical energy storage materials.

### S11 Advanced Materials and Innovative Processing Ideas for Production Root Technologies

# S11- Fundamental materials: mining, particles, bulk, and functional materials and precursors II

Room: Coquina C

Session Chair: Sungwook Mhin, Kyonggi University

#### 1:30 PM

#### (ICACC-S11-008-2025) Development Transparent (Y, Ce)α-SiAION ceramics (Invited)

J. Tatami\*1; T. Ito1; K. Aminaka1; M. Iijima1; T. Takahashi2

1. Yokohama National University, Japan

2. Kanagawa Institute of industrial Science and Technology, Japan

In recent years, highly thermal and mechanical durability is demanded for transparent materials because of high power lighting. SiAlON ceramics have been researched as typical engineering ceramics. One of the recent applications of SiAlON is phosphor for white LEDs. In this study, transparent (Y, Ce)- $\alpha$ -SiAlON ceramics were developed by controlling powder processing. The SiAlON ceramics were fabricated from Si<sub>3</sub>N<sub>4</sub>, AlN, Y<sub>2</sub>O<sub>3</sub>, and CeO<sub>2</sub> powders as raw materials, followed by gas pressure sintering (GPS) and hot isostatic pressing (HIP). As a result of experiments by changing the particle size of Y<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub>, finer particles of the rare earth oxide resulted in the finer microstructures of the (Y, Ce)- $\alpha$ -SiAlON ceramics, and they improved the transparency because of decreasing light scattering. (Y, Ce)- $\alpha$ -SiAlON ceramics fabricated by firing at 1550 °C in GPS showed higher in-line transmittance than that at 1600 °C due to the limitation of grain growth. Furthermore, firing in lower N2 partial pressure in GPS and higher N2 pressure in HIP showed higher transparency because the quantity and quality of residual glassy phase were affected by applied N<sub>2</sub> pressure.

#### 2:00 PM

#### (ICACC-S11-009-2025) Crack Healing Behavior in Environmental Barrier Coatings via Heat Treatment (Invited)

- A. Okawa\*1; S. T. Nguyen3; T. Nakayama2; T. Ishikawa4; R. Shimonishi4;
- C. Koyama<sup>4</sup>; H. Suematsu<sup>2</sup>; T. Hasegawa<sup>1</sup>; S. Yin<sup>1</sup>
- 1. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials, Japan
- 2. Nagaoka University of Technology, Extreme Energy-Density Research Institute, Japan
- 3. National Institute of Technology Kushiro College, Department of Creative Engineering, Japan
- 4. Japan Aerospace Exploration Agency, Tsukuba Space Center, Japan

This study investigates two crack healing behaviors during heat treatment processes for Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, a promising environmental barrier coating material. The first approach explores the selfhealing capability of  $\beta$ -Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>/SiC composites prepared via solid-phase reaction and hot-press sintering. Samples with induced cracks were annealed at 750-1400°C for up to 50 h in air and water vapor-rich atmospheres. Post-treatment analysis revealed crack length reduced and recovered flexural strength. The formation of metastable α-Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> under high pressure was identified, accompanied by improved fracture toughness, suggesting that strength recovery is primarily attributed to compressive stress. The second approach examines crack healing behavior potentially related to volumetric expansion caused by metastable-to-stable phase transitions in partially amorphous sprayed coatings. To investigate this phenomenon,  $Yb_2O_3$ -SiO<sub>2</sub> bulk glasses were synthesized using  $CO_2$ laser irradiation. Surface cracks were introduced and subsequently heat-treated within the crystallization temperature range. While new cracks emerged, partial healing of the initial cracks was observed. These findings contribute to the development of dense and robust environmental barrier coatings by optimizing initial composition, additives, and heat treatment processes.

#### 2:30 PM

#### (ICACC-S11-010-2025) Red clay and Black cinder of Lanao, Philippines: Indigenous minerals for low porous ceramic tiles (Invited)

I. B. Arugay<sup>\*1</sup>; F. A. Echavez<sup>1</sup>; L. R. Lumasag<sup>1</sup>; C. Saladaga<sup>1</sup>; S. D. Dionio<sup>1</sup>; J. Cahigao<sup>1</sup>; E. U. Aligno<sup>1</sup>; R. M. Dispo<sup>1</sup>; B. L. Bato<sup>1</sup>; A. R. Simplicio<sup>1</sup>; R. V. Virtudazo<sup>1</sup>

1. Mindanao State University-Iligan Institute of Technology, Department of Materials and Resources Engineering and Technology, Philippines

Several combinations of feldspars-quartz-clays (FQC) are employed in the ceramic tile production. However, importation of these minerals result to dependence on foreign suppliers placing the product less competitive in the market. Thus, replacement of these minerals by local resources is an economic advantage to local industries. In this study, red clay and black cinder from Mindanao, Philippines were investigated to possibly replace imported FQC, or even make a binary composition for ceramic tiles formed by slip casting method. Their compositions revealed that the red clay could serve as the clay substance even it contains more alumina than the usual red clays for terracotta production. The black cinder could replace commercial feldspar even if it has lower flux content than the latter. Fusion test of black cinder at 1,200 °C yielded almost negligible low water absorption. The fusion behavior of the black cinder complements the non-fused state of the red clay essential to attain a stable matrix of the tiles. This binary composition produced a ceramic tile with low water absorption with a modulus of rupture of at least 43.44 MPa. These low porous tiles are competitive for the manufacture of roof, wall and floor tiles across several standards.

#### 3:02 PM

#### (ICACC-S11-011-2025) Physicochemical Characterization of Nickel Mine Waste from Agusan Province, Philippines

M. G. Zozobrado\*<sup>1</sup>; J. Mutia<sup>1</sup>; F. A. Echavez<sup>1</sup>; C. Saladaga<sup>1</sup>; R. Aquiatan<sup>1</sup>; V. Resabal<sup>1</sup>; I. B. Arugay<sup>1</sup>

1. MSU-Iligan Institute of Technology, Department of Materials and Resources Engineering and Technology, Philippines

Clayey raw material recovered from nickel mine waste (NMW) is yet to be used as filler material for polymer/clay composites, and merits investigation to upcycle NMW. This study examined the physicochemical characteristics of untreated and sodium silicate (SS)-treated NMW from Agusan Province, Philippines, for this purpose. A slurry of <38µm NMW was treated with SS and subjected to sedimentation to obtain 1µm treated NMW. The viscosity, pH, bulk conductivity, and oxidation-reduction potential (ORP) of treated (T38) and untreated <38µm NMW (U38) were determined. The specific surface area (SSA) and cation exchange capacity (CEC) of U38 and treated 1µm NMW (T1) were measured. T38 had a higher pH (8.05 vs. 7.67), lower viscosity (10.67 cP vs 13.46 cP), and decreased ORP (81.96 mV vs. 130.40 mV) compared to U38. T1 has slightly higher SSA (52.84 m<sup>2</sup>/g vs. 49.95 m<sup>2</sup>/g) and CEC (6.75 meq/100g vs. 6.38 meq/100g) than U38. Therefore, SS treatment resulted in an alkaline shift, improved fluidity, reduction in dissolved ions, and either enhanced repulsion between particles or neutralized surface charges present within the material because of the introduction of Na-silicate into the system. This could facilitate improved compatibility between hydrophilic clay and hydrophobic polymer components, resulting in improved performance and properties of the composite material.

# S11- Innovative manufacturing processes for recycling, sustainable energy, or semiconductor industry

Room: Coquina C

Session Chair: Chisung Ahn, Korea Institute of Industrial Technology

#### 3:40 PM

# (ICACC-S11-012-2025) Analysis and optimization of the energy consumption of a CMC machining process via a data-based model approach (Invited)

R. Goller\*1; S. Unseld1; S. Kleiner1; P. von Russdorf1

1. Technische Hochschule Augsburg, Mechanical Engineering, Germany

The rising global energy demand driven by industrial production lead to considerable carbon footprint. To mitigate the impact of machining operations, research focused on energy-efficient machine tools and machining processes is becoming more frequent. Especially for the production of cost-intensive ceramic composite materials such as ceramic brake discs, with a forecast market volume of up to USD 533 million in 2032, an advancement of the energy efficiency of machining processes is an important step towards improving both economic competitiveness and the environmental carbon footprint. To realize such a transformation in systems that have already been optimized through years of experience, a data-based, model-like examination of the system is crucial. In this presentation, the drilling process of ceramic brakes will be used as an example to present such an optimization using data-based models. The model-based description includes both energetic as well as quality aspects of the drilling process. Ideal process parameters can be determined using model-based interactions from a wide variety of data sources, such as device-specific power consumption, machining force and G-code. Using a graph-based design language and approaches of similarity mechanics, specific correlations are derived from the generated data for process optimization.

#### 4:10 PM

#### (ICACC-S11-013-2025) Green and Sustainable Ceramic Materials: Developing Non-Firing Ceramic Materials from Industrial Byproducts (Invited)

R. V. Virtudazo\*<sup>1</sup>; E. Limbaga<sup>1</sup>; H. D. Melendrez<sup>1</sup>; S. Manlupig<sup>1</sup>; G. F. Maujon<sup>1</sup>;

- C. Cahimtong<sup>1</sup>; S. D. Kempis<sup>1</sup>; L. I. Cabalo<sup>1</sup>; L. M. Jabile<sup>1</sup>; I. B. Arugay<sup>2</sup>;
- V. Resabal<sup>1</sup>; M. Fuji<sup>3</sup>
- 1. Mindanao State University-Iligan Institute of Technology, Department of Materials and Resources Engineering and Technology, Philippines
- 2. MSU-Iligan Institute of Technology, Materials and Resources Engineering and Technology, Philippines
- 3. Nagoya Institute of Technology, Japan

This research study presents the development of a sustainable, non-firing ceramic materials using industrial byproducts. A combination of acid-leached waste fly ash and local siliceous raw material was employed to create a formulated non-firing ceramic product. Characterization revealed that around 20 % ratio of fly ash, exhibited good thermal insulation properties, appropriate water absorption, and suitable physio-mechanical characteristics. These results suggest its potential as a promising and environmentally friendly ceramic structural/construction material.

#### 4:40 PM

# (ICACC-S11-014-2025) Current effects on microstructural evolution of spark plasma sintered $\rm Y_2O_3$ ceramics

- L. Ji-Hwoan\*1; K. Morita<sup>2</sup>; J. So<sup>1</sup>
- 1. Korea Institute of Materials Science, Extreme Materials Institute, Republic of Korea
- 2. National Institute for Materials Science (NIMS), Japan

During spark plasma sintering (SPS), which utilizes an electric current for consolidation, various researches have reported on the possible effects of electric current on densification behavior. To investigate these effects, we employed two mold setups with different electric conductivity (conductive and insulative) while keeping sintering temperatures constant. The starting Y2O3 powder, pressure profile, and detailed sintering conditions were identical, except for the sintering temperature; the conductive set-up achieved full densification at 900°C, while the insulative set-up required 1000°C. In addition, significant differences were observed in the stage just before full densification in the two mold set ups. The conductive set up densified relatively rapidly compared to the insulative set up, and as a result, densification was completed at a lower temperature, approximately 100°C less. Each specimen was fabricated by segmenting the temperature interval from 600°C—where shrinkage begins-to the fully densified temperature. The shrinkage rate and microstructure of the specimens were subsequently analyzed. The densification behavior, characterized by normalized displacement curves, shrinkage rates, and microstructural observations at each temperature, demonstrated the effect of "current effects" in relation to the mold conductivity during the SPS process.

#### 5:00 PM

#### (ICACC-S11-015-2025) Ultra-High Cycle Stability in AZIBs via<br/> $Al_2O_3\mbox{-}Coated$ Zinc Anode and AVNF Cathode

J. Lee<sup>\*1</sup>; Y. So<sup>1</sup>; S. Lee<sup>1</sup>; S. Mhin<sup>1</sup>

1. Kyonggi University, Republic of Korea

Lithium-ion batteries are currently being used in various fields such as ESS (Energy Storage Systems). But the need for safe batteries has been increasingly emphasized recently due to the risk of fire. Aqueous zinc-ion batteries (AZIBs) are coming into focus as an alternative to Lithium-ion batteries because they use aqueous electrolytes, which have less risk of fire and explosion than organic electrolytes, and they offer high volumetric density. However, issues such as hydrogen evolution reaction, corrosion, and dendrite growth on the Zn anode can deteriorate the electrochemical performance of AZIBs. This study investigated the effects of  $Al_2O_3$ -coated Zn anode using an atomic layer deposition and ammonium vanadate nanofiber (AVNF) cathode on the cycle performance of AZIBs. The  $60Al_2O_3@Zn$  showed stable cycling for more than 100 hours in the symmetric cell tests and exhibited the lowest interfacial resistance. In the full cell test,  $AVNF//60Al_2O_3@Zn$  batteries showed ultra-high cycle stability with a capacity retention of 94% even after 5000 cycles at a current density of 10 A g<sup>-1</sup>. The results of this study indicate that the importance of cathode and anode modification to improve cycle stability.

#### 5:20 PM

#### (ICACC-S11-016-2025) Understanding Degradation Mechanisms and Evaluation Electrochemical Performance of Aqueous Zinc-Ion Batteries

E. Lee\*1; Y. So1; S. Lee1; S. Mhin1

1. Kyonggi University, Department of Advanced Materials Engineering, Republic of Korea

Aqueous zinc-ion batteries (AZIBs) offer a promising alternative to lithium-ion batteries due to their water-based electrolyte, high volumetric energy density, and abundant resource reserves, making them suitable for applications in energy storage systems (ESS). However, the electrochemical performance of AZIBs is significantly degraded by several phenomena, including dendritic growth, structural instability, and the formation of unwanted by-products. Furthermore, the charge/discharge mechanism can vary with the cathode material or electrolyte used, affecting critical battery performance metrics such as cycle stability, discharge capacity, and coulombic efficiency. This study investigates the effects of the MnO<sub>2</sub> cathode and Al<sub>2</sub>O<sub>3</sub>-coated Zn anode on the electrochemical performance of AZIBs. It was expected that cycle performance would improve by inhibiting dendrite growth with an Al<sub>2</sub>O<sub>3</sub>-coated Zn anode, but the experimental results did not exhibit a significant improvement. This degradation of cycle performance was associated with the phase transition of MnO<sub>2</sub> to Mn<sub>2</sub>O<sub>3</sub>, and the formation of by-products. Our results suggest that understanding the charge/discharge mechanism driven by structural transitions in the cathode is essential for enhancing the performance of AZIBs, and highlight the urgent need to develop advanced materials for both the anode and cathode.

### <u>S13 Development & Applications of Adv</u> <u>Ceramics & Composites for Nuclear Fission/</u> <u>Fusion Energy Sys</u>

### S13- CMC for fusion and fission energy systems

Room: Coquina D Session Chair: Theresa Davey, Bangor University

#### 1:30 PM

#### (ICACC-S13-027-2025) Tungsten fiber reinforced tungsten composite: A brittle matrix composite for fusion applications (Invited)

- H. Gietl\*<sup>1</sup>; J. Riesch<sup>3</sup>; T. Höschen<sup>3</sup>; Y. Mao<sup>5</sup>; S. Schönen<sup>2</sup>; J. W. Coenen<sup>5</sup>; W. Pantleon<sup>4</sup>; R. Neu<sup>3</sup>
- 1. Idaho National Laboratory, USA
- 2. Forschungszentrum Jülich GmbH, Institut Technology and Engineering (ITE), Partner of the Trilateral Euregio Cluster (TEC), Germany
- 3. Max-Planck-Institut fur Plasmaphysik, Germany
- 4. Department of Civil and Mechanical Engineering, Technical University of Denmark, Denmark
- 5. Forschungszentrum Jülich GmbH, Institute of Fusion Energy and Nuclear Waste Management -Plasma Physics, Partner of the Trilateral Euregio Cluster (TEC), Germany

The development of materials for plasma-facing components represents a critical challenge in the progression towards a viable fusion power plant. Due to its combination of properties, tungsten (W) is the prime candidate for these applications. However, tungsten's intrinsic brittleness and susceptibility to embrittlement under operational conditions pose significant limitations. To address these issues, ongoing research aims to overcome the limitation for operation of W through the implementation of composite structures and W fiber-reinforced W composites (W<sub>f</sub>/W) have been development. In W<sub>f</sub>/W composites, high strength and ductile tungsten fibers are surrounded by a ceramic interlayer and embedded in a brittle tungsten matrix. The interlayer between the W fiber and W matrix is crucial for the activation of extrinsic toughening mechanisms, similar to silicon carbide (SiC) fiber-reinforced SiC. Due to the brittle matrix, stresses play a critical role during the manufacturing process, and their impact on the material's performance are still under investigation. This presentation will discuss the latest achievements in the fabrication and performance of W<sub>f</sub>/W composites, including their distinctive properties after neutron irradiation, with the W fibers retaining ductility. The development challenges of W<sub>f</sub>/W composites will be compared to those of more mature ceramic matrix composites.

#### 2:00 PM

## (ICACC-S13-028-2025) Dimensional Stability of SiC Fibers under Low Temperature and High Dose Irradiation

- S. Kondo\*<sup>1</sup>; X. Yuan<sup>1</sup>; D. Geng<sup>1</sup>; K. Yabuuchi<sup>2</sup>; H. Yu<sup>1</sup>; Y. Ogino<sup>1</sup>; R. Kasada<sup>1</sup>
- 1. Tohoku University, Institute for Materials Research, Japan
- 2. Kyoto Daigaku, Institute of Advanced Energy, Japan

The irradiation stability of SiC/SiC composites is generally excellent, making them attractive structural material for neutron applications. However, at intermediate and low temperatures, under high doses, significant strength degradation has recently been found following neutron irradiation. This could be due to the smaller swelling in the SiC fibers compared to the SiC matrix. Unlike pure SiC that solely exhibit lattice expansion under irradiation, fibers could possess a contraction component, though the underlying mechanisms remain unclear. This study aims to elucidate the mechanisms mitigating swelling in SiC fibers. Highly crystalline SiC fibers (Hi-Nicalon type S, Tyranno SA3rd) were irradiated with 5.1 MeV Si-ions at room temperature or 300°C up to 100 dpa, followed by measurements of dimensional and strength changes, and microstructural analysis. The results indicated progressive amorphization (at RT) and significant strength reduction, with fiber expansion notably smaller than the SiC matrix. HRTEM revealed the dissolution of carbon packets within the irradiated fibers into the SiC grains, where shorter  $\pi$  bonds replaced the typical  $\sigma$  bonds predominantly found in the unirradiated SiC. This indicates that the excessive formation of C<sub>si</sub> antisites with shorter bonds is occurring within the SiC fibers, which may be one of the possible mechanisms responsible for the swelling mitigation.

#### 2:20 PM

#### (ICACC-S13-029-2025) Irradiation Effect on Particle Dispersion SiC Composites Fabricated by Liquid Phase Sintering

- T. Hinoki\*1; Y. Zhong1; J. Lee1; S. Kondo2
- 1. Kyoto University, Japan
- 2. Tohoku University, Japan

Silicon carbide (SiC) composites are promising materials for nuclear applications due to engineered toughness by fiber reinforcement and due to intrinsic features of SiC, including low activation, chemical and environmental inertness, exceptional irradiation stability, and very high temperature mechanical performance. The particle dispersion SiC composites were developed with the particle dispersion in matrix instead of fiber/matrix interphase. Highly crystalline SiC is required to avoid significant dimensional change due to crystallization under irradiation. Liquid phase sintering (LPS) forms highly crystalline SiC with sintering additives. Irradiation effect on particle dispersion SiC fabricated by LPS was characterized. Ion irradiation at DuET, Kyoto University and neutron irradiation at BR2, SCK CEN were carried out. Irradiation induced swelling, microstructure and mechanical properties were characterized following the irradiations. Effect of the particles like C was limited. Effect of sintering additives were limited at 800C or at low fluence. Amorphization of sintering additives were observed following ion irradiation at 300C. The design window of fluence and temperature ranges will be discussed for the particle dispersion SiC composites. Neutron irradiation and relating hot lab works have been performed by SCK CEN in the framework of SCK CEN-Tohoku Univ. collaboration.

#### 2:40 PM

#### (ICACC-S13-030-2025) Investigating the impact of neutron irradiation on SiC/SiC composites via X-ray computed tomography and finite element analysis modeling

J. D. Arregui-Mena\*1; T. Koyanagi2; Y. Katoh2

- 1. Oak Ridge National Lab, Nuclear Materials Science & Technology Group, USA
- 2. Oak Ridge National Laboratory, USA

SiC/SiC composites are emerging as potential materials for fuel cladding in LWRs and advanced reactor cores. Understanding the effects of thermal stresses, the reactor environment, and neutroninduced dimensional changes is crucial for the evaluation of SiC/SiC composite concepts. By utilizing x-ray computed tomography (XCT) scans, this study aims to quantify the neutron induced damage in SiC/SiC composites. Part of the study involved analyzing the XCT to emphasize the microstructural evolution resulting from neutron irradiation. Digital volume correlation (DVC) was used to process the XCT results and evaluate the overall neutron-induced deformation. Through the combination of these findings, one can assess plug compatibility and estimate SiC composite tube deformation via 3D characterization. Finite element analysis modeling was also conducted to understand the stress distribution. The deformation results from DVC and modeling could aid in identifying defects that could act as points of fracture initiation, thus advancing material development.

# S13- High temperature ceramics and environmental resistance I

Room: Coquina D

Session Chair: Hanns Gietl, Idaho National Laboratory

#### 3:20 PM

#### (ICACC-S13-031-2025) Ultra High Temperature Ceramics for Fusion Energy applications (Invited)

D. Sprouster<sup>1</sup>; L. Snead\*<sup>1</sup>; N. Cetiner<sup>2</sup>

- 1. Stony Brook University, USA
- 2. Massachusetts Institute of Technology, USA

Tungsten is presently the leading plasma facing component (PFC) candidate due to its attractive properties, resistance to sputtering, and chemical compatibility with tritium. However, extended exposure of W to fusion plasmas and 14 MeV neutrons raises significant concerns about its resilience against plasma-induced surface damage (cracking, erosion, and fuzz formation), and degradation of bulk properties due to neutron irradiation. Recognizing that rapid embrittlement due to neutron exposure of tungsten is a potentially insurmountable issue for the first-wall, which will experience the most extreme neutron fluence, ultra-high temperature ceramics (UHTCs) less susceptible to irradiation damage have emerged as promising first-wall materials. However, a significant technology and knowledge gap presently exists in both the materials and manufacturing methods needed for the production of integrated PFCs for viable fusion energy. In this work, we describe our efforts to fabricate UHTCs through direct current sintering with and without targeted sintering aids. Our fabrication and processing have yielded dense, uniform, monolithic UHTC compacts with no microcracks. The microstructure and thermophysical properties of several UHTC monoliths, pre- and post-neutron irradiation will also be presented. Our initial results based on the fabrication and performance testing have positive implications for future PFC research.

#### 3:50 PM

# (ICACC-S13-032-2025) Responses of SiC fiber-reinforced SiC matrix composites to high-dose neutron irradiation

- T. Koyanagi<sup>\*1</sup>; T. Nozawa<sup>2</sup>; Y. Katoh<sup>1</sup>
- 1. Oak Ridge National Laboratory, USA
- 2. National Institutes for Quantum and Radiological Science and Technology, Japan

For the development of silicon carbide (SiC) materials for nextgeneration nuclear structural applications, degradation of material properties under intense neutron irradiation is a critical feasibility issue. This study evaluated the mechanical properties and microstructure of a chemical vapor infiltrated SiC matrix composite, reinforced with nuclear grade SiC fibers coated with pyrolytic carbon, following neutron irradiation at 300 and 600 °C up to ~100 displacements per atom in the High Flux Isotope Reactor at Oak Ridge National Laboratory. Irradiation-induced degradation of the proportional limit stress and ultimate strength was associated with debonding at the fiber/matrix interface. The onset displacement damage level for the mechanical degradation depended on the microstructure of the fiber/matrix interface. The results indicate that optimization of the interface microstructure is required to overcome the lifetime limitations of the composite materials under irradiation environments. Options for developing the next-generation SiC composites with enhanced radiation resistance will be discussed. The study was supported by the US DOE Office of Fusion Energy Sciences and the National Institutes for National Institutes for Quantum Science and Technology.

#### 4:10 PM

## (ICACC-S13-033-2025) Corrosion characteristics of SiC/SiC composites in 2LiF-BeF\_ molten salt

B. W. Lamm\*1; T. Koyanagi2; H. Gietl1; J. Keiser1; J. Lee1; Y. Katoh1

- 1. Oak Ridge National Laboratory, Materials Science & Technology Division, USA
- 2. Oak Ridge National Laboratory, USA

Integration of SiC-based components in fusion reactor design requires the development of highly corrosion resistant materials. SiC/SiC composites comparing two kinds of SiC fiber (Tyranno SA3 and Hi-Nicalon type S) with chemical vapor infiltration SiC matrix were exposed to static molten salt, 2LiF-BeF<sub>2</sub>, for 1000 h at 650 and 750 °C. Both the fibers and matrix experienced localized pitting and nonuniform Si removal associated with trace metal impurities and/ or oxygen. Trace materials in the SiC fibers were associated with a reduced extent of corrosion on both fibers and matrix compared to high-purity SiC. The promising results warrant further investigations into the impact of material impurities on molten salt corrosion for reactor-grade components. This presentation is sponsored by US DOE, Office of Fusion Energy Sciences under contract DE-AC05-000R22725 with UT-Battelle, LLC.

#### 4:30 PM

# (ICACC-S13-034-2025) Compatibility of SiC sintered with $Al_2O_3/Y_2O_3$ additives and molten FLiNaK at 650°C

W. Cairang\*1; W. Zhou1; K. Vasudeva1; K. Woller2; S. E. Ferry2; M. P. Short1

- 1. Massachusetts Institute of Technology, Department of Nuclear Science and Engineering, USA
- 2. Massachusetts Institute of Technology, Plasma science and fusion center, USA

SiC-based materials remain difficult to implement as nuclear material partly due to their corrosion behavior with reactor coolants, which is highly dependent on microstructure, impurities, and processing. We investigate the corrosion behavior of liquid-phase sintered (LPS) SiC with Al<sub>2</sub>O<sub>3</sub>/Y<sub>2</sub>O<sub>3</sub> additives, exposed to molten FLiNaK salt at 650°C, using experimental techniques and DFT simulations. Experiments show that bulk LPS SiC disintegrates rapidly in contact with FLiNaK via reactions between KF and Al<sub>2</sub>O<sub>3</sub> at the grain boundaries. This reaction weakens the bond between SiC grains, allowing molten salt to infiltrate and disintegrate the SiC. DFT calculations corroborate these findings, showing that the adsorption energy of KF on O-terminated Al<sub>2</sub>O<sub>3</sub> is approximately one order of magnitude higher than that on Si-terminated SiC, indicating a stronger interaction with Al<sub>2</sub>O<sub>3</sub>. These findings show how the manufacturing and processing methods of commercial SiC greatly affect its potential for nuclear usage, as while the bulk SiC phase is largely unaffected, phases between the particles do not always fare as well. In this work, we will also present the simultaneous proton irradiation and corrosion of LPS SiC exposed to liquid lead at 675°C, showing how irradiation influences its corrosion behavior.

#### 4:50 PM

#### (ICACC-S13-035-2025) Fabrication of Advanced SiC<sub>t</sub>/SiC Composite with Improved Matrix Mechanical Properties by Particle Enhanced PIP

J. Lao\*1; C. Akaoglu1; K. Wei1; H. Liu1; P. Xiao1

1. Henry Royce Institute, University of Manchester, United Kingdom

Silicon carbide fibre reinforced silicon carbide composites (SiC<sub>f</sub>/SiC) were produced by an optimized SiC particle enhanced polymer infiltration and pyrolysis (PEPIP). The microstructure, composition and mechanical properties of the novel composites were explored by Raman, SEM, (HR)TEM, STEM, micro- and nanoindentation. Compared with the composites fabricated by conventional PIP process, the SiC matrix made by our optimized PEPIP exhibits considerably higher density, crystallinity and mechanical performance, especially the Young's modulus. The SiC matrix in PEPIP-SiC<sub>f</sub>/SiC predominantly consists of stiff crystalline SiC phase with reduced carbon content (Type A) and contains only a minimum portion of the softer, carbon-rich, nano-crystalline SiC phase (Type B), which is the dominant phase in the matrix produced by conventional PIP process. Deformed region beneath the nanoindentation mark of the matrix from PEPIP composite is found to be predominated by shear slip and exhibits a magnitude of dislocation density similar to high-quality FBCVD SiC material, and this is responsible for a higher Young's modulus. Besides, a tri-layer structure, featuring an intermediate porous carbon phase, was identified in the transitional region between the Type A and Type B matrix. This is believed to negatively impact the crystallization of PIP-SiC but can be mitigated by PEPIP methods.

#### 5:10 PM

# (ICACC-S13-036-2025) Investigating Irradiation-Induced Viscous Flow in Mullite Ceramics at Room Temperature

T. Miyagishi<sup>\*1</sup>; S. Kondo<sup>2</sup>; Y. Ogino<sup>2</sup>; H. Yu<sup>2</sup>; M. Park<sup>2</sup>; A. Hasegawa<sup>2</sup>; R. Kasada<sup>2</sup>

- 1. Tohoku Daigaku, Grauate School of Engineering, Japan
- 2. Tohoku University, Institute for Materials Research, Japan

Elucidating the mechanism of irradiation-induced viscous flow in mullite  $(3Al_2O_3 \circ 2SiO_2)$  ceramic may lead to self-healing and strength maintenance of materials used in irradiation environments. Our earlier work reported that a double-layer coating system with an alumina topcoat and a mullite bond coat on SiC did not show decrease interfacial strength even after irradiation, suggesting that the mullite might have filled microcracks. This study aims to investigate the degree of irradiation-induced viscous flow in mullite and to clarify its underlying mechanism. High purity (99.1%) polycrystalline mullite was used. Microcracks were introduced by micro-Vickers indentation prior to irradiation, with two different indentation force (0.98 N and 4.8 N) applied to create with varying opening widths. Proton irradiation at 2 MeV was conducted up to  $0.2\,$  dpa at room temperature. The damage level is considered to be well below the reported threshold of 0.35 dpa for "permanent" amorphization at this temperature. Post-irradiation analysis using laser microscopy showed some cracks closure, particularly in those created by lower indentation forces, with widths under approximately 0.5  $\mu$ m. Residual stress around the indentation may have driven the viscous flow, and cracks would be closed to decrease the surface energy. Further investigation into the degree of flow and mechanism will be presented.

### <u>S15 9th International Symposium on</u> <u>Additive Manufacturing and 3-D Printing</u> <u>Technologies</u>

#### **S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies- Design and Qualification** Room: Coquina A

Session Chairs: Meelad Ranaiefar, NASA Glenn Research Center; Michael Halbig, NASA Glenn Research Center

#### 1:30 PM

# (ICACC-S15-029-2025) Additive manufacturing of ceramics: How far can you go using computational design?

M. Pelanconi<sup>\*2</sup>; A. Ortona<sup>1</sup>

- 1. SUPSI, MEMTi, Switzerland
- 2. Scuola universitaria professionale della Svizzera italiana, MEMTi, Switzerland

This presentation is a review on the developments of complex ceramic structures at the SUPSI's Hybrid Materials Laboratory. From the first attempts to use CAD to explain the thermo-mechanical behaviour of ceramic foams by finite element modelling (FEM), this practice is now a fundamental step fully integrated in the ceramic additive manufacturing (AM). Demanding end users' requirements can be satisfied thanks to the combination of CD, simulation, and AM to solve multi-physics tasks. This presentation will show several examples of ceramic components working in high temperature, harsh conditions such as: re-entry thermal protection, porous burners, volumetric solar receivers, high temperature waste heat recovery systems, power to X components and periodic open cellular structures for catalysis.

#### 1:50 PM

#### (ICACC-S15-030-2025) Comprehensive investigation into Thermal Stability of AB-type Bio- Carbonate Hydroxyapatite synthesized via Heat-Treated Bovine Bone

H. Aeklah\*<sup>1</sup>

1. Obudai Egyetem Banki Donat Gepesz es Biztonsagtechnikai Mernoki Kar, Hungary

In recent years, interest in 3D printing of metallic biomaterials/ hydroxyapatite (HA) composites and HA coating of metallic biomaterials has increased. Rapid heating and cooling associated with 3D printing and coating processes may alter the phase composition of Bio-HA. Therefore, this study investigated the thermal stability and structural changes of Bio-hydroxyapatite (Bio- HA) prepared from heat-treated bovine bone occurring during calcination at 1000, 1100, 1200 and 1300 °C. The findings highlighted that the decomposition of AB-type CHA (ICSD NO. 261063) undergoes three stages: Dehydroxylation, formation of A-type CHA, and decomposition. Pure AB-type CHA was stable in a vacuum atmosphere, and no decomposition occurred at temperatures up to 1000 °C. Dehydroxylation and formation of A-type CHA occurred at 1100 °C. The AB-type CHA partially decomposed at a temperature of 1200 °C. A-type CHA,  $\alpha$ -TCP tricalcium phosphate (ICSD NO. 923), and TTCP tetracalcium phosphate (ICSD NO. 2631) were the main

products of the decomposition reactions, and  $\beta$ -TCP tricalcium phosphate (ICSD NO. 17082) was also detected in the system. After sintering at 1300 °C, the AB-type CHA was completely decomposed and converted into  $\alpha$ -TCP,  $\beta$ -TCP, and TTCP.

#### 2:10 PM

#### (ICACC-S15-031-2025) Designing Metamaterial Thermoelectric Generators for Optimal Energy Harvesting Efficiency

Y. Tang\*<sup>1</sup>; Y. Li<sup>1</sup>

1. Dartmouth College, Thayer School of Engineering, USA

Thermoelectric generators (TEGs) are increasingly recognized for their ability to convert low-grade waste heat into electricity via a temperature gradient, which offers a clean energy solution. Despite their significant potential, challenges such as low efficiency and high costs have limited their practical application. This paper introduces an innovative metamaterial design for TEGs with significantly improved efficiency. A Finite Element Model is validated using Bi<sub>0.5</sub>Sb<sub>1.5</sub>Te<sub>3</sub> bulk samples fabricated via the drop-cast method. This model can predict open-circuit voltage and output power as a function of an arbitrary metamaterial design. Four different metastructure designs, including 2D Triangular Honeycomb, Re-entrant, body-centered cubic (BCC), and triply periodic minimal surface (TPMS) structures, are systematically investigated. Detailed experimental and numerical analyses assess how annealing temperature, porosity, and unit cell numbers (UCNs) influence TE leg performance. The findings show that 2D Triangular Honeycomb and BCC structures effectively maintain a superior thermal gradient. Optimizing their porosity and UCNs significantly enhances output power. Compared to traditional bulk TE leg designs, adopting a 2D metastructure with 30% porosity and UCNs of 4×4×4 can approximately double the power output.

#### 2:30 PM

## (ICACC-S15-032-2025) Detecting strength-limiting defects in sintered ceramics printed via vat polymerization

L. O. Grant<sup>\*1</sup>; R. Maier<sup>1</sup>

1. National Institute of Standards and Technology, Materials Measurement Laboratory, USA

A recent interlaboratory study, jointly conducted by NIST, identified strength-limiting defects in ceramics printed with vat polymerization. When beams were tested with four-point bending, spherical and wormhole-shaped pores on the surface were key strength-limiting defects; this study highlighted the need for metrology to quickly detect surface and subsurface defects. Here, we compare two surface analysis techniques and their ability to detect strength-limiting defects.

### S15- 9th International Sym on Additive Manufacturing and 3D Printing Technologies-Design and Qualification- Materials Deposition

Room: Coquina A

Session Chairs: Lynnora Grant, Rice University; Michael Halbig, NASA Glenn Research Center

#### 3:10 PM

#### (ICACC-S15-033-2025) Effect of 3-D Printing Parameters on the Microstructure and Mechanical Properties of Ceramic and Glass Reinforced Polymer Composite Materials

L. R. Alexander-Roy\*1; M. Ranaiefar2; M. C. Halbig2; M. Singh3

- 1. Case Western Reserve University, USA
- 2. NASA Glenn Research Center, USA
- 3. Ohio Aerospace Institute, USA

In recent years, growing demand for lightweight, multifunctional components and systems have propelled the research and development on high performance materials and innovative manufacturing processes. The fused-filament-fabrication (FFF) process has been widely used for manufacturing materials in complex shapes and large sizes. In this work, two types of composite materials, namely basalt moon dust simulant and borosilicate in a polylactic acid (PLA) matrix, were 3D printed and compared with the pure PLA material. Mechanical properties (compression, tension, and Poisson's ratio) characterization was conducted. A Design of Experiments (DOE) approach was used to gain insight into the interactions between infill percentage, print orientation, and shell thickness with mechanical strength and Young's modulus. Microscopy and DIC were used to analyze the specimens before, during, and after testing and different failure modes were observed. Orienting the layer lines along the direction of load improved the strength of composite specimens but decreased the strength of pure PLA specimens. The design of experiments showed the infill percentage to be the dominant factor in determining strength, followed by shell thickness and print orientation. A significant interaction was noted between shell thickness and infill percentage.

#### 3:30 PM

#### (ICACC-S15-034-2025) 3D Printed Ceramic Reinforced Polymer Composites Microstructure and Mechanical Properties

A. P. Gyekenyesi\*1; M. Ranaiefar2; M. C. Halbig2; M. Singh3

- 1. Cleveland State University, USA
- 2. NASA Glenn Research Center, USA
- 3. Ohio Aerospace Institute, USA

In Fused Filament Fabrication (FFF) 3D printing a part is made by extruding material layer by layer. Benefits of FFF are the ability to print complex shapes quickly and at a lower cost compared to other manufacturing methods. In this work, filaments composed of either silicon carbide (SiC) or zirconium silicate ceramic particulates in a polylactic-acid (PLA) matrix were used to print specimens for microstructural analysis and mechanical testing. Pure PLA samples were also printed and tested as a baseline for comparison. A Design of Experiments approach was used to test the interactions between three different parameters and their effect on ultimate strength, Young's modulus, and yield strength. For compression test specimens, these parameters were infill percentage, number of shells, and print orientation angle. For tensile test specimens, the parameters were layer height, number of shells, and infill orientation angle. Pre- and post-compression test samples were evaluated by scanning electron microscopy for microstructural analysis. Infill percentage had the greatest effect on mechanical properties while number of shells and print orientation angle had minor effects. When changing the layer lines from perpendicular to parallel, relative to the loading direction, SiC-PLA had higher mechanical properties while pure PLA properties had decreased, and zirconium silicate-PLA had mix results.

#### 3:50 PM

#### (ICACC-S15-035-2025) Thermal Processing of Ceramic and Glass Polymer Composites 3D Printed By Fused Filament Fabrication

M. Ranaiefar\*<sup>1</sup>; L. R. Alexander-Roy<sup>2</sup>; A. P. Gyekenyesi<sup>3</sup>; M. Singh<sup>4</sup>; M. C. Halbig<sup>1</sup>

- 1. NASA Glenn Research Center, USA
- Case Western Reserve University, USA
- Cleveland State University, USA
- 4. Ohio Aerospace Institute, USA

The expansive utility of fused filament fabrication (FFF) based 3D printing technologies and demand for high-performance light-weight structures has prompted the emergence of various ceramic and glass polylactic acid (PLA) based composite filaments. However, detailed characterization of the processing-microstructure-property relationships of these materials is still required to realize their full potential. In this study, the thermal processing of basalt moon dust simulant, borosilicate, silicon carbide, and zirconium silicate, each with a PLA matrix, was investigated. Materials were characterized by thermogravimetric analysis to determine thermal processing temperatures.

Specimens of various infill percentages and shells were fabricated, and a thermal treatment was applied for de-binding and sintering. Microscopy of material cross-sections was conducted to evaluate the relationship between processing and porosity. By modifying the print parameters and thermal processing procedure, consolidated ceramic and glass specimens have been fabricated. The effect of processing parameters on the densification behavior and resulting microstructures will be discussed.

#### 4:10 PM

#### (ICACC-S15-036-2025) Process Development for Ceramic Composite Synthesis using FFF Additive Manufacturing Techniques

E. Faierson<sup>\*1</sup>; P. Collins<sup>1</sup>

1. Iowa State University, USA

Utilizing the Fused Filament Fabrication (FFF) additive manufacturing process with feedstock comprised of ceramic particles in a polymer binder is a relatively new technique for fabricating ceramic parts. This study investigated several bound-ceramic and metal filament feedstocks, with an emphasis on SiC, in order to create multi-material, spatially designed macrostructures and microstructures through the FFF process. FFF process parameters were developed to facilitate fabrication of suitable specimens using multiple materials. After fabrication the samples were consolidated using debinding and sintering techniques. Processing-Microstructure-Mechanical property relationships were investigated and optimized in order to reduce defects and obtain the best mechanical properties in the samples after sintering.

#### 4:30 PM

# (ICACC-S15-037-2025) Improving the degree of near-net-shape fabrication and the SiC content of 3D-printed C/C-SiC

N. Langhof\*1; W. Freudenberg1; J. Best1; S. Schafföner2

- 1. University of Bayreuth, Ceramic Materials Engineering, Germany
- 2. University of Bayreuth, Chair of Ceramic Materials Engineering, Germany

3D-printing of CMCs enable net-shape fabrication and 3D-shapes, that are not feasible or economically reasonable with conventionally fabrication. For C/C-SiC there are approaches with mainly direct ink writing and fused filament fabrication (FFF). Nevertheless, topics like the fiber length, the phase composition and the shape stability are challenges in this field. In this study we are trying to enhance the shape stability of FFF which is fair currently and not for all shapes and geometries reproducible. Therefore, we studied the crosslinking of PEEK by annealing the samples < 340 °C and we are trying to predict the change of dimensions by FE-Ansys. On the other hand, we are trying to increase the content of SiC, instead of Si and C. Samples with C-fiber reinforcement (13 vol. %) and fiber length of < 500  $\mu$ m were fabricated. Bending bars (5 x 10 x 60 mm<sup>3</sup>) were printed and different printing directions studied (0°, + 45°, 90°, - 45°). To study the crosslinking kinetic, DSC, TGA and rheology measurements were applied. Additionally, aqueous C-SiC slurries were infiltrated in C/C samples to increase the SiC content of C/C-SiC. For a suitable crosslinking, temperatures > 315 °C (> 12 h) are required. Shapes were predicted with Ansys and the SiC-content was increased by almost vol.50 % (strength increases: ~ 21 %). The microstructures and phase compositions were studied in detail as well.

#### 4:50 PM

# (ICACC-S15-038-2025) Solution- Based feedstock preparation for fused filament fabrication

#### O. Yucel\*1; J. Binner1

1. University of Birmingham, Ceramic Science & Engineering, United Kingdom

Additive manufacturing (AM), also known as 3D printing (3DP), has been used as a production and shaping method for polymers, ceramics and metals. Interest in this method increases due to reduced costs and providing design freedom without expensive tools. The development in AM of ceramic materials is relatively slow compared to polymers and metals. To improve 3DP of ceramics, various AM methods are proposed. Fused Filament Fabrication (FFF) is one of the ceramic AM methods. In this method, ceramic powder is mixed with a polymer binder system. This mixture is then used to produce a filament which is the feedstock for 3DP. A printer then uses the feedstock to produce pre-designed shapes on software. ZrSiO4 is the ceramic powder used in this work to produce a ceramic matrix composite. In this work, polymers are dissolved in a solvent for the mixing process instead of melting. There are several advantages of this approach. Low tool cost, low energy usage and simplicity of the method are some of them. The desired homogeneity is confirmed in this method and filament production was successful. Characterization of mixtures and filaments is going to be presented.

#### 5:10 PM

## (ICACC-S15-039-2025) Capillary rheometry to assess printability when extruding dense suspensions

L. O. Grant\*1; R. Maier1

1. National Institute of Standards and Technology, Materials Measurement Science Division, USA

The use of slurry-based feedstock, a ceramic powder mixed with an organic binder, is common in traditional ceramic processing as well as ceramic additive manufacturing. Dispensing slurry and building the ceramic part via additive manufacturing necessitates well-controlled slurries with chemical and rheological properties that are tailored to the printing process. The ceramic additive manufacturing team at NIST is developing measurements to understand the relationship between powder feedstock morphology, slurry rheology, and print parameters to increase the quality of additively manufactured technical ceramics. Using a capillary rheometer, we quantify key rheological properties (e.g. viscosity, yield stress, shear response) and compare the results to measurements are then related to the printability (extrusion, and shape retention) during direct ink writing ceramic dense suspensions.

### Friday, January 31, 2025

### **<u>S1 Mechanical Behavior and Performance of</u> Ceramics & Composites**

#### S1- Ceramics Processing-Microstructure-Mechanical Properties Correlation

Room: Coquina E

Session Chairs: Tetiana Prikhna, Institute for Superhard Materials of the National Academy of Sciences of Ukraine; Shenghuan Ding, University of Oxford

#### 8:30 AM

## (ICACC-S1-067-2025) Improving the uniformity and mechanical properties of flash sintered YSZ by doping with Ta and Nb

S. Ding\*1; R. I. Todd1

1. University of Oxford, Department of Materials, United Kingdom

To address the issue of non-uniform heat distribution in Flash Sintering (FS), a range of Ta/Nb dopants were introduced into 3YSZ. These dopants dissolve in the 3YSZ during FS, reducing electrical conductivity in regions that have experienced a high temperature and redirecting current to cooler, less sintered areas. This approach led to a more uniform sintering process, resulting in improved relative density and reduced grain size differences between the core and corners in both DC and AC FS specimens. Additionally, appropriate Ta/Nb doping preserved the tetragonal phase of 3YSZ at room temperature both by conventional and flash sintering at 1300-1500°C. This was highly transformable, leading to high frac-ture toughness of Ta/Nb-doped 3YSZ. To further optimize the properties of Ta/Nb-doped 3YSZ, a detailed investigation of compo-sitions in the Y2O3-ZrO2-Ta2O5 system was conducted. Processing variables such as dopant size and flash sintering conditions were also studied. This resulted in the successful development of uniformly flash-sintered 3YSZ with high fracture toughness.

#### 8:50 AM

### (ICACC-S1-068-2025) Improving damage tolerance of transparent ceramics using a multi-material design

A. Najafzadehkhoee\*1; A. Talimian<sup>2</sup>; A. Jabr<sup>3</sup>; R. Papšík<sup>3</sup>; D. Drdlik<sup>4</sup>; K. Maca<sup>4</sup>; D. Galusek<sup>2</sup>; R. Bermejo<sup>3</sup>

- 1. Ustav Anorganickej Chemie Slovenska Akademia Vied, Slovakia
- 2. Trencianska Univerzita Alexandra Dubceka v Trencine Centre for
- Functional and Surface Functionalized Glass, Slovakia 3. Montanuniversitaet Leoben, Institut fuer Struktur- und

Funktionskeramik, Austria

4. CEITEC - Central European Institute of Technology, Brno University of Technology, Czechia

The present study aims to utilize the build-up of residual stresses during the sintering in multi-material layered structures to improve the damage tolerance of transparent ceramics. Multi-material laminated structures and bulk samples composed of Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub>, and MgAl<sub>2</sub>O<sub>4</sub> were fabricated by stacking and thermo-compressing green layers shaped by tape-casting. Samples were consolidated using spark plasma sintering. Vickers indentation tests were used to evaluate the resistance of samples against sharp contact; the indentation load leading to the formation of an average of two radial/ median cracks per indent was used to represent the crack resistance (CR) of samples. The results showed that producing a compressive layer on the surface improved the damage resistance. The MgAl<sub>2</sub>O<sub>4</sub>/ Al<sub>2</sub>O<sub>3</sub>/MgAl<sub>2</sub>O<sub>4</sub> structure was characterized by a 500 MPa increase in damage resistance. The bonding between different layers and compatibility between the layers were found to be of paramount importance in achieving improved mechanical performance. The microstructural studies revealed that the adjacent layers affected each other's densification and grain growth through diffusion-induced grain boundary migration (DIGM). The role of neighboring layers, the stacking order, and their implications for further improving the performance of the layered ceramic by microstructural design are critically discussed.

#### 9:10 AM

# (ICACC-S1-069-2025) Design, Preparation and Application of nitride based Functionally Graded Materials

F. Chen\*1; B. Xiang1; M. Jia1; Q. Shen1

1. Wuhan University of Technology, China

Nitride ceramics are extensively used in sealing and insulation applications. In practice, it is necessary to combine nitride ceramics with metal to meet specific requirements. This necessitates addressing challenges such as ceramic/metal interface stress, interface compatibility and potential interface reactions. We have conducted systematic research on aluminum nitride based Functionally Graded Materials (FGMs), focusing on gradient material structure design, ceramic/metal system selection, gradient material preparation processes, properties testing, structural characterization and applications. We designed the gradient structure of the resulting material to address special conditions, such as high-temperature lithium vapor environments and thermal shock. For sealing applications, we designed the AlN/Mo/SS304 symmetrical gradient material. Results indicate that ceramic/metal inter-transfer network not only enhances the mechanical properties of the composite but also effectively inhibits high-temperature lithium vapor corrosion. For ceramic substrate materials, we developed AlN/Mo/Cu symmetric gradient materials for high frequency thermal shock, and the result indicates that the optimum shear strength of the FGMs is around 90 MPa and the FGMs with different diffusion interlayers failed in different ways when shear occurred, which greatly depends on the phase compositions at Cu/Mo joint.

#### 9:30 AM

## (ICACC-S1-070-2025) Thermal and Mechanical Characterization of Aluminum Fluoride Thin Films

M. Motezaker\*1; S. G. Walton3; P. E. Hopkins2

- 1. University of Virginia, Mechanical Eng, USA
- 2. University of Virginia, USA
- 3. US Naval Research Laboratory, USA

Aluminum is highly valued in UV optics for its excellent reflectivity at wavelengths as short as 90 nm; however, its performance is hindered by a rapidly forming native oxide layer that degrades reflectivity. To mitigate oxidation while maintaining optical performance, fluorine-containing coatings such as aluminum fluoride (AlF) are employed. AlF also serves as a barrier coating in advanced Li-ion batteries, preventing failures such as thermal runaway. Despite its widespread applications, the thermal and mechanical properties of AlF thin films remain underexplored. In this study, we investigated the thermal and mechanical properties of plasma-generated AlF layers with varying thicknesses. Mechanical properties were measured using picosecond acoustic techniques, while thermal properties were characterized using time-domain thermoreflectance (TDTR). We found that both the elastic modulus and thermal conductivity increase with film thickness, stabilizing for layers thicker than approximately 20 nm. This behavior correlates with a thickness-dependent chemical composition; energy-dispersive X-ray spectroscopy (EDS/EDX) analysis indicates that thinner layers have a higher aluminum content and lower fluorine content. These findings provide valuable insights for optimizing AIF films in optical and energy storage applications.

#### 10:10 AM

#### (ICACC-S1-071-2025) Experimental study of energy harvesting from mechanical load on lead zirconate titanate cement composite *WITHDRAWN*

V. Kumar<sup>\*1</sup>; S. K. Mishra<sup>1</sup>; A. Kumar<sup>1</sup>

1. Birla Institute of Technology, Mechanical Engineering, India

This paper presents the energy harvesting characteristics of cementlead zirconate titanate (PZT) composites under mechanical load. Four distinct composites were fabricated by incorporating 5%, 10%, 20%, and 40% PZT (weight%) into cement, utilising PZT powder of approximately 1-micron size. The experiment involved 28 days of water-cured unpoled composites. The study examines the waveform characteristics of the voltage generated by a unique energy harvesting circuit and the collected electromagnetic radiation (EMR) energy. The resultant peak EMR voltage and peak EMR energy are 1.47 V and 0.09 µW, respectively, with an applied mechanical energy of 500 mJ at 40% cement-PZT concentration. The sample with the maximum applied mechanical energy and the highest percentage of cement-PZT (i.e., 40% by weight) composites shows an increasing trend in the EMR voltage and energy waveforms. Both the DC voltage and the EMR energy acquired from the energy harvesting circuit exhibit an increasing pattern, corresponding to an increase in applied mechanical energy. The electromagnetic radiation energy harvesting response may be advantageous for both wired and wireless sensor applications, including fracture deformation in highways and buildings. This work advances our knowledge of impact-induced energy applications for sustainable and effective structure design.

#### S1- Ceramics for Aerospace and Other Transport Applications

Room: Coquina E

Session Chairs: B Venkata Manoj Kumar, Indian Institute of Technology Roorkee; Tetiana Prikhna, Institute for Superhard Materials of the National Academy of Sciences of Ukraine

#### 10:30 AM

## (ICACC-S1-073-2025) Sintering of TaB $_2$ modified by silicides: MoSi $_{22}$ ZrSi $_2$ and Si $_3N_4$

T. Prikhna\*1; P. Barvitskyi1; M. Karpets2; O. Borymskyi1; V. Moshchil1;

D. Zagorac<sup>3</sup>; A. Lokatkina<sup>1</sup>

- 1. Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Ukraine
- 2. National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine
- 3. Materials Science Laboratory, Vinča Institute of Nuclear Sciences, Belgrade University, Serbia

Ultra-high temperature (UHTC) transition metal borides can be used for a wide range of mechanical applications - as components of military and commercial equipment operating in extreme conditions. To UHTC belongs TaB<sub>2</sub> which exhibits high melting point (3200 °C), hardness (24.5 GPa - 25.6 GPa), fracture toughness (4.5 MPa m<sup>0.5</sup>), bending strength (555 MPa), excellent chemical stability, electrical  $(308 \times 10^4 \Omega^{-1} \times m^{-1})$  and thermal  $(0.160 - 0.161 \text{ W} \times \text{cm}^{-1} \times \text{K}^{-1} \text{ at})$ 300-1300 °C) conductivity, good corrosion resistance. In the present study we investigated modification of TaB<sub>2</sub> by MoSi<sub>2</sub>, ZrSi<sub>2</sub> and Si<sub>3</sub>N<sub>4</sub> in the amount of 20-30 wt.% and its sintering process under hot pressing conditions (30 MPa, 1750-1950 °C) and high pressure (4.1 GPa) - high temperature (1800 °C) conditions. The highest Vickers hardness  $H_v$ =31.5 GPa and fracture toughness  $K_{1C}$ =6  $MPa \times m^{0.5}$  under P= 9.8 N load was obtained for the composite sintered at 30 MPa, 1750 °C, 20 min from TaB<sub>2</sub>+20 wt.% ZrSi<sub>2</sub>, the increase of amount of ZrSi2 up to 30 wt.% leads to further increase in  $K_{1C}$ = 6.9 MPa×m<sup>0.5</sup>, but to the reduction of microhardness down to  $H_v$ =23.5 GPa. The composite sintered under 30 GPa at 1950 °C

for 40 min from TaB<sub>2</sub>+20 wt.%  $MoSi_2$  showed  $H_v$ =28.2 GPa and  $K_{1C}$ = 5.42 MPa×m<sup>0.5</sup>. AcknowledgementS: This work was supported by the Project of the NAS of Ukraine III-5-23 (0786).

#### 10:50 AM

#### (ICACC-S1-074-2025) Enhancing Mechanical Integrity in 3-YSZ Ceramic Cores for Aero-Engine Applications via Vat Photopolymerization 3D Printing: A Nanomechanical Analysis

P. P. Reddy<sup>\*1</sup>; P. Gandhi<sup>1</sup>; G. Singh<sup>1</sup>

1. Indian Institute of Technology Bombay, India

As aero engine performance advances, the production of hollow blades with intricate internal cooling cavities becomes increasingly challenging. The ceramic core, a crucial intermediate component in this process, has garnered significant attention. Vat photopolymerization (VPP) additive manufacturing technology based digital light processing (DLP) and sintering has been adopted to rapidly create these complex ceramic cores. However, variation in surface nanomechanical properties affects the performance of ceramic cores. This study presents a quantitative analysis of the nanomechanical properties of 3-YSZ (yttria stabilized zirconia) manufactured using DLP. Atomic force microscopy (AFM) and nanoindentation tests with sub-micrometer resolution were used to map the contact Young's modulus across the layered structure. The investigation focuses on the influence of DLP printing parameters on the Young's modulus in both green and sinteredparts. Parameters such as layer thickness, orientation, and light intensity were analyzed and optimization was performed to get isotropic strength parts. Findings demonstrate significant improvements in the mechanical integrity of printed parts, showcasing the potential for their application in ceramic core manufacturing.

#### 11:10 AM

# (ICACC-S1-075-2025) Fabrication of Silica Particles with Adjustable Properties for Advanced Propulsion Systems

B. Pajo<sup>\*1</sup>; R. Trice<sup>1</sup>; C. Martinez<sup>1</sup>

1. Purdue University, Department of Materials Engineering, USA

Rotating detonation engines (RDEs) represent a significant advancement in hypersonic flight technology, offering enhanced efficiency compared to traditional deflagration-based cycles. However, the high-frequency, high-amplitude dynamic loads and operational temperature of approximately 1600 °C associated with this technology present substantial challenges for a wide range of materials traditionally utilized in hypersonic propulsion, particularly brittle ceramics. Research has demonstrated that the incorporation of discrete glassy phases in ceramic materials has the potential to absorb the periodic detonation load of RDEs via its structural relaxation mechanisms near its glass transition temperature. This provides energy absorption and increases the fracture toughness of the ceramics. For this reason, we propose the utilization of an amorphous silica (SiO<sub>2</sub>) /mullite (3SiO<sub>2</sub>-2Al<sub>2</sub>O<sub>3</sub>) model system in studying the energy absorption and toughness enhancement of high-temperature ceramic composites, with silica functioning as the discrete toughening phase and mullite as the continuous elastic matrix. In this presentation, the development of chemistry and methodology to fabricate silica glass particles with various diameters and compositions that can be tailored to meet the requirements of RDEs will be discussed.

#### 11:30 AM

#### (ICACC-S1-076-2025) Boron Nitride-Nanotube - Silicon Nitride Composites for High Temperature Radome Applications

- V. Mika\*2; C. Davis1; J. P. Youngblood2; R. Trice2
- 1. Naval Surface Warfare Center Crane Division, USA
- 2. Purdue University, Department of Materials Engineering, USA

High temperature radomes necessitate a number of design constraints, including a need for stability at high temperatures while maintaining a low dielectric constant to minimize signal loss. The addition of boron nitride nanotubes to a conventional silicon

nitride system represents a potential to lower dielectric constant while not sacrificing other material properties. This study investigates the manufacturing processes needed as well as the mechanical properties of zero to 3 volume percent boron nitride nanotube loaded silicon nitride. 4-point bend testing was performed, as well as impulse excitation testing and fracture surface micrography. The results suggest the combined system shows promise in the field of radome materials, but may require further study.

### <u>S6 Advanced Materials and Technologies for</u> <u>Rechargeable Energy Storage</u>

#### **S6- Electrodes and Electrolytes for Battery Systems** Room: Coquina B

Session Chairs: Derrick Fam, Institute of Materials Research and Engineering; Palani Balaya, National University of Singapore

#### 8:35 AM

#### (ICACC-S6-035-2025) Analysis of cation-anion redox of $Na_2MS_2$ (M = Transition metal) for sodium secondary batteries (Invited)

A. Nasu\*1; R. Miyamoto1; H. Kobayashi1; M. Matsui1

1. Hokkaido Daigaku, Faculty of Science, Japan

All-solid-state sodium batteries are the one of the most potent energy sources due to the high energy density and safety. To achieve the practical development goal, novel active materials with high energy density are necessary. Reversible utilization of anion redox are focused on to improve their capacity. However structural change by anion redox heavily affects reversibility of redox and ionic transfer. Especially, anion dimer is formed in the redox reaction, and then the structural change tied to the irreversible change and spoiling ionic diffusion. In this study, we analyze cation-anion redox mechanisms based on  $Na_2FeS_2$  and  $Na_2CoS_2$  with reversible anion redox reaction. Na<sub>2</sub>FeS<sub>2</sub> showed 2  $e^-$  reaction with Fe<sup>2+/3+</sup> redox and S redox.  $Na_2CoS_2$  also showed 1.3 e<sup>-</sup>reaction with  $Co^{2+/3+}$  redox and S redox. During the cation redox in Na<sub>2</sub>FeS<sub>2</sub> and Na<sub>2</sub>CoS<sub>2</sub>, the XRD patterns showed phase transition with maintaining crystalline phases. On the other hands, their crystallinities decreased by utilizing S redox. Observing the XAFS spectra, Na<sub>2</sub>FeS<sub>2</sub> showed isolated S-S bonding. The disproportionation of Fe and S-S dimer suggested that the local phase separation was induced. On the other hands, Na<sub>2</sub>CoS<sub>2</sub> showed hybridization of sulfur dimer and iron. The reaction suppressed the irreversible change in the host structure.

#### 9:05 AM

# (ICACC-S6-050-2025) Highly reversible anode for LIB and NIB based on oxidized $Ti_3Al_{(1-x)}Sn_xC_2$ MAX phases

S. Marchionna\*1; A. Gentile1; N. Vallana2; C. Ferrara2; I. Ostroman2; R. Ruffo2

- 1. Ricerca sul Sistema Energetico RSE SpA, TGM- Materials and Generation Technologies for Energy, Italy
- 2. Universita degli Studi di Milano, Material Science department, Italy

To improve electrochemical performance of LIB and NIB batteries, conversion/alloying mechanisms are a powerful option to store alkaline ions. Unfortunately, these processes induce in common active materials low mechanical stability and a very short lifespan of the final devices. A way to overcome these main drawbacks is the nano-structuring of the materials used in the electrodes. We have tested a new approach to sinter nanocomposites based on the self-formation of nano (Ti/Sn)O<sub>2</sub> system by means the partial oxidation of the Ti<sub>3</sub>Al<sub>(1-x)</sub>Sn<sub>x</sub>C<sub>2</sub> MAX phase. Exploiting this strategy, we developed composite electrodes of (Ti/Sn)O<sub>2</sub> and MAX phase that tested in half-cells vs Li/Li<sup>+</sup> are capable of withstanding over 600 cycles in half cells with charge efficiencies higher than 99.5% and specific capacities comparable to those of graphite (>300mAh/g) and higher than lithium titanate (Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub>) or MXenes. The main experimental parameters have been deeply investigated in other to

maximize the electrochemical performances and understand the mechanisms that favorite their improve. We verify a crucial role of the unreacted MAX phase on which nucleated the Ti/Sn oxide nano-particles acting both as a conductive agent and as a buffer to preserve the mechanical integrity of the oxide during the (de-)lithiation cycles. Preliminary results about the use of the same materials as anode for NIB will be also reported.

# (ICACC-S6-051-2025) Sodium solid electrolytes- design & technology aspects MOVED TO THURSDAY, JANUARY 30, 2025 AT 4:20 p.m.

D. Wagner<sup>\*1</sup>

1. Fraunhofer-Institut fur Keramische Technologien und Systeme IKTS, Energy, Germany

Sodium-based cells, especially solid state concepts, gain more attention recently, because of more uncritical, sustainable materials, but also due to safety aspects. In addition to more efficient materials and combinations thereof, new technologies and strategies are required for creating the best possible conditions in batteries. The design and combination of cathode, electrolyte and anode can be investigated and optimized in various ways. Our work shows an overview of our activities on ceramic sodium solid electrolytes, containing systematic compositional variations, manufacturing technologies and metallic interlayers, as well as the interfacial resistance and the stability of cyclability of cells with sodium anodes. Conventional Sintering allows electrolyte thicknesses of 90 µm and conductivities of 2.5 mS/cm for NASICON (1250°C) and 1.5mS/cm for NaRSiO (1000°C). Alternative cold co-sintering performed on these materials, shaped as powder compacts and tapes, lead to 260 µm thick dense NASICON and with a conductivity of 0.3 mS/cm below 400°C. Cold co-sintering of tapes and printed active material layers is also conceivable and proven in first attempts. Using metallic interlayers has proven to be promising for improving the connection of sodium anode in terms of reduced interfacial resistance and higher cycle stability. Multiple approaches to optimize materials and processes, can lead to improved solid state cell concepts.

# S6- Recycling and Advanced Processes for Electrode Materials

Room: Coquina B

Session Chairs: Xiaonan Shan, University of Houston; Palani Balaya, National University of Singapore

#### 10:20 AM

#### (ICACC-S6-053-2025) Electrode Delamination by Induction Heating for Direct Recycling Operations for Spent Li-Ion Batteries

B. Ma\*1; O. Kahvecioglu1; B. Polzin1

1. Argonne National Laboratory, USA

A direct recycling process to reclaim active electrode materials by induction heating was developed at Argonne National Laboratory. This fast and scalable manufacturing process can quickly recover high-quality critical materials and high-purity metals from manufacturing scrap or spent Li-ion battery electrodes without the need for expensive, high-temperature, or mechanical separation processes. The principal application of this technology is in the Li-ion battery recycling industry. The materials recovered include graphite, copper, and cathode powders, are valuable and in short supply. Through induction heating delamination followed with a direct recycling process, these materials can be reused to produce new Li-ion batteries. We observed a recovery rate of ~97% using the Argonne developed technology. Electrochemical testing of battery cells made with the recovered anode materials showed comparable performance to pristine battery cells. Recycling by induction heating can reduce costs, save energy, and increase environmental sustainability in the Li-ion battery recycling industry. Implementation of this battery recycling technology will significantly increase energy savings, reduce the production of greenhouse gases, help meet the objective of improving the recovery and reuse of critical materials in end-of-life Li-ion batteries, and achieve net zero  $CO_2$  emissions by 2050.

#### 10:40 AM

#### (ICACC-S6-054-2025) Innovative method for strategic metals recovery from exhausted lithium-ion batteries based on microwave heating **WITHDRAWN**

A. Zanoletti<sup>1</sup>; A. Cornelio<sup>1</sup>; M. Scaglia<sup>1</sup>; A. Bonometti<sup>1</sup>; E. Galli<sup>1</sup>;

- E. Bontempi<sup>2</sup>; F. Alptekin<sup>\*2</sup>
- 1. Universita degli Studi di Brescia, Italy
- 2. Universita degli Studi di Brescia, DIMI, Italy

Strategic metals recovery from spent lithium-ion batteries (LIBs) is a critical step toward environmental sustainability and resource conservation. It is estimated that by 2050 the demand for lithium, and cobalt will increase by 506%, and 460%, respectively. Our work proposes a new technology based on a dedicated microwaves (MW) device for strategic metals recovery (Li, Mn, Ni and Co) derived from spent LIBs. The application of MW allows for the rapid elevation of temperature in the black mass, facilitating carbothermic reactions that enable Li recovery through a water solution and Ni, Co and Mn through environmentally friendly organic acid (L-malic acid). This new technology won the EIT RAW Materials competition in February 2022 and was selected from EU as emerging technology for energy efficiency. Experimental results obtained from a spent LCO (LiCoO<sub>2</sub>) BM sample reveal an efficiency higher than 80% within just a 5 minute treatment period. These findings support the proposition of this technology as a promising alternative to the traditional pyrometallurgical method and offer the opportunity to avoid several onerous BM pre-treatment steps.

#### 11:00 AM

#### (ICACC-S6-055-2025) New composite material based on hydrogel and combined conductive fillers for energy storage applications

G. Malyszko\*1; P. Jasinski1; S. Pawlowska1

1. Politechnika Gdanska, Department of Functional Materials Engineering, Poland

The unique properties of hydrogels combined with conductive additives have created new opportunities in the construction of innovative and low-cost systems for application as catalytic electrodes for oxygen evolution reaction (OER) and as supercapacitors. In this work new hydrogels composite materials based on N-isopropylacrylamide and conductive particles were prepared by one-stage synthesis. This method involves ultrasonic bathing of a hydrogel precursor in various solvents with suspended MnCo<sub>2</sub>O<sub>4</sub> (MCO) spinel and conductive carbon black (cCB) particles. A suitable method of dispersing the catalyst particles in the 3D hydrogel matrix was chosen to enable their separation from each other and increase their active surface area. The presence of MCO particles and cCB particles in the composite structure was confirmed by morphological analysis. The study verified electrical conductivity and catalytic activity of the hydrogels increased with the increase in the concentration of conductive carbon particles. This work demonstrates that the use of hydrogel as a matrix to suspend catalytic particles appears to be a promising technique for creating new energy conversion and storage systems with high catalytic activity.

### S10 Integrated computational-experimental modeling ad design of ceramics and composites

# S10- Modeling physical properties of advanced ceramics

Room: Coquina G

Session Chair: Dilpuneet Aidhy, Clemson University

#### 8:30 AM

#### (ICACC-S10-024-2025) Compressible Solid Electrolytes for Durable High Energy Density Batteries (Invited)

S. Adams\*1

1. National University of Singapore, Materials Science and Engineering, Singapore

Energy-dense long-life solid-state batteries require low-density catholytes that are electrochemically and -mechanically compatible with the cathode. Here, we synergize experimental characterizations with atomistic simulations to design and realize 2 classes of compressible electrolytes, that prolong cycle life by maintaining close interfacial contact with breathing cathodes. Ceramic-in-polymer Composite Electrolytes containing doped polyacrylonitrile, plasticizers and surface-active nanoceramics reach Li<sup>+</sup> conductivities of 0.1–1 mS/cm at densities <2 g/cm<sup>3</sup> and retain wide electrochemical windows by inducing a percolating network of fast-conductive interphases. Symmetric cells cycle stably with up to 2 mA/cm<sup>2</sup> over 500 h. Further improvements are expected from oriented nanoceramics. As an alternative, we exploit the correlation between conductivity and glass forming ability in glass-ceramic oxyhalides such as LiMOCl<sub>4</sub> (M=Nb, Ta) with conductivities of ca. 10 mScm<sup>-3</sup>. Our redetermination of the LiNbOCl<sub>4</sub> structure and MD simulations then find that LiNbOCl<sub>4</sub> is in a plastic-crystalline state at room temperature, explaining its favorable catholyte performance.

#### 9:00 AM

#### (ICACC-S10-025-2025) Photomechanical Effects in ZnS: Investigating Dislocation Nucleation and Behavior Under Stress and Light via Computational Simulations (Invited)

#### Q. $An^{*1}$

1. Iowa State University, Materials Science and Engineering, USA

Semiconductors, essential in electronics and solar panels, are often brittle and prone to damage. When exposed to light, they can either harden or soften-a phenomenon known as photoplasticity. Despite being recognized since 1957, the fundamental understanding of photoplasticity remains incomplete. We explore the underlying mechanisms of photoplasticity in ZnS using a quantum mechanics (QM)-based framework that integrates density functional theory (DFT), and constrained DFT. First, we discuss DFT calculations on the generalized stacking fault energy surface. We demonstrate that the bond strength in ZnS is highly sensitive to the local electron distribution, which can be effectively modified by electron-hole (e-h) pairs induced by photoexcitation. Notably, sphalerite ZnS transitions from a dislocation-dominated deformation mode in its ground state to a twin-dominated deformation mode under bandgap electronic excitations, leading to brittle failure under light illumination. Next, we examine dislocation properties in ZnS. Our simulations reveal that photoexcitation increases the energy required to break the Zn-S bond within the S-core dislocation during its glide process due to the redistribution of excited holes. This increase in bond energy raises the energy barrier for dislocation glide, reducing ZnS's dislocation mobility under light.

#### 9:30 AM

# (ICACC-S10-026-2025) Electronic Band Structure Variations in Photothermocatalytic Materials

J. K. Vanderslice\*1

#### 1. University of Missouri-Kansas City, Physics, USA

Novel photothermocatalytic devices based on layered semiconductors have great promise as efficient overall water splitting devices for hydrogen production, which can help make H<sub>2</sub> into an economically viable alternative to fossil fuels. The effectiveness of the proposed devices is sensitively influenced by the electronic structure of the different materials and their interfaces. Yet, the electronic band structure properties of many of these materials under thermal expansion is under-explored. In this study we calculate the electronic structures of a select group of sulfide semiconductors and their lattices thermal expansions, focusing on variations in key parameters such as band gap, valence band edges, and conduction band edges. The chosen materials (Ag<sub>2</sub>S, MnS, CoAsS, FeS<sub>2</sub>, etc.) were selected for their simple structures, lower electron counts and increasing band gaps compared to each other. By calculating band structures along a universal high-symmetry path that is applicable to all cell symmetries, we determine how temperature-induced asymmetric lattice changes impact the electronic properties of individual materials and the overall thermal stability of the proposed photothermocatalytic device. This approach could provide valuable insights into optimizing materials for efficient photothermocatalytic devices and guide future designs for water splitting applications.

#### 9:50 AM

## (ICACC-S10-027-2025) A Systematic ab initio Study of Electronic Transport Properties of $Ln_2NiO_4$ (Ln=La, Nd, and Pr)

S. Yang<sup>1</sup>; Y. Zhong<sup>\*1</sup>

1. Worcester Polytechnic Institute, Mechanical and Materials Engineering, USA

The  $Ln_2NiO_4+\delta$  (Ln = La, Nd, Pr) Ruddlesden-Popper (RP) family, characterized by the K2NiF<sub>4</sub>-type structure, has garnered significant attention due to its remarkable ionic and electronic conductivity. However, theoretical studies on its electronic transport properties remain scarce. In this work, we systematically investigate the electronic structures and transport properties of  $Ln_2NiO_4+\delta$  (Ln = La, Nd, Pr) using ab initio calculations. The transport properties are predicted based on Boltzmann transport theory. Specifically, the DFT+U method and the HSE06 hybrid functional are employed to predict the electronic structure of the RP phase.

#### 10:10 AM

#### (ICACC-S10-028-2025) Decipher the Materials Genome via Understanding Grain Boundary Phase-like Transitions (Invited) J. Luo<sup>\*1</sup>

1. University of California, San Diego, USA

The materials science community has long recognized that grain boundaries (GBs) can be treated as two-dimensional interfacial phases, which were also named as "complexions" to differentiate them from bulk phases. As bulk phase diagrams are arguably the most useful materials science tool, it is envisioned that their GB counterparts can be equally useful for materials design. In this talk, I will first review a series of our studies to compute the GB phase (complexion) diagrams. Recent collaborative studies within the UCI MRSEC CCAM computed a GB lambda diagram to explain activated sintering of a refractory high-entropy alloy and utilized disordered GBs in compositionally complex perovskite oxides to improve lithium-ion conduction. Another emergent concept is represented by high-entropy grain boundaries (HEGBs). In addition to temperature, chemical potentials, and pressure, an applied electric field can induce a GB transition electrochemically. A recent study utilized electrochemically-induced GB transitions to create graded microstructures and tailor microstructural evolution.

### <u>S13 Development & Applications of Adv</u> <u>Ceramics & Composites for Nuclear Fission/</u> <u>Fusion Energy Sys</u>

# S13- High temperature ceramics and environmental resistance II

Room: Coquina D

Session Chair: Takaaki Koyanagi, Oak Ridge National Laboratory

#### 8:30 AM

# (ICACC-S13-037-2025) Joining and Coating of SiC/SiC for safe nuclear energy applications

A. Pizzinat\*1; M. Ferraris1

1. Politecnico di Torino, Department of Applied Science and Technology (DISAT), Italy

SiC/SiC composites are promising options for a safer nuclear fuel cladding technology and advanced fusion and fission reactors; however, their joining process and materials are still to be optimized. Some research activity is now directed towards using SiC preceramic polymers to join and coat SiC/SiC composites. The process involves preparing a polycarbonsilane polymer mixed with SiC nanoparticles and fibers, followed by thermal treatments: curing in air at 100°C and pyrolysis in an inert atmosphere at 1450°C. The morphology, microstructure, and mechanical properties of the joined and coated SiC/SiC composites will be discussed. Acknowledgements: This research was funded by the EU's Horizon 2020 programme under grant No. 101059511 - Project SCORPION (SiC Composite Claddings: LWR Performance Optimisation for Nominal and Accident Conditions).

#### 8:50 AM

#### (ICACC-S13-038-2025) Liquid Migration of Fission Product Leakage in SiC layer of TRISO Fuel: Insights from In-situ and Ex-situ Ag-Pd/SiC and Ru-Pd/SiC Interaction Studies

J. Lao<sup>\*1</sup>; K. Wei<sup>1</sup>; H. Liu<sup>1</sup>; J. F. Martins<sup>1</sup>; C. Lin<sup>2</sup>; Y. Lei<sup>2</sup>; Z. Kho<sup>2</sup>;

- A. Eggeman<sup>2</sup>; X. Liu<sup>2</sup>; M. Smith<sup>2</sup>; P. Withers<sup>1</sup>; P. Xiao<sup>1</sup>
- 1. Henry Royce Institute, The University of Manchester, United Kingdom
- 2. The University of Manchester, Materials, United Kingdom

The effective containment of fission products (FPs) such as silver (Ag), palladium (Pd) and ruthenium (Ru) within tri-structural isotropic (TRISO) fuel particles is crucial for the safety and efficiency of High-Temperature Gas-cooled Reactors (HTGRs). The release mechanisms of Ag and Ru have been the subject of extensive research for decades, however, a comprehensive understanding of their release behaviour in TRISO fuel has vet to be fully achieved. By using the most advanced microscopy technique such as ex-situ and in-situ heating TEM, precession electron diffraction (PED) and thermodynamic analysis, this out-of-pile work studied the migration mechanism of Ag and Ru, facilitated by Pd in SiC layers of TRISO at elevated temperatures. It is found that in Ag-Pd/SiC system, Ag is dissolved in  $Pd_2Si$  to form  $(Pd_2Ag)_2$  Si phase, and in the in-situ heating work their fast liquid migration along SiC grain boundaries was directly observed at 1100°C; in the Ru-Pd/SiC system, the introduction of Pd facilitates the formation of a Ru-Pd-Si liquid phase even at minimal Pd content, and their liquid migration behaviour via grain boundaries resembles the observations made in in-pile studies. Comparing Pd's role in both systems underscores the importance of liquid phases and strongly corrosive element in facilitating the migration of FPs in SiC.

#### 9:10 AM

#### (ICACC-S13-039-2025) Aligned Boron Nitride Nanotube Reinforced Polyethylene Nanocomposite for Space Radiation Shielding

P. B. Patel\*2; N. Joseph2; C. Park1; V. L. Wiesner1; B. L. Wardle2

- 1. NASA Langley Research Center, Advanced Materials and Processing Branch, USA
- 2. Massachusetts Institute of Technology, USA

With NASA's Artemis program aiming to establish a human presence on the Moon and eventually on Mars, protecting astronauts from radiation is necessary. Flight-heritage materials, like those with high hydrogen content, such as polyethylene (PE), have proven to be effective radiation shields. This is due to hydrogen's high chargeto-mass ratio, low secondary radiation production, efficient energy absorption, and high cross-section, which increases the probability of particle interactions to slow or stop ionized particles. Boron nitride nanotubes (BNNTs) and other boron-rich materials offer more effective thermal neutron radiation-stopping capabilities due to their high cross-section and neutron absorption properties. BNNTs also enhance the mechanical properties of radiation shielding material due to their high strength-to-weight ratios. However, integrating high volumes of nanotubes in a matrix without defects presents significant manufacturing challenges. To address this, a bulk nanocomposite laminate fabricating technique, involving synthesizing millimeter-long vertically aligned BNNTs, densifying the nanotubes to high-volume fractions, and infusing the nanotubes with PE while applying heat and pressure was utilized to fabricate the BNNT-PE nanocomposite that was tested for its radiation shielding properties at NASA Langley Research Center's neutron radiation exposure lab.

#### 9:30 AM

## (ICACC-S13-040-2025) Nano-porosity characterisation of TRISO coatings using small angle X-ray scattering

E. White\*1; A. Smith2; T. Snow2; D. Kazantsev2; M. Davies3; M. Moore4;

- D. Goddard<sup>4</sup>; N. Tzelepi<sup>5</sup>; A. Seddon<sup>1</sup>; T. Martin<sup>1</sup>; D. Liu<sup>6</sup>
- 1. University of Bristol, United Kingdom
- 2. Diamond Light Source Ltd, United Kingdom
- 3. Ultra Safe Nuclear Corporation, USA
- 4. National Nuclear Laboratory Preston Laboratory, United Kingdom
- 5. National Nuclear Laboratory Ltd, Central Laboratory, United Kingdom
- 6. University of Oxford, United Kingdom

TRistructural ISOtropic fuel (TRISO) is a type of ceramic-coated nuclear fuel under consideration for the next generation of nuclear reactors. TRISO particles consist of a central fuel kernel, a porous carbon 'buffer' coating, and a SiC coating that is sandwiched between two pyrolytic carbon (PyC) coatings. The nano-porosity of these carbon coatings impacts the irradiation behaviour and transport of fission gases, so a complete understanding of the distribution is required. Conventional methods such as X-ray computed tomography and focused ion beam tomography have previously been used to characterise the coating micro-porosity. However, due to the resolution, they often struggle to resolve pores that are sub-100 nm and cannot determine the nano-porosity. There are several reasons for determining the nano-porosity. One is that variance between measurements in literature and specification values must be understood. Another is that the nano-porosity greatly influences the radiation effects which in turn affects predictions of fuel performance. The application of small angle X-ray scattering has been applied to the PyC coatings. Analysis of the scattering trace produced has allowed for a size distribution of the pores at each scan location to be determined. These results will be compared to the results from previous tomography experiments to produce a multilength scale porosity distribution.

# S13- High temperature ceramics and environmental resistance III

Room: Coquina D

Session Chair: Takaaki Koyanagi, Oak Ridge National Laboratory

#### 10:10 AM

### (ICACC-S13-041-2025) Cermet waste forms for immobilizing advanced reactor waste streams

R. Saini\*1; A. Goel1

1. Rutgers University, Materials Science and Engineering, USA

The high level waste (HWL) anticipated at the back end of advanced reactor (AR) fuel cycles shall include significant quantities of stainless steel, undissolved solids (UDS), graphite, metal oxides, and halide-based salts which makes it difficult to be immobilized into borosilicate glass, thus imposing significant challenges like low waste loading, complex processing, poor chemical durability of waste form, higher cost and longer processing time. To escalate the vitrification process and mitigate this problem, the present work emphasizes on developing high density and durable cermet waste form (WF) suitable to immobilize multiple AR wastes. These cermets comprising metals (stainless steel, Hastelloy, UDS), sodalite, halides and phosphates shall be prepared by spark plasma sintering, and hot uniaxial pressing, and characterized using x-ray diffraction (XRD), scanning electron microscope (SEM), energy dispersive spectroscopy (EDS), Electron probe microanalyzer (EPMA), Hg porosimetry and He pycnometry. The density and chemical durability of these cermets shall be optimized using different metal-to-ceramic ratios and processing variables (temperature, pressure, time). The results obtained from these investigations shall be presented.

#### 10:30 AM

#### (ICACC-S13-042-2025) First principles investigation into hydrogen solubility in defect-induced cubic silicon carbide I. Evarts<sup>\*1</sup>

1. Pacific Northwest National Laboratory, National Security Directorate, USA

Tritium and hydrogen serve critical roles across various industries. Fusion reactors, such as tokamaks, rely on a stable tritium supply for the tritium-deuterium reaction. In renewable energy applications, hydrogen storage systems (HSSs) benefit from hydrogen permeation barriers to enhance tritium retention. To improve hydrogen retention silicon carbide empirically exhibits good resistance to hydrogen permeation. Multiple investigations have modeled hydrogen diffusion in silicon carbide; however, due to its non-trivial nature, solubility has not been computationally investigated from a first principles approach. Herein, it is shown that combing ab initio techniques with statistical mechanics a model for hydrogen solubility in silicon carbide is constructed. Solubility contributions from defect sites, such as interstitials, vacancies and grain boundaries, are deconvoluted providing an in-depth understanding of hydrogen behavior. This model finds that the carbon-rich grain boundaries, silicon vacancies and interstitial sites, such as the three-center bond (Si-H-Si), adjacent to vacancies are the largest contributors to hydrogen solubility.

#### 10:50 AM

#### (ICACC-S13-043-2025) Characterization of Rapid Laser Chemical Vapor Deposition (R-LCVD) SiC Fibers

L. Mazzocco\*<sup>1</sup>; P. Cervenka<sup>1</sup>; A. Seshadri<sup>1</sup>; K. L. Williams<sup>2</sup>; S. Harrison<sup>2</sup>; J. Pegna<sup>2</sup>; P. Xu<sup>3</sup>; K. Shirvan<sup>1</sup>

- 1. Massachusetts Institute of Technology, Nuclear Science and Engineering, USA
- 2. Free Form Fibers, USA
- 3. Idaho National Lab, USA

Rapid Laser Chemical Vapor Deposition (R-LCVD) is an innovative technique for fabricating SiC fibers for SiC/SiC composites. This study systematically evaluates the mechanical behavior, manufacturing defects, and radiation damage response of near-stoichiometric and Si-enriched fibers produced by R-LCVD. These fibers were further irradiated with both Si3+ ions and at the MIT reactor, followed by extensive microstructural analysis using Transmission Electron Microscopy (TEM) at INL. The results reveal a radial crystallization gradient, with nano-grains aligning axially in the core and transitioning to an amorphous solid towards the fiber surface. Selected Area Electron Diffraction (SAED) confirms beta-SiC formation, with Si precipitates concentrated in the region between the core and surface. Manufacturing defects identified include thin material bands and nanovoids. Heat treatment at 1500 °C leads to the complete crystallization of the amorphous regions and the normalization of the partially crystallized regions, although some manufacturing defects remain. Preliminary radiation studies indicate potential void swelling and microstructural restructuring, warranting further investigation. This work represents the most comprehensive study on R-LCVD SiC fibers and provides critical data for developing theoretical models for additively manufactured SiC.

#### \* Denotes Presenter

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