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2025 Conference on Electronic Materials and Applications (EMA 2025)

ABSTRACT BOOK

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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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Wednesday, February 26, 2025

Plenary Speaker- Jian Luo

Room: Colorado E
Session Chairs: Fei Peng, Clemson University; Bai Cui, University of Nebraska-Lincoln

8:30 AM

(EMA-PLEN 01-001-2025) Computing Grain Boundary Phase (Complexion) Diagrams and Controlling Microstructures with Electric Fields

J. Luo*[1]

1. University of California, San Diego, USA

The materials science community has long recognized that grain boundaries (GBs) can be treated as two-dimensional (2D) interfacial phases, which were also named as "complexions" to differentiate them from bulk phases. Such 2D interfacial phases can process distinct interfacial structures that are neither observed nor stable as bulk phases [see, e.g., a recent perspective article: Science 368, 381 (2024)]. As bulk phase diagrams are arguably the most useful materials science tool, this presentation will first review a series of our studies to compute the GB phase (complexion) diagrams via thermodynamic models, atomistic simulations, and machine learning. In addition to temperature and chemical potentials, an applied electric field can induce a GB transition electrochemically. Recent studies further utilized electrochemically induced GB transitions to tailor micro-structural evolution and create graded microstructures.

S4 Oxide Quantum Materials: Synthesis, Properties and Application

S4- Materials synthesis

Room: Colorado B
Session Chairs: Seung Sae Hong, University of California, Davis; Jennifer Fowlie, Northwestern University

10:00 AM

(EMA-S4-001-2025) High-Mobility, Deep-Ultraviolet Transparent Conducting SrSnO3 Films with Room-Temperature Mobility Exceeding 140 cm^2/Vs (Invited)

B. Jalan*[1]

1. University of Minnesota, USA

Exploration and advancement in ultra-wide bandgap (UWBG) semiconductors are essential for the development of next-generation high-power electronics and deep-ultraviolet (DUV) optoelectronics. In this study, we implemented a thin heterostructure design to enhance conductivity, leveraging the low electron mass and relatively weak electron-phonon coupling of the materials, while maintaining high transparency through atomically thin films. Using a $SrSnO_3$/La:$SrSnO_3$/$GdScO_3$ (110) heterostructure and electrostatic gating, we successfully separated charge carriers in $SrSnO_3$ from dopants, resulting in phonon-limited transport behavior in strain-stabilized tetragonal $SrSnO_3$. This approach enabled modulation of carrier density from 10^{18} cm^{-3} to 10^{20} cm^{-3}, achieving room-temperature mobilities between 40 and 140 $cm^2V^{-1}s^{-1}$. First-principles calculations of phonon-limited mobility closely aligned with experimental results, suggesting the potential for even higher mobilities with increased electron density. Additionally, the heterostructure exhibited 85% optical transparency at a wavelength of 300 nm. I will discuss potential of heterostructure design in transparent UWBG semiconductor technologies, particularly for DUV applications.

10:30 AM

(EMA-S4-002-2025) Rethinking Epitaxial Strain with Post-Growth Functionalization (Invited)

A. Frano*[1]

1. University of California San Diego, Physics, USA

Epitaxial strain in oxide thin films and heterostructures is traditionally viewed as a static factor, fixed during growth. Once the film is deposited, the strain imposed by the substrate is typically regarded as unchangeable, with limited options for further manipulation. Furthermore, the notion that the film could strain the substrate is often overlooked. In this talk, we revisit this conventional understanding and present two cases where the strain relationship between the film and substrate is either reversed or modified post-growth. First, we demonstrate how a voltage-induced phase transition in a thin film neuromorphic device results in a lattice response in the substrate. Second, we explore how uniaxial tensile strain exerted post-growth can drive a correlated oxide from a localized to an itinerant ground state. These examples illustrate how strain can be functionalized post-growth to unlock new material properties and behaviors that are inaccessible when relying solely on the epitaxial strain imposed during growth. By revisiting the substrate-film strain relationship, we reveal new pathways for tuning the physical properties of thin films, broadening the toolkit for material design in advanced applications.

11:00 AM

(EMA-S4-003-2025) Enhancing energy storage performance via microstructure and defect design in $BaTiO_3$ related thin films (Invited)

A. Chen*[1]

1. Los Alamos National Lab, USA

In this talk, I will discuss the strategies of designing interface and domain structure in doped $BaTiO_3$ to achieve enhanced relaxor ferroelectric behavior for energy storage applications. In the first part, I will discuss the design of $(Ba_{0.7}Ca_{0.3})TiO_3$ (BCT) and $Ba(Ti_{0.8}Zr_{0.2})O_3$ (BZT) superlattices via a high-throughput combinatorial approach. In the second part of the talk, I will discuss strategies to further optimize domain structures and suppress the leakage current in BZT-BCT films via a machine learning approach. The large polarization and the delayed polarization saturation lead to greatly enhanced energy density of 80 J/cm^3 and transfer efficiency of 85% over a wide temperature range. Such a data-driven design recipe for a slush-like polar state is generally applicable to quickly optimize functionalities of ferroelectric materials.

11:30 AM

(EMA-S4-004-2025) Fractional Double Perovskites (Invited)

K. Ahadi*[1]

1. The Ohio State University, USA

Small lattice distortions could strongly modify the electronic structure. This talk will focus on a new class of complex oxides where the engineered sub-angstrom lattice distortions due to ordering of empty sites could create a highly tunable electronic structure. We will talk about the ordering of europium and empty A-sites in $Eu_{0.5}TaO_3$ ($EuTa_2O_6$). Fractional occupancy of the A-site is enforced by charge neutrality. The ordering of europium and empty A-sites, as opposed to random occupancy, could double the unit cell which is reflected in our diffraction results. The ordering is controlled by the epitaxial strain (i.e., choice of substrate) and molecular beam epitacy growth parameters. We will exhibit precise characterization of the lattice distortions, including synchrotron diffraction and advanced transmission electron microscopy results to analyze the ordering and demonstrate engineered lattice and electronic structures.

12:00 PM

(EMA-S4-005-2025) Metastable Fractional Double Perovskites Synthesis by Molecular-Beam Epitaxy

T. Schwaigert*[4]; A. Tenneti[4]; S. Hasko[5]; B. Gregory[2]; P. Malinowski[2]; B. Faith[2]; P. Woodward[1]; A. Singer[4]; K. M. Shen[2]; S. Salmani-Rezaie[3]; D. Schlom[4]; K. Ahadi[3]

1. Ohio State University, Chemistry and Biochemistry, USA
2. Cornell University, Physics, USA
3. The Ohio State University, USA
4. Cornell University, Department of Materials Science and Engineering, USA
5. Princeton University, Department of Chemical and Biological Engineering, USA

Two-dimensional states have revolutionized condensed matter physics by introducing new quantum phenomena with demonstrated device potential[1–4]. Distortions from the perovskite arisotype structure can significantly impact the physical properties[5,6]. The ability to create and control these phases is crucial yet achieving them often demands precise structural alterations at the atomic level. Prediction of quasi-2D electron systems within the 3D bulk system of the “fractional” perovskite $EuTa_2O_6$ highlights the transformative impact of such structural modifications[7]. The intrinsic crystal anisotropy of $EuTa_2O_6$ plays a pivotal role, demonstrating how targeted structural changes can enable the formation of novel quantum states. Through the single crystal synthesis of this unique perovskite derivative via molecular-beam epitaxy, we explore its crystal and electronic properties. X-ray diffraction and electron microscopy reveal the critical A-site ordering of europium atoms and the presence of vacancy planes, which are instrumental in shaping these 2D-like states. Furthermore, angle-resolved photoemission spectroscopy, combined with density functional theory calculations, provides direct insight into the electronic structure, connecting the structural distortions with electronic structure and emergence of 2D states.

12:15 PM

(EMA-S4-006-2025) Observation of Charge Transfer Phenomena in (SrCoO3)n/(SrIrO3)n Superlattices and Sr_2CoIrO_6 Double Perovskites Grown By Molecular Beam Epitaxy (MBE)

J. Ahammad*[1]; G. Rimal[2]; G. Sterbinsky[3]; G. Ortiz[4]; J. Hwang[4]; L. Lapinski[5]; U. Jayathilake[5]; A. Gray[5]; R. Comes[6]

1. Auburn University, Physics, USA
2. Western Michigan University, Physics, USA
3. Argonne National Laboratory, Advanced Photon Source, USA
4. The Ohio State University, Materials Science and Engineering, USA
5. Temple University, Physics, USA
6. University of Delaware, Materials Science and Engineering, USA

Interfacial charge transfer in superlattices consisting of perovskite metal oxides leads to emergent electronic and magnetic phenomena. Motivated by the prediction of interfacial charge transfer in 3d-5d oxide heterostructures, we grew a set of $(SrCoO_3)_n/SrIrO_3)_n$ (n= 2-5) superlattices using plasma-assisted Molecular Beam Epitaxy (MBE). In-vacuo X-ray photoelectron spectroscopy (XPS) of Co 2p in the superlattices with respect to $SrCoO_3$ (Co^{4+}) films indicated interfacial charge transfer which was further supported by ex-situ Hard X-ray Photoelectron Spectroscopy (HAXPES). We confirmed charge transfer phenomena via synchrotron-based polarization dependent hard X-ray absorption spectroscopy on Co K and Ir L edges. An anisotropy between in-plane and out-of-plane charge transfers was observed and we found a mixture of Co^{3+}/Co^{2+} in the superlattices. Scanning transmission electron microscopy confirmed the quality of the superlattices and pending EELS analysis of the Co L edge will further examine changes to the Co valence. We also grew Sr_2CoIrO_6 double perovskite films using MBE and confirmed charge transfer phenomena using XAS, with a higher ratio of Co^{2+} than the superlattices. Our findings can help explore new physics in the interface and lead to the design of novel electronic and magnetic systems with strong spin-orbit coupling.

S5 In-Situ/Operando Characterization of Nanomaterials

S5- In situ/Operando Study of Quantum and Topological Materials

Room: Colorado E
Session Chairs: Di Zhang, Los Alamos National Lab; Hao Zheng, Argonne National Lab

10:00 AM

(EMA-S5-001-2025) Operando Visualization of Ultrafast Structural Dynamics in Electronic Devices (Invited)

A. Sood*[1]

1. Princeton University, USA

The operation of many microelectronic devices is driven by ultrafast structural dynamics that occur on picometer length & nanosecond time scales. These dynamics are triggered by fast voltage or current pulses, and include a range of processes such as field-induced structural transitions, ionic diffusion, and phase change. To understand how these devices function and identify the fundamental limits of operation, it is crucial to visualize nanosecond-timescale atomic trajectories induced by electrical stimulation. In this talk, I will describe our efforts to develop operando techniques that integrate ultrafast pulsed probes with electronic devices -- in other words, electrical-pump, X-probe methods (where X = light, electrons, X-rays, etc). As one example, I will discuss our studies of the electrically-triggered insulator-metal transition in vanadium dioxide (VO2), a Mott insulator. Our ability to simultaneously measure structure and transport, as well as compare responses under electrical and optical excitation, enables us to map out the pathway underlying the transformation. These experiments point towards the existence of a voltage-induced metastable state, which could have important implications for energy-efficient switching. Looking ahead, the device-centric ultrafast operando methods we are developing can yield transformative insights into the atomic-scale changes underpinning device operation.

10:30 AM

(EMA-S5-002-2025) Ultrafast THz dynamics of novel topological polar structures (Invited)

Q. Li*[1]

1. Tsinghua University, School of Materials Science and Engineering, China

The recent discoveries of polar vortex, skyrmion, meron and other topological polar structures in $PbTiO_3/SrTiO_3$ (PTO/STO) superlattices open up exciting opportunities to explore the structure and dynamics of complex topological phases of ferroelectric dipoles and potentially leads to novel electronic functionalities. Ultrafast electric field in the form of THz laser pulses can couple with these topological phases via coherent dipole interaction, providing a well-defined, easy-to-model external control knob for probing their ultrafast structural dynamics. We studied the structural dynamics of $PbTiO_3/SrTiO_3$ superlattices hosting different types of topological polar structures using THz pump, X-ray probe and second harmonic generation probe spectroscopies. We observed subterahertz collective excitation modes of the topological polar structures stemming from the lattice dipoles, and further demonstrated their electric-field tunabilities and temperature evolutions. These observations were jointly corroborated by the dynamical phase-field models and atomistic calculations. Altogether, topological polar structures could be potentially ultilized in terahertz optoelectronics that will enable next-generation wireless communication technologies.

11:00 AM

(EMA-S5-003-2025) Atomic Visualization of Polar Order across Temperatures in Ferroelectric Oxides (Invited)

Y. Zhang*[1]; I. El Baggari[1]

1. Harvard University, Rowland institute, USA

In condensed matter systems, the disorder generally gives way to order when temperature is reduced as thermal fluctuations subside. In a rare phenomenon known as "inverse melting", however, more disordered configurations appear at lower temperatures. To date, inverse melting has not been observed nor visualized in atomic- and nanoscale fluctuations of order parameters. In this work, we discovered an inverse melting of the polar order in a ferroelectric oxide with quenched chemical disorder ($BaTi_{1-x}Zr_xO_3$) through direct atomic-scale visualization using in situ scanning transmission electron microscopy (including heating and cryogenic). In contrast to the clean $BaTiO_3$ parent system in which long range order tracks lower temperatures, we observe in the doped system that thermally driven fluctuations at high temperature give way to a more ordered state and then, surprisingly, to a re-entrant disordered configuration at even lower temperature. Additionally, we visualized the origin of polar order in a polar metal (NaV_6O_{11}) with cryogenic microscopy, which is contributed by the subtle atomic shift of Na below room temperature. These visualizations highlight a rich landscape of polar order in ferroelectric oxide, and maybe key to understanding the colossal and unusual responses of materials with quenched disorder.

11:30 AM

(EMA-S5-004-2025) Polarization Switching and Domain Propagation in Novel Ferroelectrics via Electron Microscopy (Invited)

S. Calderon*[1]; E. C. Dickey[1]

1. Carnegie Mellon University, Materials Science and Engineering, USA

The discovery of ferroelectricity in hafnium oxide and wurtzite-based materials like AlScN and AlBN has drawn great attention due to their compatibility with CMOS processes and potential use in non-volatile memory devices. Unlike traditional ferroelectrics, these materials retain strong ferroelectric properties even at thicknesses below 20 nm, opening new doors for integrating ferroelectrics into modern microelectronics, including low-power and in-memory computing. We use scanning transmission electron microscopy (STEM) to examine the polarization inversion, and ferroelectric domain behavior in fluorite and wurtzite ferroelectrics. Using differential phase contrast, we observe light and heavy atomic columns, allowing for precise determination of the local structure. We also use pair correlation functions to map local phase distributions and quantify disorder and polarization at the nanoscale. Lastly, our in-situ experiments offer insights into polarization inversion, domain nucleation, and propagation, shedding light on the ferroelectric switching mechanisms in these novel materials. This material is based upon work supported by the center for 3D Ferroelectric Microelectronics (3DFeM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE-SC0021118.

12:00 PM

(EMA-S5-005-2025) Unveiling Behavior of Nanoscale Spin Textures in van der Waals Ferromagnets Using Cryo Lorentz Electron Microscopy (Invited)

Y. Li*[1]

1. Argonne National Laboratory, Materials Science Division, USA

Magnetic van der Waals (vdW) materials have unique crystal structures, which consist of layered atoms separated by vdW gaps, leading to strong intra-plane interaction and weak inter-plane vdW interaction. This unique structure gives rise to exotic physical phenomena, such as rich magnetic spin textures, including maze domains, skyrmion and merons etc. Thus, it is essential to understand the behavior of spin textures in the vdW materials in response to external stimuli, such as magnetic field, temperature and strain, in order to control them. Lorentz transmission electron microscopy (LTEM) allows for imaging the local spin textures and microstructure at high resolution in such materials. We will explore the creation and the control of Néel magnetic spin textures in the metallic vdW Fe3GeTe2 (FGT) by temperature and magnetic field using the cryo LTEM. We also gain insight into the order and interaction in the collective skyrmion lattice by the combination of machine learning approach. $Cr_2Ge_2Te_6$ (CGT) is a semiconducting vdW ferromagnet with the Curie temperature of 65 K, which however has weaker uniaxial anisotropy compared to FGT. The Bloch-type stripes and bubble domain are formed in CGT. We will demonstrate the effect of local strain on stripe and bubble domains, which provides another degree of freedom to controlling the order of spin texture in such materials.

S8 New Frontiers and Science in Additive Manufacturing of Ceramic Materials

S8 -Additive Manufacturing of Ceramics

Room: Matchless

Session Chairs: Joe Cesarano, Robocasting Enterprises LLC; Russell Maier, National Institute of Standards and Technology

10:00 AM

(EMA-S8-001-2025) The State of Robocasting: Extrusion-Based AM Technology (Invited)

J. Cesarano*[1]

1. Robocasting Enterprises LLC, USA

Robocasting is a specific subset of extrusion-based additive manufacturing (AM) techniques utilizing concentrated fine-particulate pastes carried in a volatile solvent medium. The technology is amenable to printing multiple materials and is scalable. Robocasting has been used to produce millions of parts. A review of robocasting technology and its utility for AM of dense and porous ceramics and multi-material components will be presented. In particular, results for functionally graded materials, pressureless sintered SiC, and components with utility in extreme applications will be presented. Finally, it is important to elucidate the advantages, disadvantages, and limitations of the current state of the technology.

10:30 AM

(EMA-S8-002-2025) An Additive Manufacturing Approach to Produce Silicon Nitride (Si3N4) Fibers via Laser Chemical Vapor Deposition (LCVD) (Invited)

J. Vervlied*[1]; S. Harrison[1]; J. Pegna[1]; S. Shuster[1]

1. Free Form Fibers, US, USA

Microstructure, morphology, and processing of Silicon Nitride (Si3N4) fibers, produced via a disruptive additive manufacturing technology called Laser Chemical Vapor Deposition (LCVD), will be reviewed. Early developments in creating composites and joining of ceramic matrix composites (CMC's) based upon Si3N4 fibers, will be discussed.

11:00 AM

(EMA-S8-003-2025) Development of contact dispense reactive ink printing of SiO_x film for replacement of ARC deposition in III-V solar cell fabrication

M. P. Nicodemus*[1]; J. Selvidge[2]; M. Steiner[2]; O. Hildreth[3]

1. Colorado School of Mines, Chemical Engineering, USA
2. National Renewable Energy Laboratory, USA
3. Colorado School of Mines, Mechanical Engineering, USA

High-efficiency III-V space solar cells rely on thin film oxide anti-reflective coatings to improve light coupling from the environment into the active portions of the cell. These coatings are manufactured using expensive thermal or electron-beam evaporation processes that create high amounts of wasted material and take significant time. To reduce costs, we have developed an ambient pressure-compatible contact dispense printing ink that reacts on printing to form a continuous, patternable silicon oxide film. Using sol-gel chemistry as a basis, we explore changes to composition and processing conditions to create thin films. We can control the printed liquid's reaction rate by utilizing an acidic catalyst mixture, minimizing the solution mixing time, and printing onto a 90°C heated substrate. Optimal conditions appear to suppress nanoparticle formation and drive a directional solidification reaction, reducing crack formation in the film, and enabling low-temperature processing compatible with III-V solar cells. Switching to an organic/inorganic acid mixture, we demonstrate continuous printed films with uniform thickness, low roughness, and limited edge effects. This work demonstrates the promise of silicon oxide printing for additive manufacturing of thin film ceramic optical coatings, including an anti-reflective coating for III-V solar cells.

11:15 AM

(EMA-S8-004-2025) Reactive selective laser sintering of compositionally complex carbide ceramics

B. Cui*[1]; L. Trinh[1]; Z. Hua[2]; K. Bawane[2]; L. He[3]; L. Malakkal[2]; X. Chen[1]; L. Wadle[1]; Y. Lu[1]

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

Reactive selective laser sintering (SLS) process has been successfully developed towards additive manufacturing of compositionally complex ceramic (CCC) from a powder mixture of constitute mono-carbides. A continuous-wave Yb fiber laser source was employed for SLS, resulting in a single-phase non-equiatomic CCC phase. While (Zr,Nb,Hf,Ta)C has a uniform distribution of four metal elements, (Zr,Nb,Hf,Ta,Ti)C and (Zr,Nb,Ta,Ti,W)C exhibit three-layer microstructures with different metal element distributions. Cellular structures with W, Zr, and Ti element segregation and dislocations on cell boundaries were observed in the SLSed (Zr,Nb,Ta,Ti,W) C sample, indicating the effect of non-equilibrium conditions on microstructure formation during laser melting followed by rapid cooling and solidification process. Compared to the CCC sample prepared by spark plasma sintering, the SLSed CCC samples showed enhanced hardness and reduced thermal conductivity, which may be related to unique cellular structures.

11:40 AM

(EMA-S8-005-2025) Metrology and Standards Development of Ceramic Additive Manufacturing (Invited)

R. Maier*[1]; A. J. Allen[1]; I. Levin[1]

1. NIST, Materials Measurement Science Division, USA

The development of new and improved testing standards and research grade test materials for ceramic additive manufacturing (AM), as cited by industrial stakeholders, would help to open critical bottlenecks in commercialization of the technology. To aid in efforts to improve reliable testing of ceramic AM parts and feedstocks, we are currently making progress in improving metrology and developing feedstock standards for ceramic direct-ink writing (DIW) and digital light processing (DLP) techniques. Advances in commercial DLP techniques to print high resolution ceramic parts has led to questions regarding the applicability of conventional test standards and procedures used on AM parts. Defects control the strength of ceramic materials, and pores, voids, agglomerates, etc., introduced to the material through the printing process act as critical stress concentrators leading to failure. Results will be presented from a recently completed interlaboratory study (ILS) of Al_2O_3 printed using a vat photopolymerization process. Six participating labs printed specimens that were tested at NIST using four-point bend fracture followed by extensive fractography analysis. The results of this ILS reveal characteristic types of defects that can be separated into categories based on process vs. user-controlled sources. Lessons learned from this study and follow-up metrology research underway at NIST will be presented.

12:10 PM

(EMA-S8-006-2025) Localized domain switching and tunable functional properties in 3D printed architected ferroelectric ceramics

A. Pramanick*[1]; C. Baboori[1]; F. Albertini[2]; F. Gjørup[4]; A. Kumar[3]; M. Jorgensen[4]; L. Daniel[1]

1. Universite Paris-Saclay, CentraleSuepelec, France
2. Université Paris-Saclay, Université de Versailles Saint-Quentin-en-Yvelines, France
3. Indian Institute of Technology, Bhilai, India
4. Aarhus Universitet, Denmark

Advances in 3-D printing have enabled fabricating architected ceramics with tunable properties at reduced weight and cost. An essential cornerstone of materials design is to determine structure-property relations. For ferroelectrics, such relationships can be complex due to several microscopic mechanisms, such as lattice strains and/or domain-switching. For architected ceramics, these mechanisms can also be orientation-dependent and also spatially non-uniform. This entails development of appropriate methodology to correlate functional properties of architected ferroelectrics with spatial- and orientation-resolved structural mechanisms. Here, using in situ X-ray micro-diffraction, we show that sharp geometric features causes highly inhomogeneous distribution of microscopic structural changes in architected ferroelectrics under applied electric fields. Based on a comparative study of $BaTiO_3$ ceramics with two different geometric forms, we demonstrate that the macroscopic dielectric and electromechanical response can be enhanced by at least a factor of two through a change in material architecture, which is primarily dependent on spatially localized progression of non-180 domain switching in the two different ceramics. The current study paves a new way to engineer modified dielectric and electromechanical properties in ferroelectric ceramics using 3-D printed architecture.

12:25 PM

(EMA-S8-007-2025) Digital Light Processing of Yttria Stabilized Zirconia Scaffolds

B. Cui*[1]; L. Wadle[1]; M. Krishnan[2]; R. Wall[1]; L. Trinh[1]; B. Duan[2]

1. University of Nebraska-Lincoln, USA
2. University of Nebraska Medical Center, USA

3 mol.% yttrium-stabilized tetragonal zirconia polycrystal (3Y-TZP) is a promising biocompatible ceramic for craniofacial bone reconstruction and regeneration applications. A digital light processing (DLP) based process has been developed for 3D printing of 3Y-TZP scaffolds for cellular growth, which aims to utilize commercially available 3Y-TZP slurry (Zircolite) and optimize the DLP parameters using a binary optimization approach. This research lays the groundwork for rapid and repeat fabrication of scaffolds with sub-millimeter pores. The as-sintered samples feature a high purity, density, and hardness. Cellular proliferation tests have verified the viability as scaffolds and shown promising results of adipose derived mesenchymal stem cell culture.

S10 Structure, dynamics and functionalities in high-entropy and compositionality complex oxides

S10- Structure, dynamics, and functionalities in high-entropy and compositionally complex oxides I

Room: Colorado D
Session Chair: Raphael Hermann, Oak Ridge National Laboratory

10:00 AM

(EMA-S10-001-2025) Exploring Disorder-Driven Phenomena in High-Entropy Oxides (Invited)

C. M. Rost*[1]; G. R. Bejger[1]; J. Barber[1]; G. Niculescu[2]; S. Ayyagari[3]; M. Webb[4]; L. Min[3]; S. S. Almishal[3]; M. Caucci[3]; Y. Son[3]; J. Sivak[3]; B. Yang[3]; N. Alem[3]; J. Heron[4]; Z. Mao[3]; J. Maria[3]; S. Sinnott[3]; S. Trolier-McKinstry[3]

1. Virginia Polytechnic Institute and State University, Materials Science & Engineering, USA
2. James Madison University, Physics and Astronomy, USA
3. The Pennsylvania State University, USA
4. University of Michigan, USA

Disorder plays a key role in shaping the properties of materials, particularly in high-entropy oxides (HEOs), where a high level of disorder presents a wealth of opportunities for investigation. Here, we focus on the synthesis and characterization of novel HEOs in powder, thin film, and single crystal forms to explore how compositional disorder influences structural evolution and functional properties. We examine the structural evolution of thin-film HEOs under varying oxygen partial pressures, identifying a transition from rock salt to spinel structures. Through high-temperature magnetization, combined with neutron and synchrotron-based measurements, we observe distinct ferrimagnetic transitions at elevated temperatures for different compositions in single crystal HEO spinels. In high-entropy perovskite oxide (HEPO) films, we show that B-site disorder can be used to tune the time stability of remanent polarization. Transmission electron microscopy (TEM), X-ray absorption fine structure (XAFS), and machine learning techniques are employed to probe nanoscale structural variations. This talk highlights how lattice distortions in the high-entropy phase lead to significant changes in material behavior, deepening our understanding of the relationship between disorder and material properties. These insights advance the field of HEOs and open pathways to future applications in functional materials.

10:30 AM

(EMA-S10-002-2025) Disorder by design in strongly correlated materials (Invited)

A. Mazza*[1]

1. Los Alamos National Laboratory, USA

Generally, uniformity in materials is seen as critical to phase order, with disorder and defects being thought to result in lower ordering temperatures and the prevention of long-range percolation. However, disorder is an important aspect of many materials systems – from alloys to dilute magnetic semiconductors. It can be used to manipulate superconductivity, magnetic ordering, and design degeneracies. High entropy materials are an evolution of this understanding and work in this field has begun to demonstrate that disorder is a parameter which can drive local microstates into globally ordered behaviors. In this talk, theoretical and experimental results exploring the role of disorder in manipulating spin, charge, lattice and electronic order parameters in single crystal high entropy oxide epitaxial films are discussed. The results discussed suggest cation size, spin, and charge variance, such as that accessible only in high entropy oxides, can be critical in the design of next generation electronic, structural, and magnetic materials.

11:00 AM

(EMA-S10-003-2025) Impact of synthesis method on the structure and function of high entropy oxides (Invited)

M. Gonzalez Rivas*[1]; S. S. Aamlid[2]; M. Rutherford[1]; J. Freese[4]; E. Villalobos Portillo[5]; H. Castillo Michel[5]; M. Kim[3]; N. Chen[6]; R. Sutarto[6]; H. Takagi[3]; R. Green[4]; A. Hallas[1]

1. The University of British Columbia, Blusson Quantum Matter Institute/Physics and Astronomy, Canada
2. University of British Columbia, Stewart Blusson Quantum Matter Institute, Canada
3. Max Planck Institute for Solid State Research, Germany
4. University of Saskatchewan, Physics and Engineering Physics, Canada
5. ESRF, France
6. Canadian Light Source Inc, Canada

The term sample dependence describes the troublesome tendency of nominally equivalent samples to exhibit different physical properties. High entropy oxides (HEOs) are a class of materials where sample dependence has the potential to be particularly profound due to their inherent chemical complexity. In this work, we prepare a spinel HEO of identical nominal composition by five distinct methods, spanning a range of thermodynamic and kinetic conditions. By structurally characterizing these five samples across all length scales with a variety of x-ray methods, we find that while the average structure is unaltered, the samples vary significantly in their local structures and their microstructures. The most profound differences are observed at intermediate length scales, both in terms of crystallite morphology and cation homogeneity. These structural differences in turn significantly alter the observed functional properties, which we demonstrate via characterization of their magnetic response. While ferrimagnetic order is retained across all five samples, the sharpness of the transition, the magnitude of the saturated moment, and magnetic hardness all show marked variations with synthesis method. We conclude that the chemical flexibility inherent to HEOs is complemented by strong synthesis method dependence, providing another axis along which to optimize these materials for a wide range of applications.

11:30 AM

(EMA-S10-004-2025) Investigating Size Effects on the Phase Stability of High Entropy Oxide

W. J. Deary*[1]; J. Barber[1]; G. R. Bejger[1]; S. Muhlenberg[1]; C. M. Rost[1]

1. Virginia Polytechnic Institute and State University, Materials Science and Engineering, USA

The effect of particle size on oxide phases is an important consideration in materials processing, where the surface energy and other size effects can significantly influence thermodynamic stability. In this work, we explore the phase stability in the $(MgCoNiCuZn)_{0.2}O$ high entropy oxide system as a function of average particle size using a top-down approach. From as-reacted single-phase powders, we use conventional powder milling methods to systematically reduce particle size. Samples are characterized using several techniques including X-ray diffraction for phase analysis (XRD), laser diffraction for particle size analysis (PSA), and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDS) for microstructure and compositional mapping. Phase stability in the context of particle size variation as well as milling energetics are considered and discussed.

11:45 AM

(EMA-S10-005-2025) 2D High Entropy Perovskites for Electrocatalysis

S. N. Gonzalez*[1]

1. Colorado School of Mines, Chemistry, USA

A challenge for the next generation of field dispatchable power sources is transitioning the electrocatalyst from platinum group metals to earth abundant materials while improving catalytic efficiency and durability. The community has demonstrated that nanostructuring specially-selected compositions while controlling the morphology of the final products is useful. High Entropy Oxides (HEOs) are a class of materials that can accommodate catalytically active earth-abundant elements while also offering the ability to tailor both composition and morphology. Such attributes make them an excellent candidate for electrocatalysis. This "high entropy" designation can be extended to the perovskite structure as High Entropy Perovskites (HEPs) are characterized by the presence of five or more cations on the A or B site in equimolar concentrations. The resulting increase in the configurational entropy allows the entropic term to dominate the free energy, thus stabilizing the structure. Through solution-based methods, HEPs can be synthesized in 2D nanostructured sheets, improving the surface-to-volume ratio and catalytic activity. This work presents the aerogel synthesis of Ba, Sr, Ca, Co, and Fe-containing HEPs to promote nanomaterial production. Pseudo-supercritical drying allows for solvent removal while circumventing the kinetics of aggregation. A powder product results, ready for validation using symmetric electrochemical cells.

12:00 PM

(EMA-S10-006-2025) Rock Salt High-Entropy Oxide Heterostructures: Structural and Magnetic Properties

S. S. Almishal*[3]; P. Kezer[6]; S. Ayyagari[5]; T. Charlton[2]; N. Alem[3]; C. M. Rost[4]; J. Heron[6]; J. Maria[1]

1. Penn State, Materials Science and Engineering, USA
2. Oak Ridge National Lab, USA
3. Pennsylvania State University, Department of Materials Science and Engineering, USA
4. Virginia Polytechnic Institute and State University, Materials Science and Engineering, USA
5. The Pennsylvania State University, USA
6. University of Michigan, Materials Science and Engineering, USA

High entropy oxides (HEOs) are inherently metastable, with properties that are highly sensitive to their thermal history and formation kinetics. In this study, we investigate epitaxial thin films of $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ derivatives grown via pulsed laser deposition. We systematically explore how variations in substrate temperature, oxygen partial pressure, and growth rate influence their out-of-plane lattice parameters and physical properties. By incorporating a sixth cation, such as Sc or Cr, into $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$, we achieve fine control over the out-of-plane lattice parameter, with up to a 6% change across a 200°C temperature range. We use this lattice parameter tunability to engineer vertically stacked pseudomorphic heterostructures. These HEOs heterostructures present an intriguing system for studying how variations in cation chemical environments within a disordered medium influence the overall magnetic properties.

12:15 PM

(EMA-S10-007-2025) Structural Complexity and Properties of Entropy Enhanced Yttrium Iron Garnets

R. Tanveer*[1]; C. Overstreet[2]; T. Kanyowa[1]; B. Hu[1]; M. Lang[2]; V. Keppens[1]; W. J. Weber[3]

1. The University of Tennessee Knoxville, Materials Science and Engineering, USA
2. The University of Tennessee Knoxville Tickle College of Engineering, Nuclear Engineering, USA
3. University of Tennessee, Materials Science & Engineering, USA

Yttrium Iron Garnets (YIG) are interesting due to their high magnetic moment, low magnetic damping, large frequency dependence, and enhanced magneto-optic properties with diverse existing and potential applications. The incorporation of compositional diversity, or "enhanced configurational entropy," in these oxides at specific lattice sites can enhance the tunability of their magnetic and optical properties, facilitate the introduction of new cation species for additional functionalities, and induce structural disorder that may lead to yet unexplored characteristics. Designing such compositionally complex multifunctional oxides, however, presents significant challenges due to various limiting factors, including structure-to-cation compatibility, the compositional restrictions of specific lattice sites, high-mixing enthalpy, and variable oxidation states. This study aims to dilute the Fe sites of YIG with five distinct transition metals to modify its magnetic and optical properties, as well as to develop a spin glass characterized by magnetic ion disorder. X-ray diffraction (XRD) and synchrotron-derived Pair Distribution Function (PDF) analyses were employed to examine the global and local structural ordering, in conjunction with room temperature Raman spectroscopy. The magnetic, optical, and elastic properties will be illustrated based on various cation species for multifunctionality assessment.

S12 Advanced semiconductors and microelectronics

S12- Semiconducting thin films I

Room: Colorado G

Session Chairs: Aiping Chen, Los Alamos National Lab; Ludi Miao, New Mexico State University; Chonglin Chen, University of Texas San Antonio

10:00 AM

(EMA-S12-001-2025) Emergent magnetism and superconductivity through tailored strain and charge gradients at epitaxial interfaces (Invited)

M. Brahlek*[1]

1. Oak Ridge National Lab, materials science, USA

Understanding and designing functional phenomena is challenging due to the complexity involved in integrating structurally dissimilar materials and controlling factors like valence, spin, orbital, and structural degrees of freedom. In this talk, I will showcase recent findings that reveal how new phenomena emerge when interfacing materials as high-quality thin films using molecular beam epitaxy. These findings include emergent and controllable ferromagnetism, interfacially enhanced superconductivity, and proposed altermagnetism. The key takeaway is that achieving these successes requires a strong integration of synthesis and various characterization steps to understand the origins of functional quantum phenomena and how these phases can be manipulated, potentially paving the way for future microelectronic devices.

10:30 AM

(EMA-S12-002-2025) A New Rhombohedral R3 Phase in Mn-doped Hf0.5Zr0.5O2 Epitaxial Films with Robust Ferroelectricity (Invited)

J. Guo[3]; X. Xu[1]; L. Tao[2]; S. Du[2]; J. Ma[4]; C. Chen*[1]

1. University of Texas San Antonio, Physics, USA
2. Chinese Academy of Sciences Institute of Physics, China
3. Tsinghua University, China
4. Tsinghua University, School of Materials Science, China

HfO_2-based ferroelectric materials are emerging as key components for next-generation nanoscale devices, owing to their exceptional nanoscale properties and compatibility with established silicon-based electronics infrastructure. Despite the considerable attention garnered by the ferroelectric orthorhombic phase, the polar rhombohedral phase has remained relatively unexplored due to the inherent challenges in its stabilization. In this study, we report the successful synthesis of a distinct ferroelectric rhombohedral phase, i.e., the R3 phase, in Mn-doped $Hf_{0.5}Zr_{0.5}O_2$ (HZM) epitaxial thin films, which stands different from the conventional $Pca2_1$ and R3m polar phases. Our findings reveal that this R3 phase HZM film exhibits a remnant polarization of up to 47 μC/cm^2 at room temperature, along with an exceptional retention capability projected to exceed a decade and an endurance surpassing 10^9 cycles. Moreover, we demonstrate that by modulating the concentration of Mn dopant and the film's thickness, it is possible to selectively control the phase transition between the R3, R3m, and $Pca2_1$ polar phases. Our research not only sheds new light on the ferroelectricity of the HfO_2 system but also paves the way for innovative strategies to manipulate ferroelectric properties for enhanced device performance.

11:00 AM

(EMA-S12-003-2025) Capacitive Energy-density and Colossal Electrocaloric and Pyroelectric Effects of Sm-doped PMN-PT Thin Films (Invited)

M. Spreitzer*[1]; Z. Hanani[1]; J. Belhadi[2]; U. Trstenjak[1]; N. A. Shepelin[3]; T. Lippert[3]; A. Razumnaya[4]; I. Lukyanchuk[2]; Z. Kutnjak[1]

1. Jozef Stefan Institute, Slovenia
2. University of Picardie Jules Verne, France
3. Paul Scherrer Institut PSI, Switzerland
4. Southern Federal University, Faculty of Physics, Russian Federation

Sm-doped $Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ (Sm-PMN–PT) bulk materials have revealed outstanding ferroelectric and piezoelectric properties due to enhanced local structural heterogeneity. In this study, we further explore the potential of Sm-PMN–PT by fabricating epitaxial thin films, revealing that Sm doping significantly improves the capacitive energy-storage, piezoelectric, electrocaloric, and pyroelectric properties of PMN–PT thin films. These Sm-PMN–PT thin films exhibit fatigue-free performance up to 10^9 charge-discharge cycles and maintain thermal stability across a wide temperature range from −40°C to 200°C. Notably, the films demonstrate a colossal electrocaloric effect with a temperature change of 59.4K, and a remarkable pyroelectric energy density. By using scanning transmission electron microscopy and phase-field modeling, we revealed that these exceptional properties arise from the increased local structural heterogeneity and strong local electric fields along spontaneous polarization directions, which in turn facilitates the nucleation of polymorphic nanodomains characterized by a slush-like polar structure.

11:30 AM

(EMA-S12-004-2025) Germanium based photocathode for green hydrogen production

L. Bučar*[1]; M. Spreitzer[1]

1. Jozef Stefan Institute, Advanced materials department, Slovenia

Controlled integration of oxide materials on semiconductors is an important aspect in semiconductor devices and with the ability of semiconductors to convert solar energy into chemical energy, such devices can be used for green hydrogen production via photoelectrochemical water splitting. Due to the difficulty of controlling the interface quality between silicon and other oxides, we instead used germanium as a substrate and deposited strontium titanate (STO) using pulsed laser deposition method (PLD). The crystallinity of the film was determined with x-ray difraction and surface was investigated with atomic force microscope (AFM). To achieve epitaxial growth of STO it was crucial the STO seed layer was deposited on clean Ge at room temperature, followed by annealing so the STO crystallized in (001) orientation. This step provided a stable STO template for further STO deposition. Photoelectrochemical measurements were preformed and onset potential was improved when using sputtered Pt nano-islands on top of the film as a co-catalyst. Cycling of the samples showed poorer stability, which was due to the pinholes in the film observed by AFM. Nevertheless, STO/Ge heterostructures can be a promising candidate for photocathode for green hydrogen production.

11:45 AM

(EMA-S12-005-2025) Expansion of compositional space of Gd^{3+} in wurtzite $Al_{1-x}Gd_xN$ heterostrcutural alloys via reactive HiPIMS technique

B. Paudel*[1]; K. Yazawa[1]; R. Smaha[2]; G. Brennecka[1]

1. Colorado School of Mines, USA
2. National Renewable Energy Laboratory, USA

The substitution of cations in wurtzite AlN (e.g., $Al_{1-x}M_xN$, M=Sc, B) has shown exceptional ferroelectric and electromechanical properties, spurring significant interest in this materials family. Expanding these wurtzite alloys to include rare earth (RE) cations can potentially unlock new ferroelectric materials and enhanced optoelectronic and luminescence properties. An understanding of phase evolution as a function of RE content is desired. Of particular interest is Al1−xGdxN alloy due to the potential magnetic ordering, highest known neutron capture cross-section of ^{157}Gd, and potential for ferroelectricity. Our previous synthesis via radio frequency (RF) sputtering achieved x=0.24 in wurtzite Al1−xGdxN films, lower than the x=0.82 maximum predicted from enthalpy calculations. Here, we expand the Gd content in wurtzite Al1−xGdxN alloys using reactive high-power impulse magnetron sputtering (HiPIMS) to x>0.35, as confirmed by the grazing incidence synchrotron X-ray scattering. Moreover, we have observed that a nitrogen-rich (poor) environment results in higher (lower) maximum achievable Gd concentrations. In-situ optical emission spectroscopy reveals that increasing the nitrogen flow leads to higher Gd ionization in HiPIMS compared to RF sputtering. This work shows higher ionization during HiPIMS can achieve higher cation contents in Al1−xMxN alloy systems.

12:00 PM

(EMA-S12-006-2025) Investigating the Resistive Switching Mechanism of Nitride-based Memristor Devices (Invited)

D. Zhang*[4]; R. Dhall[2]; M. Schneider[1]; C. Song[2]; H. Dou[3]; S. Kunwar[4]; N. Yazzie[4]; J. Ciston[2]; N. Cucciniello[4]; P. Roy[4]; M. T. Pettes[4]; J. Watt[4]; W. Kuo[4]; H. Wang[5]; R. McCabe[1]; A. Chen[4]

1. Los Alamos National Lab, USA
2. E O Lawrence Berkeley National Laboratory, Molecular Foundry, USA
3. Purdue University, Materials Engineering, USA
4. Los Alamos National Lab, Center for Integrated Nanotechnologies, USA
5. Purdue University, School of Materials Engineering, USA

Resistive switching (RS) observed in a variety of transition metal oxides and nitrides is of great research interest since it opens up enormous possibilities in the next-generation integrated electronics such as nonvolatile memory and neuromorphic computing devices etc. A new interface-type RS devices with lower operation current and more reliable switching repeatability exhibits great potential in the applications of ultra-low-energy memory and data storage devices. In this work, we fabricate a Metal/TiO_x/TiN/Si (001) thin film memristor by using a one-step pulsed laser deposition. In situ transmission electron microscopy (TEM) imaging and current-voltage (I-V) characteristic demonstrate that the device is switched between high resistive state (HRS) and low resistive state (LRS) in a bipolar fashion with sweeping the applied positive and negative voltages. In situ scanning transmission electron microscopy (STEM) experiment with electron energy loss spectroscopy (EELS) reveal the charge carriers (such as oxygen vacancies) migration as well as Ti valence states variation inside the device during RS. Without forming an obvious conductive filament, the charge carriers can move through the intrinsic grain boundaries of TiO_x insulating phase under electric field, leading to the modulation of Schottky barriers at the upper and lower metal/semiconductor interfaces.

12:30 PM

(EMA-S12-007-2025) Disentangling electronic and ionic effects of LRS relaxation in valence change memory

J. Hellwig*[1]; C. Funck[1]; D. Spithouris[1]; R. Dittman[1]

1. Forschungszentrum Julich GmbH, Peter Grünberg Institute, Germany

In neuromorphic computing, volatile memory devices based on the valence change mechanism (VCM) are often used to mimic volatile processes in the human brain. These exceed the time constants of conventional CMOS hardware. However, the relaxation processes are poorly understood and may be a combination of electronic and ionic processes. Here we present an evaluation of the VCM-decay process of the low-resistive state (LRS) in terms of its time constants using a crystalline Pt/$SrTiO_3$/Nb:$SrTiO_3$ device as a model system. We show how the electrical transport of these devices and the contributions of ions and electrons during decay can be modelled using the Tsu-Esaki formalism. We identify unique features of the electrons and ions that are visible in the relaxation measurement. We verify these findings with recent transient spectroscopy measurements and show how electronic and ionic processes can be disentangled experimentally. Furthermore, we propose how transient spectroscopy can be used to measure the evolution of defects during memristive switching, as the method gives us a unique spectroscopic insight into the defect distribution, defect type and concentration.

12:45 PM

(EMA-S12-008-2025) Enhancing the surface treatment of Nb-doped $SrTiO_3$ substrates: effects on structural and chemical properties

M. Son*[1]; K. Kang[1]

1. Kyungpook National University, Physics, Republic of Korea

Using $SrTiO_3$ substrates with either TiO_2- or SrO-terminated surfaces is crucial for achieving high-quality epitaxial perovskite oxide thin films. Introducing niobium doping into $SrTiO_3$ imparts new functionalities and alters both its metallic and structural characteristics. This study thoroughly investigates the physical and chemical processes involved in chemical etching and annealing, aiming to obtain an atomically flat, single-terminated surface on (001)-oriented Nb-doped $SrTiO_3$ (Nb:STO) and optimize its performance. Atomic force microscopy (AFM) identified the optimal treatment, consisting of annealing at 950 °C for 6 hours coupled with a 90-second etching process, resulting in a clearly defined step-terrace structure on the substrate. Additionally, angle-resolved X-ray photoelectron spectroscopy (AR-XPS) revealed significant shifts in the dominant chemical species in the near-surface region due to variations in thermal parameters despite maintaining consistent temperature and duration. Reflection high-energy electron diffraction (RHEED) confirmed the creation of a single-terminated surface under these annealing conditions. This study provides important insights into surface treatment techniques for Nb:STO substrates and their effects on the substrates' structural and chemical properties.

S13 Defects and transport in ceramics

S13- Defects and Transport in Ceramics I

Room: Colorado H
Session Chairs: Xin Xu, Arizona State University; Dong Hou, Clemson University

10:00 AM

(EMA-S13-001-2025) Discovery of New Fast Oxygen Conductors with Vacancy and Interstitial Mechanisms (Invited)

D. Morgan*[1]; J. Meng[1]; R. Jacobs[1]; J. Liu[2]; L. Schultz[1]

1. University of Wisconsin-Madison, Materials Science and Engineering, USA
2. NETL, USA

In this talk I describe some of our recent work demonstrating that molecular simulation-based screening can discover new materials with outstanding oxygen kinetics mediated through both vacancy and interstitial mechanisms. I will focus first on using cluster algorithms to find similar materials to known fast oxygen conductors, which led to the identification of the Sillén oxychloride $LaBi_2O_4Cl$ (LBC) as a potentially promising material. We then used ab initio methods to predict that LBC has very intriguing defect behavior, including ready formation of Frenkel pairs of oxygen vacancies and interstitials, ultrafast vacancy diffusion (with vacancy migration barriers ~0.1 eV), and good interstitial transport. I will then discuss recent work on discovering oxygen interstitial diffusers. A review of known materials strongly suggests that electron availability and structural flexibility are requisites for being a good interstitial mediated oxygen conductor. We combined these qualitative requisites with ab initio calculations to discover new families of interstitial conductors. We then studied $La_4Mn_5Si_4O_{22+d}$ in detail and found it to have fast interstitial oxygen conduction and outstanding oxygen surface exchange rates. Together these results help illustrate the capabilities of emerging tools of modern materials discovery and design for developing new ceramics with targeted defect and transport properties.

10:30 AM

(EMA-S13-002-2025) Exploring tranpsort processes in solid oxide electrochemcial cells (Invited)

S. Skinner*[1]

1. Imperial College London, United Kingdom

Advances in the development of solid oxide cell technologies have led to the rapid uptake of both fuel cell and electrolyser devices, with increased focus on extending lifetime. To achieve this it is essential that the critcal processes leading to performance loss in the cells and stacks are fully understood. Loss of electrochemical performance is typified by interfacial reactions between the functional components, and through interaction with atmospheric contaminants.

Degradation mechansims are often apparent only at, or after, the point of failure, with increasing demands now to model lifetime based on correlative studies of physical propoerties. Identifying the inital stages of chemcial and microstructural changes that underpin performance loss requires advanced techniques that enable transport phenomena to be unambiguously measured and linked to performance. This is acheived using a combination of advanced analytical techniques with isotopic labelling to probe both anion and cation mobility in the key functional components of solid oxide cells. Here we will explore ion transport processes in both oxide ion and proton conducting cell technologies using a combination of microscopy and scattering techniques, allowing surface chemistry and grain boundary phenomena to be identified.

11:00 AM

(EMA-S13-003-2025) The effect of controlling the defect chemistry of $Na_{0.5}Bi_{0.5}TiO_3$-based ceramics on its solid solutions

S. Bauer[1]; T. Frömling*[1]

1. Technische Universität Darmstadt, Materials Science, Germany

$Na_{0.5}Bi_{0.5}TiO_3$ (NBT) based ceramics are considered to be excellent lead-free replacements for lead zirconate titanate. However, NBT can actually be modified from highly oxygen-conductive to highly resistive. This shows that the defect chemistry is quite complex. Therefore, a detailed understanding of the defect chemistry of NBT is highly important. This also counts for the solid solutions with $SrTiO_3$ (ST) and $BaTiO_3$ (BT). These are the materials that show merits for ferroelectric applications. However, while BT forms homogeneous solid solutions, materials with ST are prone to develop core-shell structures. Furthermore, NBT-ST exhibits unusually high strain and almost antiferroelectric behavior. In this work, we will illustrate how core-shell structures are generated and controlled in NBT solid solutions and which materials are prone to show these features. This will elucidate the extraordinary opportunities to alter the properties of NBT-based material for multiple applications.

11:15 AM

(EMA-S13-004-2025) Defect chemistry regulated dislocation nucleation in oxides: an electromigration and nanoindentation study

C. K. Okafor*[1]; S. Bruns[2]; A. Sayyadishahraki[4]; K. Durst[2]; T. Frömling[4]; P. Carrez[3]; P. Hirel[3]; X. Fang[1]

1. Karlsruher Institut fur Technologie, Institute of Applied Materials, Germany
2. Technical University Darmstadt, Physical Metallurgy, Germany
3. Universite Lille, Materials and Transformation Unit CNRS, France
4. Technische Universität Darmstadt, Materials Science, Germany

Modern functional oxides are mainly tailored by tuning the defect chemistry, which essentially is the study of point defects and their interaction in the solid state. Recently, dislocations (line defects) offer a new perspective for improved mechanical and functional properties. This raises the question regarding the interaction of dislocations and point defects in functional oxides for performance stability evaluation. Here, we report the impact of defect chemistry change on the mechanical response of single-crystal strontium titanate, a prototype perovskite. Doping and/or electromigration (field-assisted vacancy migration), facilitated the defect chemistry changes which are reflected in the maximum shear stresses for dislocation nucleation (pop-in event) and the nanoindentation creep rate via nanoindentation testing. Molecular dynamic simulation validates the experimental data by showing that oxygen vacancies promote dislocation nucleation. The lattice friction stress, a measure of the resistance for dislocation glide hence its mobility and the plasticity of the materials, is estimated based on the dislocation etch pits. These findings and mechanisms will shed new light on the interaction between dislocations and point defects, and hold the potential to be transferred to other functional oxides that can be tuned by dislocations for functional applications.

11:30 AM

(EMA-S13-005-2025) Fundamental design principles for fast oxygen exchange: the interplay of surface and bulk properties of mixed conducting oxides (Invited)

M. Siebenhofer*[1]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria

The oxygen exchange reaction (OER) at high temperatures is critical for a variety of technologies, such as solid oxide fuel/electrolysis cells (SOFCs/SOECs) or oxygen permeation membranes, so being able to modulate and optimize its kinetics is key for these technologies. Experimentally, strong correlations between fast OER kinetics and high oxygen nonstoichiometry or high oxygen diffusivity have been found. Computationally, Lee et al. have identified the bulk O 2p band center as a powerful descriptor for the OER kinetics. On the other hand, Nicollet et al. have recently shown that the OER kinetics (and the work function) of $Pr_{0.1}Ce_{0.9}O_{2-\delta}$ can be systematically modified over several orders of magnitude depending on the acidity of a binary oxide that is used to infiltrate the surface. Here, we discuss in detail the desired material properties for fast OER kinetics on mixed conducting oxide surfaces at high temperatures, focusing both on bulk and surface. In the process, we want to bridge the gap between experiment and computation by clarifying connections between the electronic structure of a material and relevant properties, such as oxygen nonstoichiometry, adsorption energies and surface acidity. Thus, we aim to lay the groundwork for a comprehensive framework to design material systems with optimal catalytic properties for the high temperature OER.

12:00 PM

(EMA-S13-006-2025) Design Rules for Ionic Conduction in Amorphous Thin-Film Metal Oxides

D. Shin*[1]; A. V. Levlev[2]; Y. Li[1]

1. University of Michigan, Materials Science and Engineering, USA
2. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA

Ion conduction in ceramic materials is vital for the performance and reliability of various functional materials, such as batteries, gate dielectrics, electrochemical transistors, and memristors. In crystalline materials, ion conduction relies on point defects like vacancies and interstitials, making ionic conductivity directly proportional to defect concentration and mobility. However, in amorphous materials, such crystallographic point defects are undefined. Our study measured oxygen tracer diffusion in amorphous hafnium oxide thin films and found that sub-stoichiometric hafnium oxide exhibits diffusivity two orders of magnitude lower than that of stoichiometric hafnium oxide. Furthermore, among stoichiometric amorphous hafnium oxide thin films, higher-density films show lower diffusivity compared to their lower-density counterparts. This indicates that traditional defect chemistry fails to describe diffusion trends in amorphous hafnium oxides. Instead, free volume and film density significantly influence oxygen diffusivity. Further investigation using pair distribution function analysis from electron diffraction supports the finding that denser films have lower free volume, which hinders oxygen diffusion. This study reveals that density and free volume are crucial factors in ionic conduction for amorphous materials, with broad implications for batteries, memristors, and transistors.

12:15 PM

(EMA-S13-007-2025) Defect chemistry - transport - chemical strain coupling of mixed-conducting (Pr,Ce)$O_{2-\delta}$ nanoparticles: role of interfaces

S. Zhang*[1]; Z. Fang[2]; M. Chi[2]; N. H. Perry[1]

1. University of Illinois Urbana-Champaign, Materials Science & Engineering, USA
2. Oak Ridge National Laboratory Center for Nanophase Materials Sciences, USA

Mixed ionic-electronic conductors (MIECs), having the ability to exchange oxygen with the gas phase, serve in many applications, e.g. fuel/electrolysis cells. However, large chemical strains in MIECs, arising from the changes in oxygen stoichiometry, may lead to significant mechanical stresses that induce cracking. Studies of chemical expansivity have predominantly focused on bulk ceramics, while as electrodes, MIECs are typically nanostructured for efficient performance at medium-to-low temperatures. The objectives of this work are 1) to investigate how nanostructuring impacts the chemical expansion behavior and 2) to control the chemical strain by means of interfaces/microstructure, with the ultimate goal of promoting device stability and efficiency. $Pr_{0.2}Ce_{0.8}O_{2-\delta}$ (PCO20), a model MIEC, was prepared as nanopowders by co-precipitation. The nanopowders were first in-situ sintered in a dilatometer with impedance feedthroughs for microstructure evolution, followed by simultaneous chemical strain-transport measurement on stable microstructures at four isotherms (550 – 400 °C) with pO_2 steps. We found the chemical strains can be successfully suppressed by decreasing the particle size. This trend can be explained by the decrease of reduction enthalpy, verified through pO_2- and temperature-dependent conductivity. The underlying defect chemistry will be discussed.

S16 Controlling grain boundary structure, chemistry, and their network as a function of material processing

S16- Microstructure evolution

Room: Colorado C
Session Chair: James Wollmershauser, U.S. Naval Research Laboratory

10:00 AM

(EMA-S16-001-2025) Microstructure by Design: Thin Film Grain Growth Experiments, Simulations, Data Analytics (Invited)

K. Bramak*[1]

1. Columbia University, Applied Physics and Applied Mathematics, USA

A grand challenge problem in engineering of polycrystals is to develop prescriptive process technologies capable of producing an arrangement of grains that provides for a desired set of materials properties. One method by which the grain structure is engineered is through grain growth or coarsening of a starting structure. Grain growth can be viewed as the evolution of a large metastable network, and can be mathematically modeled by a set of deterministic local evolution laws for the growth of an individual grain combined with stochastic models to describe the interaction between grains. This talk will address not only the challenges of generating suitable nanocrystalline film samples for experiments, but also the challenges of extracting the relevant microstructural metrics from bright-field transmission electron images and crystal orientation maps. A machine learning approach to automated grain boundary detection and integration of experiments with simulations, mathematical models and theory will be discussed.

10:30 AM

(EMA-S16-002-2025) Surface composites synthesized through the incorporation of atomic layer deposited AlO_x into nanoporous fuzzy tungsten (Invited)

P. Bandaru*[1]

1. University of California San Diego, Mechanical & Aerospace Engineering, USA

The incorporation of energetic helium gaseous species into plasma facing materials such as tungsten (W), imparts intrinsic surface fragility, yielding fuzzy tungsten. To enhance the robustness of the surface layers, aluminum oxide (AlO_x) was deposited by atomic layer deposition into the fuzzy W. The conformally deposited ceramic yields a new class of surface composites. Structural characterization of the fuzzy W-AlO_x composites through nanoindentation testing indicated enhanced indentation modulus (E_{ind}) and hardness (H_{ind}) and was modeled through various rules of mixtures approaches. The distribution of AlO_x in fuzzy W was explored and a systematic study of the extent of incorporation of the AlO_x into the fuzzy W was carried out. The synthesized composites may be utilized for improved structural characteristics, e.g., in reducing crack initiation and fracture

11:00 AM

(EMA-S16-003-2025) Reverse-Engineering A Legacy Ferroelectric Material of Known Composition and Microstructure

G. Kamm*[1]; E. Neuman[1]; W. Dong[1]; S. Bishop[2]; P. Yang[1]; R. Trujillo[1]; W. Bachman[1]; C. Bailey[1]; S. Ehlers[1]

1. Sandia National Laboratories, USA
2. Sandia National Laboratories, Materials, USA

Lead zirconate titanate (PZT) compositions are ubiquitous in explosive-electric transducers as on-demand power sources that are reliable even after decades of storage. These devices exploit the pressure-induced phase transformation from a polar to non-polar phase to rapidly produce current. Here, we investigate the processing and properties of Ba, Bi co-doped PZT to reverse-engineer the microstructure and composition of a relaxor ferroelectric material. Preparation of a material with identical properties is challenging due to lack of availability of original processing records. To address this, we examine the role of sintering aids, second phase additions, processing, and sintering conditions to replicate the legacy composition and microstructure. A design of experiments approach was utilized to predict and validate the optimal conditions. The reverse engineering approach and the effects of additives and processing conditions on the microstructure and electrical properties of the reverse engineered ceramic will be discussed. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

11:15 AM

(EMA-S16-004-2025) Effects of Grain Size on Plasticity Mechanisms of Nanocrystalline $MgAl_2O_4$ Spinel under Nanoindentation: Hall-Petch vs. Inverse Hall-Petch

Z. S. Arenella*[1]; S. Rommel[1]; Z. H. Aitken[2]; H. Ryou[3]; J. Wollmershauser[3]; E. Gorzkowski[3]; B. N. Feigelson[4]; Y. Zhang[2]; M. Aindow[1]; S. Lee[1]

1. University of Connecticut, Materials Science and Engineering, USA
2. Agency for Science, Technology and Research, Institute of High Performance Computing, Singapore
3. U.S. Naval Research Laboratory, Material Science & Technology Division, USA
4. U.S. Naval Research Laboratory, Electronics Science & Technology Division, USA

Understanding the relationship between grain size and mechanical properties of nanocrystalline magnesium aluminate ($MgAl_2O_4$) spinel are important due to their strong potential for transparent structural applications. In this study, $MgAl_2O_4$ with grain sizes ranging from 3.7 to 80nm has been synthesized by environmentally controlled pressure assisted sintering, and the effect of grain size on plasticity mechanisms under nanoindentation was investigated for the grain size within the Hall-Petch regime (80nm), the inverse Hall-Petch regime (3.7nm), and near the transition grain size (10.5nm). Transmission electron microscopy of an 80nm grain size sample revealed the significant local lattice distortion and grain boundary decohesion caused by dislocation plasticity. In contrast, a 3.7nm grain size sample does not show the dislocation plasticity even right below the indent. Also, grain boundary decohesion was observed within shear bands. Atomistic simulation of 3.7nm grain size shows that plastic strain is developed mostly at grain boundaries without dislocation nucleation even after extensive plastic deformation, indicating that the grain boundary sliding is the unit mechanism of plasticity. The results of this work provide an important insight into understanding the indentation plasticity of nanocrystalline ceramics with different grain sizes.

S16- Processing parameters

Room: Colorado C
Session Chairs: Hadas Sternlicht, The Pennsylvania State University Department of Materials Science and Engineering; Ece Gunay, Carnegie Mellon University; Sai Venkata Gayathri Ayyagari, The Pennsylvania State University

11:30 AM

(EMA-S16-005-2025) The Impact of Bismuth on the Nonlinearity and Reliability of Cold Sintered ZnO Varistors

K. Chuong*[1]; Y. Liu[1]; T. Forbes[1]; D. Senthilkumar[1]; L. Graber[1]; L. Garten[1]

1. Georgia Institute of Technology, USA

ZnO based varistors are critical for shunting voltage surges in DC circuit breakers (DCCBs), but most research has focused on AC circuits where operational stressors are dissimilar from DCCBs. Cold sintering (CS) – a low-temperature, liquid phase dependent, high-pressure processing method – is proposed as a route to increase grain size uniformity, reduce grain size, and increase nonlinearity to improve varistor performance in DCCBs. In traditionally sintered ZnO varistors, bismuth doping influences nonlinearity and voltage breakdown, but the effects of bismuth doping in CS varistors is not yet established. This study investigates the impact of bismuth on the electrical properties of ZnO varistors fabricated through CS. ZnO was doped with 0, 0.1, 0.5, and 1.0 mol% Bi_2O_3 which was either cold sintered at 300 °C under 700 MPa for 1 hour or traditionally sintered at 1100 °C for 1 hour. Scanning electron microscopy showed an increase in grain size uniformity and an average grain size decrease of 3.8 μm for CS samples. Impedance, C-V, and I-V measurements were taken to analyze changes in device behavior and quantify the increase in nonlinearity and Schottky barrier height. It was found that Bi-doping increased nonlinearity in CS ZnO more than its traditional counterpart, and 0.1 mol% Bi_2O_3 increased nonlinearity the most. Such improvements increase device reliability, which is suitable for DCCBs.

11:45 AM

(EMA-S16-006-2025) A systematic study of Black Light Sintering (BLS): Dependence of grain growth on processing parameters, thermal and optical properties

P. Zahler*[1]; J. N. Ebert[2]; D. Jennings[4]; T. Froemmling[3]; W. Rheinheimer[2]

1. Universitat Stuttgart, Institute for Manufacturing Technologies of Ceramic Components and Composites, Germany
2. Universitat Stuttgart, IFKB, Germany
3. Technische Universitat Darmstadt, Germany
4. Forschungszentrum Julich GmbH, Germany

Conventional sintering techniques are energy intensive and rather inefficient processes. Illuminating ceramics with high intensity blue or UV light has been proven to be an effective method of sintering dense ceramics, yet many of the processing parameters still need optimization. The current studies investigate the impact of processing parameters, thermal properties (heat capacitance, thermal conductivity) and optical properties (absorbance, reflectance) on the microstructure evolution during BLS of $SrTiO_3$ ceramics. SEM images of microstructures are compared to FEM simulation of the temperature distribution inside the sample during the BLS process. The goal of this research is to identify parameters and properties most relevant for the BLS process. The data of this study will then be used to design a processing route that can be transferred to other materials.

12:00 PM

(EMA-S16-007-2025) Free Carbon and Processing Considerations in Entropy Stabilized Carbides

A. Salanova Giampaoli*[1]; H. Ryou[1]; K. P. Anderson[1]; E. Patterson[1]; S. C. Mills[1]; H. Keshmiri[1]; L. Backman[1]; B. N. Feigelson[1]; E. Gorzkowski[1]; J. Wollmershauser[1]

1. US Naval Research Laboratory, USA

High–entropy carbides have demonstrated improved properties relative to the individual metal carbide constituents. The general class of high–entropy ceramics leverage an increase in configurational entropy to improve the material properties such as increases in thermo-mechanical stability and decreases in thermal conductivity. High–entropy ceramics require four or more individual constituents at or near equimolar ratios. The typical synthesis route of high–entropy carbides involves mixing the individual carbide precursors and heat treating them to form a single solid solution. The assumption that the final solid solution maintains the equimolar ratios that were batched initially must be reconsidered. The individual carbides often contain free carbon that may remain out of solid solution through heat treatment, resulting in a final material that can paradoxically be stoichiometrically carbon deficient while containing excess free carbon. This work investigates processing and free carbon content on high–entropy carbides and their properties.

12:15 PM

(EMA-S16-015-2025) Polycrystal Microstructure Informatics (Invited)

J. Hu*[1]

1. University of Wisconsin-Madison, USA

An important topic of materials research is to predict the processing–microstructure–property relationship as well as the dynamical evolution of microstructures under complex 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 $Tb_xDy_{1-x}Fe_2$ and ceramic solid electrolytes $Li_7La_3Zr_2O_{12}$ 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 physics-informed 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 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.

S17 Emerging semiconductor materials and interfaces

S17- 2D Materials

Room: Colorado I
Session Chairs: Sanghoon Bae, Washington University, St. Louis; Nidhin Kalarickal, Arizona State University

10:00 AM

(EMA-S17-001-2025) Atomically-thin nonvolatile memory based on sliding ferroelectricity (Invited)

K. Yasuda*[1]

1. Cornell University, Applied and Engineering Physics, USA

Achieving atomically thin ferroelectric materials for the use in ferroelectric nonvolatile memory remains a significant challenge in materials science, primarily due to the depolarization effects in ultra-thin scales. To address this challenge, we present a novel approach to engineering atomically thin ferroelectrics using van der Waals heterostructures. Our method involves artificially inducing ferroelectricity by manipulating the stacking angle of non-ferroelectric materials such as bilayer boron nitride and bilayer transition metal dichalcogenides. This technique enables us to produce one of the thinnest out-of-plane ferroelectrics that operates as a nonvolatile memory at room temperature. We specifically highlight its device performance as a ferroelectric field effect transistor. Artificial ferroelectrics offers atomically-thin devices that enables ultrafast and high-endurance switching, which overcomes some of the traditional constraints. This exceptional performance stems from the unique ferroelectric mechanism, called sliding ferroelectricity, where the polarization is switched by the interlayer sliding motion between the van der Waals layers.

10:30 AM

(EMA-S17-002-2025) Controlling Structure and Symmetry in 2D Semiconductors and Heterostructures (Invited)

A. J. Mannix*[1]

1. Stanford University, Materials Science and Engineering, USA

Atomically thin van der Waals materials offer precise control over composition, symmetry, moiré superlattices, and interfacial coupling, but scaling these innovations for practical applications remains challenging. In this talk, I will present several recent advances in the growth and device fabrication of 2D semiconductors and their heterostructures. Optimizing the growth of transition metal dichalcogenides (TMDCs) like MoS2 and WSe2 is crucial for creating devices that can surpass silicon CMOS and enable scalable photonics. We developed a hybrid metal-organic chemical vapor deposition (HyMOCVD) process for precise compositional control, enabling tunable WS2 growth via doping, alloying, and selection of growth promoting additives. By adjusting growth kinetics, we achieved polytype-selective growth of ferroelectric 3R-phase TMDCs, opening avenues for ferroelectric devices and nonlinear optics. Improving electrical contacts to 2D semiconductors is another critical challenge. Evidently, Ni forms effective contacts with n-type WS2 despite its suboptimal work function. We observe that the mechanical strain from Ni electrode deposition can significantly enhance device performance, with strain effects yielding up to a 2.7× increase in transistor on-state current and a 78% reduction in contact resistance. This effect is widely neglected but shows great potential for further device engineering.

11:00 AM

(EMA-S17-003-2025) Improving the planar growth of SnSe by tuning substrate surface energy and lattice match

J. R. Chin*[1]; M. Frye[1]; D. Liu[2]; M. Yu[3]; M. Hilse[4]; S. Law[2]; L. M. Garten[1]

1. Georgia Institute of Technology, School of Materials Science and Engineering, USA
2. The Pennsylvania State University, Department of Materials Science and Engineering, USA
3. University of Delaware, Materials Science and Engineering, USA
4. The Pennsylvania State University, Materials Research Institute, USA

The direct growth of wafer-scale, high-quality 2D chalcogenide films is a critical challenge in realizing the potential of 2D nanoscale electronics. SnSe is an emerging 2D material whose relatively high binding energy (146 meV/atom) increases the impact of the substrate on planar growth, film morphology, and crystallographic orientation. Tailoring the substrate lattice parameters and surface energy can control the crystallographic orientation and morphology of SnSe thin films deposited by molecular beam epitaxy (MBE). SnSe films were deposited with a 1.35 Se:Sn flux ratio onto substrates heated to 285 °C. The MBE-grown films exhibited greater surface coverage on substrates with higher surface energies, such as mica (5 J/m^2), compared to c-Al_2O_3 (3.36 J/m^2). The substrate surface preparation also affects grain orientation and morphology; MgO substrates that were cleaved and annealed at 900 °C show increased planar SnSe growth compared to films on untreated substrates. The cleaving exposes an internal surface clear of atmospheric contaminants, while high temperature annealing increases surface energy. SnSe grows with a predominant [010] orientation on MgO, with which it has a lattice mismatch of 1.42%. Understanding how the growth of SnSe is affected by substrate selection and preparation will help to develop deposition procedures for similar chalcogenide thin films for nanoscale devices.

S17- Wide bandap (WBG) and ultra-wide bandgap (UWBG) materials

Room: Colorado I
Session Chairs: Nidhin Kalarickal, Arizona State University; Hari Nair, Cornell University

11:15 AM

(EMA-S17-004-2025) MOCVD of Ga_2O_3 (Invited)

H. Zhao*[1]

1. The Ohio State University, USA

Ultra-wide bandgap gallium oxide (Ga_2O_3), with a bandgap energy of 4.8 eV and a predicted critical field strength of 8 MV/cm, emerges as a promising material for power electronics. Significant progress has been made in Ga_2O_3 substrate development, thin film epitaxy, defect and doping control, and device demonstrations. I will discuss recent MOCVD advancements, focusing on impurities and doping, phase stabilization, and p-type oxide developments. This includes the growth of high-purity (010) and (001) β-Ga_2O_3, the challenges in developing high quality thick Ga_2O_3 films, and MOCVD of p-type NiO and n-Ga_2O_3/p-NiO pn junctions.

11:45 AM

(EMA-S17-005-2025) High-Throughput Ab Initio Study of Ultra-Wide Bandgap Materials (Invited)

A. Singh*[1]

1. Arizona State University, Physics, USA

Ultra-wide bandgap (UWBG) materials present an exciting area of research in high-power and RF electronics, deep ultraviolet optoelectronics, and quantum information science. However, investigating the fundamental properties of UWBG materials and their heterostructures, such as impact ionization rates, bandgaps, band offsets, and point defect energy levels, is an enormously challenging task due to the vast configuration space associated with these studies.

In this talk, I will show how we have developed an open-source Python package, pyGWBSE, to perform automated first-principles calculations within the GW-BSE framework to investigate the fundamental properties of UWBG materials and their heterostructures in a high-throughput manner. GW approximation accurately predicts the electronic structure of materials, for instance, it overcomes the bandgap underestimation issue of the more widely used density functional theory. BSE formalism accurately predicts the excitonic properties of materials producing absorption spectra that are directly comparable with experimental observations. Furthermore, I will show how we used pyGWBSE for benchmarking studies, predicting the properties of $B_xAl_{1-x}N$ alloy structures across the entire x = 0 to 1 range, and how we used it to develop machine learning models for the discovery of electronic materials and their properties.

12:15 PM

(EMA-S17-006-2025) Damage recovery due to high-temperature Ge ion implantation in β-Ga_2O_3 ***WITHDRAWN***

A. Sardar*[1]; T. Isaacs-Smith[1]; S. Schaefer[4]; B. Tellekamp[4]; T. Kaspar[3]; R. Comes[2]; M. Park[1]
1. Auburn University, Physics, USA
2. University of Delaware, Department of Materials Science and Engineering, USA
3. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
4. National Renewable Energy Laboratory, Materials Science, USA

Monoclinic Beta Gallium Oxide (β-Ga_2O_3) is emerging as a promising wide bandgap semiconductor material for power electronic applications. Ion implantation enables precise and selective doping of material regions, making it effective for device processing. Our previous study reported that high temperature (HT) Si ion implantation improved the conductivity and maintained better crystallinity even at high concentrations of dopants, although the damages and defects were not fully explored. In this work, we are comparing room temperature (RT) and HT Ge ion implantation to study the change in structural morphology of β-Ga_2O_3. We performed RT (25 °C) and HT (600 °C) Ge implants into MBE-grown (010) β-Ga_2O_3 films with energies of 325 keV and 675 keV, followed by annealing in flowing nitrogen to activate the dopants. HRXRD and rocking curve showed structural defects after the implantation and partial crystallization recovery upon annealing, with fewer defects after HT implantation. Currently we are investigating beam damage using STEM measurements of implanted films, dopant activation using electron paramagnetic resonance and transport, and changes in electronic structure using spectroscopic ellipsometry. These results are highly encouraging for achieving Ge-doped β-Ga_2O_3 layers with low crystalline defects using HT ion implantation as we will discuss in this presentation.

S18 Characterization of struture-property relationships in functional ceramics

S18- Integrating computational-imaging techniques and machine-learning into the structural measurement workflow

Room: Colorado J
Session Chair: James LeBeau, Massachusetts Institute of Technology

10:00 AM

(EMA-S18-001-2025) From Data to Discovery: AI's Transformative Role in Thin Film Research (Invited)

S. R. Spurgeon*[1]
1. National Renewable Energy Laboratory, USA

The advancement of thin film technologies is pivotal for progress in numerous fields, including energy, electronics, and quantum computing. However, the traditional trial-and-error approach to materials discovery is inherently slow and inefficient. This presentation will showcase how artificial intelligence (AI) is transforming thin film research by enabling a data-driven paradigm shift. We will highlight our past successes in applying AI to understand radiation damage in thin film oxides, demonstrating how graph analytics can unravel complex material behavior. Additionally, we will provide insights into our current work at the National Renewable Energy Laboratory, where we are leading the charge in autonomous materials science. Backed by a $14M investment in our characterization facility, we are developing AI-guided workflows that seamlessly integrate experimentation and AI-guided decision-making. By harnessing the power of AI, we aim to accelerate the discovery and design of high-performance thin films, propelling innovation across a multitude of industries.

10:30 AM

(EMA-S18-002-2025) Robust multislice ptychography for quantiative imaging of ceramics

C. Gilgenbach*[1]; J. LeBeau[2]
1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. Massachusetts Institute of Technology, USA

Multislice electron ptychography is a developing 4D STEM technique that promises three-dimensional, quantitative phase contrast imaging for a wide range of materials science problems. However, it remains difficult to implement because of the large set of acquisition and computation parameters required for a successful reconstruction. In this talk, we discuss the optimization of acquisition parameters for multislice ptychography. We introduce two physically informed metrics, areal oversampling and Ronchigram magnification, which are sufficient to inform the selection of experimental parameters. We evaluate these metrics over a wide range of metrics in simulation and experiment. Through application of these metrics, we achieve reconstructions with large scan step size, which enables large field-of-view reconstructions with minimal redundant data. Finally, we discuss the application of optimized multislice electron ptychography for quantitative phase contrast imaging of ceramic materials.

10:45 AM

(EMA-S18-003-2025) AI's Promise and the Limits: Unpacking Structure-Property Relationships in Functional Ceramics Amid Infrastructure Constraints (Invited)

J. Agar*[1]
1. Drexel University, USA

Science uses data for decision-making. The emergence of advanced sensing technologies has led to a flood of large, fast-moving data from varied sources. Despite advancements like ChatGPT, their limitations are evident. We explore the co-design of experimental systems, encompassing algorithms and hardware, all aimed at actualizing scientific ML. We then tackle the challenges inherent in applying ML within the context of ferroelectrics, where concepts like symmetry form essential semantic relationships. Our discussion extends to computational tools for deploying resilient, self-repairing services in materials science. We spotlight innovations in parsimonious NN, adept at learning geometric transformations in reciprocal space. We emphasize the role of stochastic averaging in enhancing noise robustness, surpassing algorithmic approaches. We apply these techniques to a variety of common synthesis and characterization techniques in ferroelectrics. We examine the progress in AI co-design, wherein algorithms are optimized for FPGAs for real-time <1 ms inference. This optimization enables rapid, intelligent analysis, decision-making, and control on ultra-low-cost, low-power devices at unparalleled speeds. We illustrate how this approach is instrumental in real-time data analysis, data reduction, and dose-controlled imaging in including electron microscopy.

11:15 AM

(EMA-S18-004-2025) Next-Generation Gaussian Processes for Function Approximation, Uncertainty Quantification, and Decision-Making (Invited)

M. M. Noack*[1]

1. Lawrence Berkeley National Laboratory, Applied Mathematics, USA

Gaussian processes (GPs) and Gaussian-related stochastic processes are powerful tools for function approximation, uncertainty quantification, global optimization, and autonomous data acquisition due to their robustness, analytical tractability, and natural inclusion of Bayesian uncertainty estimates. Even so, Gaussian processes are often criticized for poor approximation performance and neck-breaking computational costs in real-life applications. The reason for this gap, however, is not the methodology itself but rather a user-caused lack of flexibility and domain awareness of the underlying prior probability distribution, the likelihood, poor training, and insufficiently expressive utilization of the posterior for decision-making. In this talk, I want to address many challenges of GPs that might inhibit optimal performance, guiding the audience to "Next-Generation Gaussian Processes". We will begin our journey by looking at a few motivating examples and some theoretical preliminaries before diving into commonly encountered challenges and what can be done to address them. We will discover hands-on solutions and tools that make implementation easy. The key takeaway for the audience will be a better understanding of Gaussian processes and ways to customize them for optimal performance.

11:45 AM

(EMA-S18-005-2025) Unveiling the Impact of Electrode Materials on the Structure and Ferroelectric Properties of Hf0.5Zr0.5O2 Thin Films using 4D-STEM

G. Baucom*[1]; T. Tharpe[1]; R. Tabrizian[1]; H. Kim[1]

1. University of Florida, USA

Ferroelectric hafnium zirconium oxide (HZO) stands as a promising candidate material for next-generation ferroelectric memory devices due to its unique ability to sustain ferroelectricity in ultrathin condensed geometries and its compatibility with established semiconductor fabrication technologies. However, optimization of synthesis strategies has numerous challenges, most notably that HZO possesses many similar structural polymorphs and that the phase responsible for ferroelectric behavior is only metastable. Synthesis of thin film devices containing pure ferroelectric phase HZO has yet to be attained. Additionally, due to the extreme structural similarity between the polymorphs, precise identification and quantification of the phases present in samples is often challenging using conventional bulk techniques such as x-ray diffraction. Here, we leverage four-dimensional scanning transmission electron microscopy (4D-STEM), a technique that collects 2D electron diffraction patterns over a 2D scan area, to examine the structural origins of the dependence on the choice of the electrode material on device performance in metal-ferroelectric-metal capacitor HZO devices. Automated crystal orientation mapping reveals the differences in the phase composition and orientation between devices fabricated on different electrode materials.

12:00 PM

(EMA-S18-006-2025) Combinatorial synthesis and characterization of thin film $Al_{1-x}RE_xN$ (RE = Pr^{3+} and Tb^{3+})

R. Smaha*[1]; B. Paudel[2]; J. Mangum[1]; C. Lee[2]; K. Yazawa[1]; P. Gorai[2];
G. Brennecka[2]

1. National Renewable Energy Laboratory, USA
2. Colorado School of Mines, USA

Cation-substituted AlN-based materials with wurtzite-derived structures, such as $Al_{1-x}Sc_xN$ and $Al_{1-x}Ga_xN$, have a range of exceptional electronic, electromechanical, and dielectric properties, spurring research into this broad materials family. Rare earth (RE) cations are appealing to impart optoelectronic or magnetic functionality, but success in incorporating a significant level of RE cations into AlN has been limited because it is thermodynamically challenging to stabilize such heterostructural alloys. Building upon our previous success achieving nearly x = 0.25 for $Al_{1-x}Gd_xN$ thin films, we next explore the phase diagrams of $Al_{1-x}RE_xN$ (RE = Pr, Tb) both experimentally and computationally. We perform a rapid survey of the composition-structure-property relationships as a function of RE substitution using high-throughput combinatorial co-sputtering and synchrotron grazing incidence wide angle X-ray scattering and electron microscopy to study the crystal structure and composition. We find that synthesis conditions far from equilibrium are required to stabilize wurtzite $Al_{1-x}RE_xN$ (RE = Pr, Tb) with significant amounts of Pr/Tb, and we uncover trends in the optoelectronic properties with RE substitution level. This work shows the importance of advanced scattering and microscopy techniques in the development of synthesis-property design rules in these emerging multifunctional materials.

S22 Advanced Electronic Materials- Processing structures and applications

S22- Advanced electronic materials, including ferroelectric, piezoelectric, dielectric, electrostrictive, and pyroelectric materials

Room: Colorado F
Session Chairs: Eric Patterson, Naval Research Laboratory;
Tadej Rojac, Jozef Stefan Institute

10:00 AM

(EMA-S22-001-2025) Discovery and Design of AlN-based Ferroelectric Materials (Invited)

K. Yazawa*[1]; N. Bernstein[2]; D. Drury[4]; B. Hanrahan[4]; C. Lee[1]; P. Gorai[1];
N. Haegel[3]; A. Zakutayev[3]; G. Brennecka[1]

1. Colorado School of Mines, USA
2. Colorado School of Mines, Materials and Metallurgical Engineering, USA
3. National Renewable Energy Laboratory, USA
4. US Army Combat Capabilities Development Command Army Research Laboratory, USA

AlN-based wurtzite ferroelectrics are a promising candidate for microelectronics applications due to their chemical, process, and crystallographic compatibilities to tetrahedrally bonded semiconductors such as Si and GaN. The ferroelectricity in this material class is achieved by cation substitution such as (Al,Sc)N, (Al,B)N, and (Al,Y)N, but the ferroelectric property predictors and underlying mechanisms of cation substitution are not fully understood. Those insights are important for efficient material discovery and strategic material property tuning demanded in applications. This talk covers AlN-based ferroelectric material discovery and its design strategies. Systematic experimental and computational approaches reveal that local displacement associated with Sc substitution is key to realize ferroelectricity in (Al,Sc)N properties. Based on those insights, we extend the chemistry space of (Al,M)N (M = rare-earth elements and Hf) to broaden ferroelectric material candidates and functionalities. We demonstrate the mechanistic understanding and the identification of the predictor enabling ferroelectric switching, which provides a rational approach to discovering and designing AlN-based wurtzite ferroelectric materials.

10:30 AM

(EMA-S22-002-2025) Ferroelectricity of Wurtzite Aluminum Hafnium Nitride Heterovalent Alloys

N. Bernstein*[1]; D. Drury[3]; K. Yazawa[4]; G. R. Fox[5]; A. Zakutayev[4]; B. Hanrahan[3]; G. Brennecka[2]

1. Colorado School of Mines, Materials and Metallurgical Engineering, USA
2. Colorado School of Mines, USA
3. US Army Combat Capabilities Development Command Army Research Laboratory, USA
4. National Renewable Energy Laboratory, USA
5. Fox Materials Consulting, LLC, USA

Thin films of Aluminum Hafnium Nitride ($Al_{1-x}Hf_xN$) were synthesized via reactive magnetron sputtering with three different cation ratios x. XRD measurements showed a c-axis oriented wurtzite phase. Polarization vs. electric field measurements showed hysteresis attributed to ferroelectric switching. Additional verification of polarization reversal was observed using two different measurement methods: phosphoric acid etching rate and film displacement using a double beam laser interferometer (DBLI). This shows that $Al_{1-x}Hf_xN$ is a wurtzite ferroelectric nitride alloy. Ellipsometry and X-ray Photoelectron Spectroscopy results will be discussed. These results signify the compositional and valency flexibility of ferroelectric AlN-based systems and, therefore, present a new foundation for understanding and engineering the electrical properties.

10:45 AM

(EMA-S22-003-2025) Ferroelectricity in ternary (Al,B,Ga)N thin films

B. DeBastiani*[1]; J. Maria[1]

1. The Pennsylvania State University, Earth and Mineral Sciences, USA

Wurtzite aluminum nitride is grown in a substitutional solid solution with compositions across the aluminum nitride, boron nitride and gallium nitride ternary phase diagram. This is achieved through physical vapor deposition (PVD) by reactive magnetron sputtering of aluminum, boron nitride, and gallium nitride targets with pulsed direct current (PDC) and radio frequency (RF) power. The films are grown on plasma treated conductive n-silicon wafers. The crystallinity of the resulting films is interrogated using X-Ray diffraction (XRD) techniques. Compositional information was collected via energy dispersive spectroscopy (EDS). Metallic electrodes are sputtered for polarization – electric field (PE) measurements taken at 1 kHz. By spanning the compositional landscape, the electrical properties as well as the crystallinity can be tuned. In this work, for approximately 18% Ga, ferroelectric hysteresis is observed throughout the sampled boron concentrations (3-12%). Over this range the out of plane lattice parameter decreases by 0.48% and the rocking curve FWHM's range from 2.00-3.48°. Films show a promising PE response despite significant oxygen contamination. Current work is focused on utilizing a higher purity gallium target as it is thought to be the contamination source.

11:00 AM

(EMA-S22-004-2025) Ferroelectric $Al_{1-x}B_xN$ Sputtered thin films on n-type Si bottom electrodes

I. Mercer*[1]; C. Skidmore[1]; S. Calderon[2]; E. C. Dickey[2]; J. Maria[1]

1. The Pennsylvania State University, Materials Science and Engineering, USA
2. Carnegie Mellon University, Materials Science and Engineering, USA

Ferroelectric $Al_{1-x}B_xN$ thin films at compositions x = <0.01, 0.02, 0.06, 0.08, 0.13, and 0.17 are grown on n-type Si, which fulfills the role as both substrate and bottom electrode. Polarization hysteresis reveals remanent polarization values between 130-140 μC/cm^2 and coercive field values down to 4 MV/cm at 1 Hz, maintaining RMS roughness below 1 nm. Films with compositions x = 0.06 and 0.13 showed the most robust hysteresis and leakage resistance. The affect of plasma treatment utilizing a high substrate bias also primes the n-type Si surface for enhanced leakage resistance and crystallinity. Cross-sectional TEM and EELS shows an amorphous 3.5 nm Si_3N_4 at the $Al_{1-x}B_xN$ interface post plasma treatment and deposition. The first ~5 nm of $Al_{1-x}B_xN$ is highly crystallographically defective with much higher mosaicity but electrical properties are unfazed. Using this substrate the prospects of thickness scaling is also highlighted and discussed. By combining the bottom electrode and substrate, the n-type Si enables a streamlined growth process for $Al_{1-x}B_xN$ at a wide range of BN compositions and layer thicknesses.

11:15 AM

(EMA-S22-005-2025) Developing Processing Routes to Stabilize Hexagonal Transition Metal Oxides (Invited)

M. Frye[2]; I. Graham[1]; J. R. Chin[1]; L. M. Garten*[1]

1. Georgia Institute of Technology, School of Materials Science and Engineering, USA
2. Georgia Institute of Technology, USA

Developing synthesis routes to stabilize metastable materials is critically needed in order to realize the many predicted piezoelectric hexagonal transition metal oxides. For example, while the ground state of $BaNiO_3$ (BNO) and $ScFeO_3$ (SFO) are centrosymmetric, both materials have a 6mm piezoelectric phase within 100 meV/atom above the convex hull. In this talk, I will discuss how interface design, deposition timing, and oxidation control can be used to access these metastable materials. BNO and SFO thin films were deposited from ceramic targets onto (0001) Al_2O_3 substrates using pulsed laser deposition. These films were deposited over a range of temperatures from 400-900 °C, and laser fluences of 2.0-3.5 J/cm^2. In SFO, (0001) textured $P6_3cm$ phase of $ScFeO_3$ forms on (0001) Al_2O_3 despite the 17% lattice mismatch between the film and substrate. Transmission electron microscopy shows a (111) Fm-3m FeO phase forms at the interface of (0001) Al_2O_3 which promotes the stabilization of the metastable SFO phase. In BNO, x-ray diffraction results indicated that varying the oxygen partial pressure 0.009-0.16 mbar can be used to select between multiple polymorphs of BNO. The mechanisms of stabilization described here provide a toolbox for accessing piezoelectric polymorphs of complex transition metal oxides.

11:45 AM

(EMA-S22-006-2025) Synthesis-structure-property relationships in co-sputtered Zn1-xMgxO thin films

W. A. Prudnick*[1]; J. Maria[1]; S. Yang[1]

1. The Pennsylvania State University, USA

This presentation will summarize ferroelectric zinc-magnesium oxide (Zn1-xMgxO or ZMO) thin film synthesis using RF magnetron sputtering with attention to connections between low and high-field electrical properties and deposition conditions. Current efforts focus on low temperature growth–exluding unitnended substrate heating–so as to maximize compatibility with the broadest substrate spectrum while preserving crystallinity, controlling composition, and minimizing coercive field. ZMO is grown by RF magnetron sputtering using metallic Mg and Zn targets in a mixture of Ar and 10% ozone in molecular oxygen. Generally we find that lower pressures yields the best crystallinity, crystal texture, smoothness, and the highest insulation resistance, especially at high electric fields. Moreover, we find that high kinetic energy conditions produce the lowest coercive fields–with values approaching 2 MV/cm. Additionally, these conditions produce exceptionally square hysteresis loops with margins separating breakdown strength and coercive field exceeding 1 MV/cm. The most interesting electrical properties occur for Mg concentrations approaching the solubility limit, which is near 40% Mg for these conditions. Challenges to ZMO synthesis shall be discussed–namely, the strong dependency of film composition on total pressure and oxidant-to-Ar ratio under constant relative Zn:Mg cathode power ratios.

12:00 PM

(EMA-S22-007-2025) Operando Assessment of Mixed Neutron and Gamma Radiation Effects on Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ Capacitors

C. Sharma*[1]; J. Nimmagadda[1]; M. Lee[2]; J. Kim[3]; J. C. Nino[1]

1. University of Florida, Materials Science and Engineering, USA
2. The University of Texas at Dallas, Electrical and Computer Engineering, USA
3. The University of Texas at Dallas, Materials Science and Engineering, USA

High-κ HfO_2 dielectrics have been extensively studied to replace SiO_2 and enhance microelectronics' operation lifetime and performance in high-radiation environments. The development of ferroelectric memory architectures using Zr doped-HfO_2 (HZO) marked a significant advancement, improving data storage technology with increased speed, efficiency, and durability, especially for space and defense applications due to its promising ferroelectric properties. This study investigates the effects of bipolar cycling in HZO-based metal-ferroelectric-metal capacitors pre-, operando, and post-exposure to mixed neutron and gamma radiation. Over time, high neutron irradiation increases oxygen vacancy concentrations in HfO_2 thin films but also reduces neutral and charged defects. The study leverages thermal, epithermal, and fast neutron fluxes combined with gamma radiation inside a thermal nuclear reactor's beam port. Operando characterization is performed at neutron fluences up to 10^{12} n/cm^2, while high-fluence neutron irradiation and post-radiation analysis extends up to 10^{14} n/cm^2. This research provides critical insights into data retention, imprint, and polarization relaxation in high-radiation environments. The findings aim to inform the impact of neutron irradiation on the long-term reliability and performance of HZO-based ferroelectric capacitors.

12:15 PM

(EMA-S22-008-2025) Correlative Mapping of Ion Irradiated Aluminum Nitride

B. Dryzhakov*[1]; S. J. Randolph[1]; K. Kelley[1]

1. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA

Through strategic ion irradiation, the aluminum nitride wurtzite framework is enhanced with defect landscapes conducive to ferroelectric switching. In particular, we show He-ion irradiation can induce ferroelectricity in pure aluminum nitride and reduces the ferroelectric switching barrier of boron substituted aluminum nitride ($Al_{0.94}B_{0.06}N$) by >40%. Essentially, locally patterned defect chemistries allow the aluminum nitride lattice to follow a low-energy heterogeneous domain inversion pathway. This presentation highlights the use of correlative spectroscopic techniques that map a systematically patterned region of localized states with enhanced piezoresponsivity and defect signatures. SEM-cathodoluminescence, photoluminescence, and Raman mapping demonstrate intrinsic point defects evolution with the observed local reductions in coercive fields and enhancements in ferroelectric switching, as probed by piezoresponse force microscopy. The combined spatially resolved analyses demonstrate the direct-write tunability of ferroelectric properties in aluminum nitride via ion irradiation.

12:30 PM

(EMA-S22-009-2025) Low concentration ($x \leq 0.01$) doping impact on defect dipole stabilization in $BaTi_{1-x}Fe_xO_3$

S. C. Mills[1]; E. Patterson[2]; R. Maier[3]; M. Staruch*[2]

1. US Naval Research Laboratory, Material Science and Technology, USA
2. Naval Research Laboratory, USA
3. National Institute of Standards and Technology, USA

In ferroelectric $BaTiO_3$ (BTO) single crystals with <1% of iron, the alignment of defect dipoles to the ferroelectric dipoles in the material was demonstrated to result in large and reversible electrostrains (up to 0.8%). In previous work, we verified large strains in (001) oriented 0.5% Fe doped single crystals, but those exhibit a large hysteresis relaxation effect. Here we expand this work to look at a wider range of compositions in Fe doped BTO ceramics ($BaTi_{1-x}Fe_xO_3$; $0 \leq x \leq 0.02$) that were produced by traditional solid-state processing. Samples were characterized by X-ray diffraction (XRD) and scanning electron microscopy and these results correlated to the dielectric, piezoelectric, and ferroelectric properties. Polarization-electric field loops show that, at concentrations between 0.1 and 1% Fe doped BTO, pinched hysteresis loops are observed, which originate from the pinning of domain walls as the walls interact with defects. The saturation polarization and strain values correlate well with the c/a ratio from XRD and electron paramagnetic resonance measurements of the defects, in alignment with previous work that has emphasized the role that composition and the c/a ratio play in stabilizing this effect. This comprehensive study elucidates the systematic behavior of the ferroelectric properties at very dilute dopant levels and demonstrates the optimal compositions for this system.

S4 Oxide Quantum Materials: Synthesis, Properties and Application

S4- Oxide electronics

Room: Colorado B
Session Chairs: Alex Frano, University of California San Diego; Elizabeth Nowadnick, University of California, Merced

2:00 PM

(EMA-S4-007-2025) Evolutionary and neuromorphic intelligence with complex oxides (Invited)

S. Ramanathan*[1]

1. Rutgers University, ECE, USA

About 15 years ago, T. Nakagaki et al demonstrated a stunning result that non-neural organisms can predict periodic events, suggesting an analogy to the Egyptian civilization evolving around the flooding of the river Nile. More recently, studies on monkeys in Khao Sam Roi Yot National Park in Thailand have shown that mastering tool-use can affect maturation of shellfish (prey). Such observations in nature highlight the power of learning and force a fundamental re-think of hardware design for sustainable AI. I will discuss how the adaptive and reconfigurable electronic band structures in complex oxides can inspire disruptive and unconventional approaches for information processing grounded in evolutionary and neural intelligence. I will illustrate with specific examples from our collaborative research on phase transitions in perovskite nickelates and related correlated electron systems as well as their monolithic integration with CMOS electronics.

2:30 PM

(EMA-S4-008-2025) Emerging Functional Heterointerfaces Enabled by Ferroelectric Oxide Thin Films and Membranes (Invited)

X. Hong*[1]

1. University of Nebraska-Lincoln, Department of Physics and Astronomy, USA

Integrating ferroelectric oxides with strongly correlated oxides and 2D van der Waals materials opens the opportunities for achieving novel interfacial coupling and nonvolatile field effect control that are programmable at the nanoscale. In this talk, I will discuss a range of emerging functionalities in heterostructures based on $Pb(Zr,Ti)O_3$ (PZT) thin films and membranes. Leveraging the charge transfer effect between two correlated oxides $LaNiO_3$ and $(La,Sr)MnO_3$, we achieve a record high room temperature resistance switching ratio of 384,400% in PZT-gated Mott transistors. Microwave impedance microscopy studies show that the switching ratio is stable at up to 1 GHz, confirming the electronic nature of the conductance modulation. Negative capacitance (NC) transistors are developed based on polycrystalline PZT gated MoS_2, which exhibit up to 8×10^6 current ratio within small gate voltage of ±0.5 V and ultralow subthreshold swing of 9.7 mV/decade at 300 K. Theoretical modeling and PFM studies suggest that the NC mode is enabled by the metastable polar states of domain walls. We also observe unconventional tuning effect of second harmonic generation capitalizing on the polar coupling of monolayer MoS_2 with either the polar domain or domain wall in PZT thin films and free-standing membranes. Our study showcases the rich functionalities of ferroelectric oxide based heterointerfaces.

3:00 PM

(EMA-S4-009-2025) High electroresistance in all-oxide ferroelectric tunnel junctions enabled by a narrow bandgap Mott insulator electrode

Y. Zhang*[1]; Y. Hao[1]; L. Zhang[1]; K. Wang[1]; X. Hong[1]

1. University of Nebraska-Lincoln, Department of Physics and Astronomy, USA

All-oxide ferroelectric tunnel junctions (FTJs) are promising building blocks for developing nonvolatile memories and neuromorphic computing. FTJs with correlated oxide electrodes offer notable advantages in size scaling. However, due to the challenges in achieving high asymmetric interfacial screening and significant modulation of the tunneling potential profile, they only yield moderate electroresistance (ER) at room temperature. In this talk, we report high ER in all-oxide FTJs by paring a correlated metal with a narrow bandgap Mott insulator as electrodes. We fabricate epitaxial FTJs with 2.8 and 4 nm $PbZr_{0.2}Ti_{0.8}O_3$ tunnel barriers sandwiched between correlated oxides electrodes $LaNiO_3$ and $Sr_3Ir_2O_7$. An large ER of 6,500% has been observed at room temperature, which increases to over 10^5% at 100 K. The high ER can be attributed to the metal-insulator transition induced by ferroelectric polarization in interfacial $Sr_3Ir_2O_7$, resulting in enhanced asymmetry for the tunneling potential barrier. Our study presents an effective material strategy for designing all-oxide FTJs with high room temperature ER, paving the way for their application in energy-efficient memory and computing devices.

S4- Superconductivity

Room: Colorado B
Session Chairs: Jennifer Fowlie, Northwestern University;
Seung Sae Hong, University of California, Davis

3:45 PM

(EMA-S4-010-2025) Superconducting phase diagram of the layered square-planar nickelates (Invited)

G. A. Pan*[1]

1. Harvard University, USA

The discovery of superconductivity in square-planar nickelates has offered a rich materials platform to explore the origins of cuprate-like superconductivity. Experimental investigations however have largely been limited to within the infinite-layer RNiO2 (R=rare-earth) nickelates. Here, we construct a phase diagram of the multi-layer square-planar $Nd_{n+1}Ni_nO_{2n+2}$ compounds and discover signatures of a superconducting dome for n = 4 – 8. Upon decreasing the dimensionality n, the superconducting anisotropy evolves due to 4f electron effects, and electronic structure characteristics approach cuprate-like behavior. Magnetic fluctuations persist from within the superconducting dome and into the over-doped, non-superconducting regime. Our work establishes this layered structural template, complementary to chemical doping, for creating new nickel-based superconductors. We further demonstrate underlying commonalities and distinct differences across varying structural realizations of superconducting square-planar nickelates.

4:15 PM

(EMA-S4-011-2025) Uncovering the ground state of the infinite-layer nickelate parent compound, $NdNiO_2$ (Invited)

C. T. Parzyck*[1]; Y. Wu[1]; L. Bhatt[2]; N. Gupta[3]; V. Anil[1]; B. H. Goodge[2]; D. Muller[2]; L. F. Kourkoutis[2]; D. Hawthorn[3]; D. Schlom[4]; K. M. Shen[1]

1. Cornell University, Laboratory of Atomic and Solid State Physics, USA
2. Cornell University, School of Applied and Engineering Physics, USA
3. University of Waterloo, Department of Physics and Astronomy, Canada
4. Cornell University, Department of Materials Science and Engineering, USA

The infinite-layer nickelates, $RENiO_2$, RE=La, Nd, Pr, offer a novel platform to study the nature of high T_c superconductivity, and the normal state from which it emerges. Comparison between the nickelates and their structural (and electronic) analogs – the cuprate superconductors – may allow for discernment of the universal elements of the high T_c phase diagram. However, synthesis of the undoped, parent nickelates poses a significant challenge which must be overcome to reveal their intrinsic ground state properties. Here, we discuss synthesis of the infinite-layer nickelate, $NdNiO_2$, by a combination of reactive oxide molecular-beam epitaxy and atomic hydrogen reduction, demonstrating improved control of the reduction process and integrability with in situ structural probes. We leverage this technique to shed light on some of the properties of the parent nickelates, including a reexamination of the presence of putative charge order and observed superconductivity in the undoped compounds. Utilizing a multimodal approach, we show that the previously reported $3a_0$ charge ordering is attributable to interstitial oxygen ordering rather than a correlation driven density wave. Finally, we discuss observations of superconductivity in the parent nickelates and examine both intrinsic and extrinsic scenarios for its origin.

4:45 PM

(EMA-S4-012-2025) Structural Basis for Achieving Superconductivity in an Ultrathin Multilayer-Nickelate

H. Zhou*[1]; X. Yan[2]; H. Zheng[2]; Y. Li[2]; D. P. Phelan[2]; H. Hong[1]; Y. Liu[3]; A. Bhattacharya[2]; D. Fong[2]

1. Argonne National Laboratory Advanced Photon Source, USA
2. Argonne National Laboratory, Materials Science Division, USA
3. Argonne National Laboratory, Center for Nanoscale Materials, USA

WITHDRAWN

The discovery of infinite-layer and multilayer superconducting nickelates heralds a new chapter of superconductivity after a long time extensive pursuit in nickelate compounds for achieving cuprate-like unconventional superconductors. However, it is still a formidable experimental challenge in the thin film synthesis and the subsequent chemical reduction to attain superconductivity in nickelate heterostructures. We utilize in situ synchrotron X-ray scattering performed during growth of the parent phase, e.g. Nd6Ni5O16, to reveal that the necessary layer-by-layer deposition sequence does not follow the sequence of the formula unit but an alternate order due to the relative stability of the perovskite unit cell. We exploit this insight to grow ultrathin Nd6Ni5O16 heterostructures and report the appearance of superconductivity in single unit cell Nd6Ni5O12, exhibiting a transition temperature as high as that of thicker films. Our in situ studies of topotactic reduction find that formation of the square-planar phase occurs rapidly and is highly sensitive to reduction temperature. The fluorite layer within the unit cell facilitates reduction by initially stabilizing the square-planar phase in the upper half of the unit cell. Our findings provide insight into growth of the Ruddlesden-Popper nickelates, highlighting the need for in situ studies of the metastable phases key to superconductivity.

*Denotes Presenter

S5 In-Situ/Operando Characterization of Nanomaterials

S5- In situ/Operando Study of Energy and Functional Materials

Room: Colorado E
Session Chairs: Alessandro Mazza, Los Alamos National Lab; Katherine Harmon, Stanford University

2:00 PM

(EMA-S5-006-2025) Advances in In-situ Multi-Modal X-Ray Characterization of Nanomaterials (Invited)

S. Nemsak*[1]

1. E O Lawrence Berkeley National Laboratory, Advanced Light Source, USA

In the last two decades, Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) has established itself as a go-to technique to study heterogeneous and complex material systems under reaction environments. Multimodal approaches, which correlate information from two or more complementary techniques, are currently one of the forefronts of the APXPS development. In the past years, Advanced Light Source contributed one such setup: a combined Ambient Pressure PhotoEmission and grazing incidence X-ray Scattering (APPEXS) instrument commissioned and operated at beamline 11.0.2 The combination of the two in-situ techniques allows correlating structural and chemical information, which is critical for describing processes that transform materials in both these domains. For example, by using APPEXS, we observed dynamics of the exsolution process of catalyst metallic nanoparticles, studied arrays of patterned nano-objects under reaction conditions, and explored chemistry of ligands capping nanoparticles. Future developments of the technique and applications to a wider variety of scientific problems will be discussed.

2:30 PM

(EMA-S5-007-2025) Probing Ion Hopping in Solid-State Electrolytes (Invited)

K. W. Orr*[1]

1. Stanford University, USA

Large-scale deployment of batteries is an essential part of global decarbonization strategies, but significant concerns of safety, longevity, and material supply chains persist. All-solid-state batteries offer great promise for addressing these issues. However, despite being integral to their operation, an atomistic understanding of the ion hopping events in solid electrolytes is lacking, having primarily been studied from theoretical and computational standpoints. In this talk, I will outline our current work using pump-probe measurements to understand ion hopping in solid ion conductors, specifically in beta-aluminas ($M_2Al_{22}O_{34}$, M=Na, K, Ag,…) and in LLZO ($Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$). The principle of our approach is to pump these materials with short, single-cycle THz pulses, which induce ion hopping along the direction of THz polarization. Following this, we monitor ion hopping as a function of time spectroscopically using Kerr effect measurements to track the memory of ion migration through these materials. In future measurements, we will probe the transient structure of the materials induced by the THz pumps using ultra-fast X-ray diffraction measurements, to understand how these materials distort to facilitate ion transport.

3:00 PM

(EMA-S5-008-2025) Shaping lithium phosphate polycrystals in the flow (Invited)

V. Starchenko*[1]; A. Ladd[2]; P. Szymczak[3]; M. Emmanuel[4]; Á. Tóth[4]; D. Horváth[4]

1. Oak Ridge National Laboratory, USA
2. University of Florida, USA
3. Uniwersytet Warszawski, Poland
4. Szegedi Tudomanyegyetem, Hungary

Comparison between pore-scale models and in-situ experimental observations became an indispensable strategy to study physics and chemistry behind crystal nucleation and growth, shaping materials for applications in nano-, micro-electronics, thermoelectric and energy storage devices. Here we use reactive transport pore-scale model with explicit moving boundary based on Arbitrary Lagrangian-Eulerian (ALE) approach to understand chemical kinetics and reaction pathways during precipitation of polycrystalline lithium phosphate (Li3PO4). In this study we demonstrate that the shape of precipitate solid particles can be controlled by the reaction pathway and by the ion transport regime rather than by the reaction kinetics. We show how ALE approach allows to capture numerically evolution of solid material interface observed in the in-situ experiment. Most unique advantage of the ALE approach is ability to predict interface dynamics and overall system evolution governed by coupled processes using fundamental values without fitting parameters if they can be calculated ab initio or obtained from prior measurements. By comparing modeling and experiment we test an earlier proposed hypothesis that the reaction to form solid happens in separate steps. We find that the kinetics of the surface reaction is very slow. Additionally, we will discuss the role of a limiting step in the reaction mechanism to form solid Li3PO4.

4:00 PM

(EMA-S5-009-2025) Electrochemistry combined in situ/operando neutron reflectometry for a greener future (Invited)

H. Wang*[1]

1. Oak Ridge National Laboratory, CNMS, USA

Neutron reflectometry (NR) is a powerful tool to investigate surface and interfacial structures of thin films in a non-destructive and non-invasive fashion. The Liquids Reflectometer (LR) at Oak Ridge National Lab provides valuable information over a wide variety of scientific applications, e.g., interfacial reactions in energy conversion and storage materials, phase separation in polymer films, protein adsorption, etc. LR offers the capability to conduct in situ electrochemistry to probe the structural change at surfaces/interfaces as a function of chemical and electrochemical gradients over time. Meanwhile, event mode at LR helps elucidate the kinetic behavior of surface/interfaces under dynamic conditions and bring a unique perspective to equilibrium studies. A specific application in ionomer-based water electrolysis by using in situ/operando NR will be presented. The study sheds light on fundamental understanding of the complex interaction of ionomer with catalysis, in the typical operation condition of PEM electrolyzer. In addition to neutron techniques, some complementary capabilities for surface chemistry and electrochemistry available at user facilities Center for Nanophase Materials Sciences and Neutron Scattering Division will be outlined. Together, they play a key role in creating new, and more efficient systems through rationally design of the structure and operating conditions.

4:30 PM

(EMA-S5-010-2025) Local Structural Changes as a Response to Heating: In-Situ Characterization using 4D-STEM (Invited)

T. M. Kucinski*[1]

1. Los Alamos National Laboratory, MST-16, USA

Local lattice changes are essential to understanding structure-performance relationships. In-situ characterization can provide powerful observations of the response of materials to environmental stimuli in real time but can be limited due to technical capabilities. Studying the structure of materials at the nanoscale remains challenging due to measurement techniques that only provide global averages; lack of spatial resolution; or in the case of transmission electron microscopy (TEM), multiple/dynamical scattering from thick samples. Overcoming these challenges is possible with four-dimensional scanning transmission electron microscopy (4D-STEM), in which a series of diffraction patterns are measured at each probe position in a conventional STEM image. This remarkable tool enables statistical structural analysis that can produce maps of local strain, crystalline structure and orientation, and thermal expansion. 4D-STEM can be easily combined with in-situ holders for observing nanoscale changes as a response to heating, cooling, and strain. We demonstrate 4D-STEM characterization of materials heated in-situ to determine local lattice structure as a function of temperature. These results could expand our knowledge on the evolution of structure in response to environmental stimuli such as temperature, which has significant implications for understanding the structure/property connection.

5:00 PM

(EMA-S5-011-2025) Structural Explanation of the Dielectric Enhancement of Barium Titanate Nanoparticles (Invited)

A. Suzana*[2]; S. Liu[2]; J. Diao[3]; L. Wu[2]; T. Assefa[2]; M. Abeykoon[2]; R. Harder[1]; W. Cha[1]; E. Bozin[2]; I. Robinson[2]

1. Argonne National Laboratory, USA
2. Brookhaven National Laboratory, USA
3. University College London, United Kingdom

Perovskite transition-metal oxides have been studied for decades because of both their many applications and to answer fundamental scientific questions. $BaTiO_3$ (barium titanate, BTO), is frequently chosen as a lead-free functional material for sensor applications and in the fabrication of devices such as multilayer ceramic capacitors. The present work reports a detailed characterization of domain walls in BTO nanoparticles using state-of-the-art synchrotron techniques. A hydrothermal approach is used to synthesize BTO nanocrystals, which are characterized by a range of methods, including X-ray Rietveld refinement and the Williamson–Hall approach, revealing a mixture of metastable cubic and tetragonal phases at room temperature and the presence of significant inhomogeneous strain associated with the cubic phase. However, X-ray pair distribution function measurements clearly show the local structure is lower symmetry than cubic. This apparent inconsistency is resolved by examining 3D Bragg coherent diffraction images of selected nanocrystals, which show the existence of ≈50 nm-sized domains, which are interpreted as tetragonal twins, and yet cause the average crystalline structure to appear cubic. The ability of these twin boundaries to migrate under the influence of electric fields explains the dielectric anomaly for the nanocrystalline phase.

S6 Two-Dimensional Quantum Materials-Synthesis, theories, properties and applications

S6 – Two dimensional quantum materials: Synthesis, theories, properties & applications

Room: Gold Coin
Session Chairs: Haozhe Wang, Duke University; Cheng Gong, University of Maryland

2:00 PM

(EMA-S6-001-2025) Observations on Transport in Contacts to 2D Semiconductors Using Diverse Contact Structures (Invited)

A. D. Franklin*[1]

1. Duke University, ECE, USA

Most semiconducting nanomaterials would be perfect for use in nanoscale transistors if only the transport between metal contacts and the atomic-scale crystal could be mastered. Over the years, we (speaking both personally for my lab and collectively for the field) have cleaned, damaged, preserved, gapped, removed, and doped the 2D semiconductor beneath the source/drain contacts – so, where does that leave us? While I won't pretend to have a definitive answer, I will offer a few observations from my group. We've observed that intentional damage to MoS_2 and WS_2 immediately prior to contact metal deposition can be beneficial for few-layer films with a few seconds of ion beam exposure. With further ion beam bombardment, we explored clean edge contacts to 2D semiconductors that showed superb and consistent scalability, but at a notable cost to contact resistance – a tradeoff that would have to be carefully managed. Finally, we discovered an intriguing asymmetry in the scaling of top contacts to MoS_2 that suggests greater scalability of the drain-side – perhaps asymmetry worth embracing for 2D transistor technologies. There is much more to understand and improve in the metal-2D interface; these observations will hopefully provide some insights for moving forward.

2:30 PM

(EMA-S6-002-2025) Chemically Functionalized 2D Materials for Quantum Photonic Science and Technology (Invited)

M. C. Hersam*[1]

1. Northwestern University, Materials Science and Engineering, USA

Layered two-dimensional (2D) materials interact primarily via van der Waals (vdW) bonding, which has created opportunities for heterostructures that are not constrained by epitaxial lattice matching. However, since any passivated surface interacts with another via non-covalent forces, vdW heterostructures are not limited to 2D materials alone. In particular, 2D materials can be integrated with a diverse range of other materials, including those of different dimensionality, to form mixed-dimensional vdW heterostructures Furthermore, chemical functionalization allows tailoring of the properties of 2D materials and the degree of coupling across heterointerfaces. In this talk, the prospects of mixed-dimensional heterostructures for quantum photonic science and technology will be discussed with a focus on how chemical functionalization can manipulate and enhance single-photon emission in strained 2D transition metal dichalcogenides. In addition to technological implications, this talk will explore fundamental issues including band alignment, doping, trap states, and charge/energy transfer across heterointerfaces.

3:00 PM

(EMA-S6-003-2025) Materials innovation through single crystalline 2D and 3D nanomembranes: From energy storage to AI hardware (Invited)

S. Bae*[1]

1. Washington University in St Louis, USA

Thin film technology involves the deposition of thin layers of material, typically ranging from a few nanometers to several micrometers thick, onto a substrate. While Silicon has traditionally dominated thin-film innovation due to its mature processing, the demand for higher performance and novel functionalities has spurred the exploration of new materials. Emerging freestanding nanomembranes, including 2D materials and ultrathin 3D nanomembranes, represent a promising avenue for material innovation, offering unique properties and enabling the development of novel devices and the discovery of new physical phenomena. Our team has been at the forefront of material innovation, focusing on the development of freestanding 2D and 3D nanomembranes. We have devised novel methodologies to create these materials, which possess characteristics such as extreme thinness, low stiffness, and low internal stress. These features facilitate easy vertical stacking and 3D integration, making them ideal platforms for exploring new physical phenomena and realizing innovative device architectures through the formation of artificial heterostructures. In this presentation, I will discuss the general principles and their electronic applications from energy storage to AI hardware.

3:30 PM

(EMA-S6-004-2025) Atomristors: Resistance Switching at the Atomic Limit and Low-Energy Electronic Applications (Invited)

D. Akinwande*[1]

1. The University of Texas at Austin, USA

This presentation examines the nonvolatile resistance switching memory effect in two-dimensional (2D) materials, known as atomristors; the atomic limit of memristors. These memory devices exploit defect engineering, particularly the interaction of vacancies and metal adsorption, to achieve nonvolatile memory functionality. The discussion highlights the defect energetics and introduces emerging applications, including zero-power switches for RF, 6G, and THz systems. Atomristors offer high energy efficiency and rapid switching, presenting significant potential for reducing energy consumption in mobile systems, cloud computing, and data centers.

4:00 PM

(EMA-S6-005-2025) Maxwell-Wagner interfacial charge driven MoS_2 synaptic devices and their applications for reservoir computing (Invited)

X. Zhang*[1]

1. Carnegie Mellon University, USA

Synaptic devices with tunable weight hold great promise in enabling non-von Neumann architecture for energy efficient computing. In this work, we present a binary oxide based three-terminal MoS_2 synaptic devices, in which the channel conductance can be modulated by interfacial charges generated at the oxide interface driven by Maxwell-Wagner instability. The binary oxide stack serves both as an interfacial charge host and gate dielectrics. Both excitatory and inhibitory behaviors are experimentally realized, and the presynaptic potential polarity can be effectively controlled by engineering the oxide stacking sequence, which is a unique feature compared with existing charge-trap based synaptic devices and provides a new tuning knob for controlling synaptic device characteristics. The programming channel and reading channel are physically separated and the programming power consumption can be kept constantly low (~50 pW) across a wide dynamic range of 10^5. The MoS_2 synaptic devices show great potential in building a highly efficient reservoir computing system for processing temporal signals at low training cost.

S10 Structure, dynamics and functionalities in high-entropy and compositionality complex oxides

S10- Structure, dynamics, and functionalities in high-entropy and compositionally complex oxides II

Room: Colorado D
Session Chairs: Megan Butala, University of Florida; Thomas Ward, Oak Ridge National Lab

2:00 PM

(EMA-S10-008-2025) Exploring the Landscape of Entropy Stabilized Oxides (Invited)

V. R. Cooper*[1]

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA

Recently, an oxide analogue of high entropy metal alloys comprised of MgO, CoO, NiO, CuO and ZnO was synthesized. These entropy stabilized oxides (ESOs) exhibit a reversible phase transition from a multiphase to a rock salt-ordered single phase compound above 850-900°C. ESOs may engender unique properties, such as high melting temperatures, radiation resistance and other anomalous responses. Here, we discuss a design strategy for the prediction of synthesizable ESOs based on the relationship between pairwise enthalpies of formation, ΔH, and the configurational entropy of the disordered material. A similar chemical identity-to-ΔH map for high entropy alloys was previously employed to correlate the stability of multicomponent metal alloys to the enthalpy of mixing of binary and ternary compounds. Combining these pairwise formation enthalpies with Monte Carlo simulations we explore the temperature dependent phase transitions of these materials. We extend this concept to study the role of oxygen partial pressure; allowing for the synthesis of metastable phases like the recently synthesize Fe-based ESOs. This work presents a roadmap for the discovery of a host of new entropy stabilized materials. Work supported by the U.S. D.O.E., Office of Science, BES, MSED (first principles calculations) and the LDRD Program of ORNL (simulations), managed by UT-Battelle, LLC, for the U. S. DOE using resources at NERSC and OLCF.

2:30 PM

(EMA-S10-009-2025) Oxygen vacancy formation energetics in MgO-based high entropy oxides from DFT and experimental validation

O. Opetubo[1]; T. Shen[1]; R. Bordia[1]; D. Aidhy*[1]

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 (VFEs) 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 the cation charge where significantly low VFEs are observed in Cu-containing oxides due to limited charge transfer from Cu to oxygen. In addition, we find significant lattice distortion and a range of vacancy volumes in these oxides. 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 calculations. This understanding contributes to oxygen vacancy transport useful in microstructure evolution and electrochemical applications.

2:45 PM

(EMA-S10-010-2025) Element-sensitive characterization of high-entropy oxide perovskite thin films (Invited)

A. Farhan*[1]

1. Baylor University, Department of Physics, USA

Employing the entropy-driven stabilization concept into the perovskite structure showed first promising results demonstrating the potential unlimited freedom in designing ferroic properties in high-entropy oxide perovskite (HEOP) thin films. Here, I will show how element-sensitive characterization with x-ray absorption spectroscopy (XAS), employing x-ray magnetic circular- and linear dichroism (XMCD and XMLD) can shed light into how each transition metal element contributes to the overall ferroic order in HEOP thin films with a primary focus on rare-earth-based R(Ni0.2Co0.2Fe0.2Mn0.2Cr0.2)O2 (R: Tb, Lu and Dy). The results highlight the important role of elevated Co2+ concentrations, likely iduced via strain, in introducing long-range ferromagnetic order and the occurrence of spin-reorientations in Dy-based HEOPs.

3:15 PM

(EMA-S10-011-2025) Magnetism in bulk iron-base rocksalt high-entropy oxide

R. Hermann*[1]; M. Manley[1]; J. Yan[1]; D. Moseley[1]; S. Calder[1]; D. Abernathy[1]; B. Winn[1]

1. Oak Ridge National Laboratory, USA

Rocksalt high entropy oxides based on transition metals have, to date, found only two realizations in (Mg,Co,Ni,Cu,Zn)O (i.e. ‘J14’) and (Mg,Mn,Fe,Co,Ni)O, though a larger family of materials has been predicted. We have investigated magnetism in (Mg,Mn,Fe,Co,Ni)O by neutron diffraction and spectroscopy and my Mossbauer spectroscopy. In contrast to ‘J14’ the iron-manganese based material exhibits a twice larger Néel temperature near 200 K that can be rationalized by a larger fraction of magnetic elements and larger average spin. The propagation vector is (1/2,1/2,1/2) similar to NiO. Mossbauer spectral data reveals a discrete distribution of near neighbor environments for magnetic coupling. Calorimetry shows a clear lambda-transition which provides information on the magnetic entropy across the phase transition. Work supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division. This research used resources at the Spallation Neutron Source and at the High Flux Isotope Reactor, facilities supported by DOE, BES, Scientific User Facilities Division.

4:00 PM

(EMA-S10-012-2025) Entropy-stabilized oxide memristors for efficient data processing (Invited)

S. Chae*[1]

1. Oregon State University, School of Electrical Engineering and Computer Science, USA

Energy demand by computation is growing exponentially with the emergence of machine learning (ML) technology. While conventional computers have memory and processing units segregated, memristor arrays are a promising computing platform which provides reduced data path for efficient data processing in machine learning tasks. However, memristors based on traditional amorphous oxides suffer from device stochasticity and a lack of tunability which limits applications requiring adaptive networks. Here I present entropy-stabilized oxide (ESO) memristors where tunable transport and memristor dynamics are allowed by tunable defect formation via composition control. Systematic control of characteristic decay time constants in ESO memristors allows the implementation of task-specific reservoir computing neural network with improved energy efficiency for temporal data processing. While rocksalt-(Mg,Ni,Co,Cu,Zn)O entropy-stabilized oxide memristors exhibit short-term memory effects, I will present new composition systems that enable long-term memory effects such as entropy-stabilized chalcogenides and structures beyond rocksalt.

4:30 PM

(EMA-S10-013-2025) Resolving Local Structure of Pb-based High Entropy Perovskites via Combined X-ray and Neutron Fitting

J. Barber*[1]; Y. Son[2]; S. Trolier-McKinstry[2]; C. M. Rost[1]

1. Virginia Polytechnic Institute and State University, Materials Science and Engineering, USA
2. The Pennsylvania State University, Materials Science and Engineering, USA

Understanding the local structure of high entropy perovskites is crucial for understanding the polarization mechanisms across the material. The electrocaloric effect (ECE) offers a promising method for efficient refrigeration, with significant ECE observed in lead zirconate-titanate (PZT) thin films and relaxor ferroelectrics. PZT-based perovskites were synthesized with a compositionally disordered B-site occupied by Hf, Zr, Ti, Nb, and either Fe or Sc (Pb(HfZrTiNbX)0.2 O3, X=Fe, Sc), exhibiting relaxor behavior in P-E hysteresis loops indicative of polar nanoregions. X-ray absorption spectroscopy (XAS) collected at the Advanced Photon Source, Argonne National Lab, characterized the local geometry of hafnium, zirconium, and niobium. Neutron total scattering data from the Spallation Neutron Source, Oak Ridge National Laboratory, provided absolute atomic positions within the compound. Combined fitting of these datasets reveals local structure trends based on B-site cation species, offering insights into the material’s behavior and potential applications in cooling technologies.

4:45 PM

(EMA-S10-014-2025) Unraveling the Local Disorder in High Entropy Oxides with XAFS and DFT-Assisted Analysis

G. R. Bejger*[1]; M. Caucci[2]; J. Sivak[2]; L. Anderson[1]; J. Maria[2]; S. Sinnott[2]; C. M. Rost[1]

1. Virginia Polytechnic Institute and State University, Materials Science and Engineering, USA
2. The Pennsylvania State University, USA

High entropy oxides (HEOs) have garnered increasing attention in the scientific community since the original synthesis of $(MgCuCoZnNi)_{0.2}O$ (J14) in 2015 due to their unique properties and potential applications in catalysis, energy storage, and electronic materials. However, the analysis of these HEOs is difficult because of their high configurational disorder and inherent complexity. One of the primary techniques used to investigate these materials is X-ray absorption fine structure (XAFS) measurements. XAFS is invaluable for probing the electronic structure of individual cations within the material, providing insights into the local environment, bond lengths, and electronic states of each constituent element. This technique is especially useful for studying HEOs since their complex and disordered nature makes traditional characterization methods insufficient for capturing the full extent of their atomic-scale interactions. To aid the experimental analysis of X-ray absorption near edge structure (XANES) spectra, theoretical simulations based on density functional theory (DFT) and the FEFF9 software have been employed. By incorporating a fitting software, the effects of local distortions on the simulated XANES spectra are systematically investigated and compared to experimental data, advancing our understanding of how structural disorder influences the electronic properties of HEOs.

5:00 PM

(EMA-S10-015-2025) Local and Average Crystallographic and Magnetic Structure and Magnetic Dynamics in Compositionally Complex Perovskite Oxides

N. Arndt*[1]; B. L. Musicó[2]; K. Sahebkar[1]; K. Puri[1]; L. Pattison[1]; G. Young[1]; R. Baral[3]; J. Paddison[3]; Q. Zhang[3]; A. Mazza[4]; V. Keppens[2]; T. Z. Ward[3]; S. Calder[3]; R. Need[5]; M. M. Butala[1]

1. University of Florida, Materials Science and Engineering, USA
2. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science and Engineering, USA
3. Oak Ridge National Laboratory, USA
4. Los Alamos National Lab, USA
5. University of Florida, USA

Large configurational disorder in compositionally complex oxides (CCOs) can be leveraged to synthesize unique functional properties by extending the already rich composition-structure-property phase space found in complex oxides. In particular, previous work on CCOs has shown the formation of mixed phase magnetic structures and the tunning of magnetic and electronic properties. In this study, we have focused on determining the effect of compositional disorder on the local and average crystallographic and magnetic order in disordered ABO_3 perovskites. We alloyed perovskites with A-site dopants, (5A) = $La_{0.2}Nd_{0.2}Pr_{0.2}Tb_{0.2}Y_{0.2}$, that average to the ionic radii and unpaired magnetic moment of Nd^{3+}. Using a combination of bulk magnetometry, temperature-dependent neutron diffraction, and pair-distribution function analysis of neutron total scattering we have determined the ground state average magnetic and crystallographic order as well as the local ordering of our $(5A)BO_3$ materials, B = Fe and Mn. To elucidate the interplay between the type of compositional complexity, magnetic or ionic size, and crystallographic site alloyed, we have compared the $(5A)BO_3$ materials to undisordered $NdBO_3$ analogs. This work lays the groundwork for structure-property relationships that can guide rational design in the functionalizing of CCOs.

S11 Complex oxide thin films and heterostructures- from synthesis to strain/interface-engineered emergent properties

S11- Freestanding Metal Oxide Membranes

Room: Colorado A
Session Chair: Ludi Miao, New Mexico State University

2:00 PM

(EMA-S11-001-2025) Atomic scale imaging of freestanding oxide membranes (Invited)

S. Hong*[1]

1. University of California, Davis, USA

The unique electromagnetic properties of complex oxides are often closely linked to their lattice structures. Imaging these structures is essential for understanding the functionalities that arise from structural phase transitions. Freestanding oxide membranes provide an ideal platform for studying these transitions via electron microscopy due to the absence of bulk substrates. This presentation will discuss early examples of atomic-scale imaging of phase transitions in oxide membranes, with an emphasis on topotactic phase transitions between metallic ferromagnet and insulating antiferromagnet. Advanced electron microscopy imaging reveals the delicate balance between strain, oxygen transport, and domain structures.

2:30 PM

(EMA-S11-002-2025) Advanced Strain Engineering for Large-Area Freestanding Ti-Based Metal Oxide Membranes

H. Rostaghi Chalaki*[1]; D. Kamleshkumar[1]; J. Tindal[1]; D. Lee[1]

1. University of South Carolina, Mechanical Engineering, USA

Freestanding oxide membranes provide remarkable structural tunability and flexibility for next-generation electronic devices. Among the various fabrication methods, using a water soluble sacrificial layer facilitates the creation and manipulation of freestanding oxide membranes. However, producing large-area membranes free of cracks and wrinkles remains challenging. The quality of these membranes is strongly dependent on the choice of supporting layers and sacrificial layers. Here, we show a novel method for fabricating large-area oxide membranes free from cracks and wrinkles by precisely controlling the thickness of supporting layers and epitaxial strain between the membrane and sacrificial layer. Engineered sacrificial layers combined with a polypropylene carbonate support enable precise control of epitaxial strain in three oxide membranes: $La_{0.7}Ca_{0.2}Ni_{0.25}Ti_{0.75}O_3$, $SrTiO_3$, and $Sr_{0.95}Ti_{0.76}Ni_{0.05}Nb_{0.19}O_3$ during the growth, releasing, and transfer processes. High-resolution X-ray diffraction and reciprocal space mapping reveal detailed strain engineering in these heterostructures. Finally, through strain relaxation and support layer flexibility, we successfully fabricate 5 x 5 mm membranes without cracks and wrinkles. Our findings establish a foundation for further exploration of strain engineering in transferred oxide membranes and innovative transfer techniques for a wide range of oxides.

2:45 PM

(EMA-S11-003-2025) Emerging phase transitions in sodium niobate heterostructures and membranes (Invited)

R. Xu*[1]

1. North Carolina State University, USA

Sodium niobates ($NaNbO_3$), known as the most structurally complex perovskite oxide material, exhibits a wide variety of structural phases with distinct symmetries, ferroic orders, and oxygen octahedral tilts. The intricate energy landscape of these phases presents unique opportunities to induce and control phase transitions via external stimuli. In this presentation, I will present our recent work on $NaNbO_3$ heterostructures and membranes, highlighting their enormous potential as a platform for emerging phase transitions and enhanced susceptibilities. We demonstrate a strain-induced mixed-phase state, where competing monoclinic distorted ferroelectric phases coexist, akin to strain-induced morphotropic phase boundary in $BiFeO_3$. The structural instability near the emerging phase boundaries in $NaNbO_3$ heterostructures leads to significantly enhanced ferroelectric and dielectric properties. Furthermore, we investigate the intrinsic size dependence of antiferroelectricity in freestanding $NaNbO_3$ membranes by decoupling substrate effects. Through a combination of experimental and theoretical approaches, we reveal an intriguing surface-driven antiferroelectric-to-ferroelectric transition as membrane thickness decreases, resulting in a mixed-phase state with coexisting ferroelectric and antiferroelectric phases.

S11- Emergent phenomena in complex oxide thin films I

Room: Colorado A
Session Chair: Xin Xu, Arizona State University

4:00 PM

(EMA-S11-004-2025) Two-dimensional magnetic monopole gas at oxide interfaces (Invited)

L. Miao*[1]; Y. Lee[2]; P. Timsina[1]; M. Lawler[3]; K. M. Shen[4]

1. New Mexico State University, Physics, USA
2. Cornell University, USA
3. Binghamton University, USA
4. Cornell University, Physics, USA

Magnetic monopoles have been proposed as emergent quasiparticles in spin ice compounds (e.g. $R_2Ti_2O_7$, R = Dy, Ho). However, up to date, all the experimental researches have been focused on ensembles comprised of equal number of monopoles and antimonopoles in bulk spin ice crystals. In this project, we proposed the formation of a novel two-dimensional monopole gas (2DMG) that can carry a net magnetic charge, at the interface between a spin-ice compound (e.g. $R_2Ti_2O_7$, R = Dy, Ho) and an isostructural antiferromagnetic (AFM) pyrochlore iridate (e.g. $R_2Ir_2O_7$). The 2DMGs display a lot of other exciting properties including metallic behavior, gate controllability, and an exotic entropy-induced two-dimensionality. These results not only represent the first magnetically charged system in condensed matter physics, but also provide a completely new and exciting platform to study fundamental physics about monopoles as well as to develop future monopole devices.

4:30 PM

(EMA-S11-005-2025) Emergent tunability in polar vortices

N. Orloff*[1]; F. Bergmann[1]; P. Meisenheimer[2]; S. Das[2]; R. Ramesh[3]

1. NIST, Communications Technology Laboratory, USA
2. University of California Berkeley, USA
3. Rice University, USA

Superlattice films of layers of $PbTiO_3$ and SrTiO3 form polar vortices under the right lattice periodicity conditions. Low frequency and terahertz experiments observed both negative permittivity and interesting collective dynamics that could lead to other emergent behavior. Gigahertz complex permittivity data could provide a new insight into polar vortices dynamics and how emergent behavior develops with periodicity, but the measurements present challenges given the anisotropic nature of these complex thin films. Here, we present our dielectric spectroscopy data and theory to explain the emergence of tunability in polar vortices. Our experiment tested 12 different 100 nm thick films with periodicities to understand how dispersion and tunability emerge with the formation of polar vortices. Taken together, these results provide new insights into the high frequency dynamics of polar vortices and how they may lead to new devices.

4:45 PM

(EMA-S11-006-2025) Observation of high out-of-plane tunability and low loss in Ruddlesden-Popper films

F. Bergmann*[2]; S. Freed[2]; M. Papac[2]; M. R. Barone[1]; Z. Tian[3]; A. Ross[4]; D. Schlom[1]; N. Orloff[2]

1. Cornell University, Department of Materials Science and Engineering, USA
2. NIST, Communications Technology Laboratory, USA
3. University of California Berkeley, USA
4. The Pennsylvania State University, USA

Microwave circuits like tunable filters and phase shifters rely on high tunability and low loss dielectrics. About a decade ago, scientists observed a record-breaking combination of high in-plane tunability and low loss in strained Ruddlesden-Popper phase $Ba_xSr_{1-x}TiO_3$ thin films at microwave frequencies. However, most voltage-tunable devices employ out-of-plane geometries, hindering the implementation of Ruddlesden-Popper films in microwave circuits. Still, theory predicts that engineering strainless Ruddlesden-Popper phase $Ba_xSr_{1-x}TiO_3$ with a high barium content should result in high out-of-plane tunability. Here, we report on measuring this high out-of-plane tunability in Ruddlesden-Popper phase $Ba_xSr_{1-x}TiO_3$ thin films and show that we can engineer the Ruddlesden-Popper phase to result in low dielectric loss at microwave frequencies. This result shows that Ruddlesden-Popper phase dielectrics can indeed be tunable out-of-plane while retaining their low dielectric loss. Our observations set a new benchmark for low loss out-of-plane tunable microwave dielectrics.

5:00 PM

(EMA-S11-007-2025) Topotactic redox reactions in thin film transition metal oxides (Invited)

J. Fowlie*[1]

1. Northwestern University, USA

Topotactic redox reactions have emerged as a promising pathway to engineer novel crystal phases. In these reactions, oxygen anions can move in an out of the crystal while the cation sublattice remains intact -- effectively oxygen breathing. Centering the discussion on nickel oxides, iron oxides, and others, I will discuss some of the prospects, as well as some of the limitations, of the approach.

S12 Advanced semiconductors and microelectronics

S12- Semiconducting thin films II

Room: Colorado G
Session Chairs: Hua Zhou, Argonne National Lab; Chonglin Chen, University of Texas San Antonio

2:00 PM

(EMA-S12-009-2025) II-VI based organic-inorganic hybrid superlattices: structure, stability, properties, and potential applications (Invited)

Y. Zhang*[1]

1. UNC Charlotte, ECE, USA

A group of II-VI organic-inorganic hybrid nanostructures have been shown to exhibit nearly perfect crystal structures, manifesting as high crystallinity comparable to that of a high quality III-V or II-VI binary and better than any known semiconductor superlattices. For instance, β-$ZnTe(C_2N_2H_8)_{0.5}$ exhibits a 20-30″ XRD rocking-curve linewidth, below 1 cm^{-1} low-temperature Raman linewidth, and band-edge free exciton emission (3.56 eV) without below-bandgap emission. More interestingly, it offers various highly desirable properties, e.g., room temperature excitonic emission due to a large exciton binding energy around 300 meV, strongly enhanced optical absorption as high as 10^6 cm^{-1}, close to 100% internal quantum efficiency in room-temperature photoluminescence, zero-thermal expansion over a broad temperature range, and much reduced density and dielectric constants. Uniquely, it is the only hybrid crystalline structure that exhibits an over-15-year shelf life, benefiting from a large formation energy and kinetic barrier. On the one hand, it offers a new approach to form perfect heterostructures beyond the conventional wisdom of requiring lattice match; on the other hand, the novel properties suggest many potential applications, such as room-temperature exciton-polariton condensation, efficient UV emission and detection, transparent p-type conductive material.

2:30 PM

(EMA-S12-010-2025) The role of interface in mixed dimensional van der Waals heterostructures (Invited)

M. Cotlet*[1]

1. Brookhaven National Laboratory, Center for Functional Nanomaterials, USA

We discuss mixed dimensional heterostructures incorporating atomically thin van der Waals materials as potential active nanostructures for optoelectronic applications. We address the importance of the heterostructure interface in providing the desired optoelectronic function, and how this can be achieved using bandgap engineering. Specifically, I will be discussing mixed heterostructures based on TMDs, quantum dots and perovskites and the realization of photodetectors and valleytronic devices.

3:00 PM

(EMA-S12-011-2025) Anisotropic Semiconductors for Infrared Opto-electronics (Invited)

J. Ravichandran*[1]

1. University of Southern California, Chemical Engineering and Material Science, USA

Infrared opto-electronics is at crossroads, where very mature II-VI and thermal detector technology dominates the detector markets with much of the focus on the scaling and device advances over materials. Nevertheless, the sustained growth of infrared optoelectronics relies on the development of novel materials with additional functionalities in the modulation and sensing of infrared light. To this end, in this talk, I will introduce a new class of materials known as quasi-1D hexagonal chalcogenides as a new semiconducting platform with large optical anisotropy in the mid- and long-wave infrared energies. First, I will discuss the origin of large linear optical anisotropy in $BaTiS_3$ in terms of birefringence, dichroism. Second, I will discuss the role of modulations in $Sr_{1+x}TiS_3$ towards dramatic improvements in the optical anisotropy. Lastly, I will also discuss our efforts in understanding the anisotropic photoconductance response towards polarization sensitive infrared detection. Finally, I will provide a general outlook for future studies and applications of these exciting new class of materials.

S12- Characterization and applications of semiconducting materials

Room: Colorado G
Session Chairs: Ruijuan Xu, North Carolina State University; Aiping Chen, Los Alamos National Lab

4:00 PM

(EMA-S12-012-2025) Dielectric Screening and Breakdown of 2D Hybrid Organic-Inorganic Perovskites (Invited)

Q. Tu*[1]

1. Texas A&M University System, Materials Science and Engineering, USA

2D hybrid organic-inorganic perovskites (HOIPs) have emerged as promising low-cost, high-performance direct bandgap semiconductor materials in a plethora of energy and electronic applications. Understanding the interaction of 2D HOIPs with charges and electric field is crucial for device engineering and device design for durable applications. In this talk, I will show our most recent results on the dielectric screening and dielectric breakdown of 2D HOIPs investigated by advanced scanning probe techniques, using a prototypical family of 2D HOIPs, $(BA)_2MA_{n-1}Pb_nI_{3n+1}$ (BA = butylammonium, MA = methylammonium cation, and n = 1 to 5) as model examples. First, we will show the screening length study of 2D HOIPs by Kelvin probe force microscopy and its dependence on the structural parameters of 2D HOIPs to shed light on the fundamental mechanism behind the screening behavior of these materials when interfaced with charged impurities and molecular dipoles. We further employ conductive AFM to investigate the dielectric breakdown of 2D HOIPs under various loading conditions and quantify the thickness-dependent dielectric breakdown strength of these materials as well as the underlying stochastic behavior of the breakdown behavior. The talk will be concluded by a discussion of guidelines and potential applications derived from these studies.

4:30 PM

(EMA-S12-013-2025) Nanovolumetric Surface Milling and Tomography of Functional Materials Properties: Pushing the Limits (Invited)

K. Lizu[1]; K. Del Cid-Ledezma[1]; A. Akoma[1]; A. Chen[2]; B. Huey*[1]

1. University of Connecticut, Materials Science and Engineering, USA
2. Los Alamos National Lab, USA

Variants of Atomic Force Microscopy have long been leveraged to probe surfaces, or for basic lithographic patterning, in order to investigate local materials properties and device functionalities in incessantly shrinking microelectronics and other advanced semiconductor systems. However, current and future devices increasingly depend upon 3-dimensional designs and functionalities. Recent AFM advances enable truly Angstrom scale depth control during nanopatterning, while novel nano-volumetric property mapping can also be achieved via in situ polishing and AFM to effectively achieve tomography. Examples proving Angstrom scale depth control in single crystals, epitaxial thin films, superlattices, and polycrystalline ceramics are shared, extending the resolution limits in X, Y, and Z. Primarily focused on piezoelectricity and conductivity, mechanical strength is also assessed even including the shear strength of interfaces in layered structures.

5:00 PM

(EMA-S12-014-2025) Engineering antiphase domain boundaries boosted tunable ferromagnetic insulation

X. Jia[1]; Y. Chen[1]; C. Nan[1]; J. Ma[1]; C. Chen*[2]

1. Tsinghua University, China
2. University of Texas San Antonio, Physics, USA

Interface-engineered superlattices composed of perovskite $PrCoO_3$ and brownmillerite $CaCoO_{2.5}$ ($[(PCO)_n/(CCO)_n]_m$) were designed and fabricated on (001) $SrTiO_3$ substrates with integrated antiphase domain boundaries (APBs) for investigating ferromagnetic insulating phenomenon. The APBs were formed at the surface-step-terrace edges and the densities of APBs can be regulated by the periods of the superlattices. In these superlattices, ferromagnetic insulating properties were found to be significantly modulated by the APBs. The room-temperature resistivity of the n = 1 superlattice increases by more than three orders of magnitude than that of the n = 5 superlattice and more than five orders of magnitude than that of the $Pr_{0.5}Ca_{0.5}CoO_{3-\delta}$ alloy films. The insulation behavior is primarily derived from the charge carriers scattering at the APBs, which block the charge carriers transferring along the in-plane direction. These results could propel the advancement of multifunctional material genetics and provide a strategic approach for the development of artificial materials with tunable properties.

5:15 PM

(EMA-S12-015-2025) De-embedding interconnects from mmWave flip-chip integrated photodiodes

A. Osella*[1]; B. Bosworth[2]; N. Jungwirth[2]; A. Feldman[2]; N. Orloff[2]

1. Colorado School of Mines, Metallurgy and Materials Engineering, USA
2. NIST, Communications Technology Laboratory, USA

6G technologies are pushing electronics and materials testing into mmWave (30 GHz - 300 GHz) and low THz regime, however, conventional up-conversion methods are band limited and noisy. We have previously presented a method for signal generation that relies on flip-chip integration of photodiodes onto lithographically patterned, electrooptic waveguides for low-noise, high power signal generation in the hundreds of GHz. While this method proved to be more broadband than traditional vector network analyzer extender heads, the on-wafer reference plane poses challenges such as de-embedding the bonding interconnect from the photodiode performance. This work focuses on characterizing, diagnosing, and correcting for the effects of those interconnects.

5:30 PM

(EMA-S12-016-2025) Study of an enhanced photocatalytic hybrid semiconductor Z-scheme ZnO@CdS nano heterojunction for efficient H_2 Production ***WITHDRAWN***

A. Ali*[1]; K. Kang[1]

1. Kyungpook National University, Physics, Republic of Korea

Nano heterojunctions of hybrid semiconductor metal oxide offer a platform to enhance visible light absorption and improve the efficient separation of photogenerated charges, which is crucial for maximizing the potential of metal oxides in photocatalytic water splitting for H_2 production. These materials can absorb a broad range of light wavelengths, enabling the separation and migration of charge carriers necessary for efficient water splitting. In this study, we synthesized ZnO@CdS nano-heterostructures with varying weight percentages, effectively combining the wide bandgap of ZnO with the narrow bandgap of CdS to amplify photocatalytic efficiency. These advanced heterostructures demonstrated significant improvements in light absorption and charge separation. The optimized sample achieved H_2 production rates of 3.91 times higher than pure ZnO rods and 3.22 times higher than CdS nanoparticles. Using various techniques, we thoroughly examined the ZnO@CdS nano heterojunction, investigating their crystal structure, chemical state, elemental composition, morphology, bandgap energy, and photocatalytic charge transfer mechanisms. Our work employed a straightforward sol-gel method under ambient pressure and low temperatures, offering a cost-effective and scalable approach for large-scale H_2 production.

S13 Defects and transport in ceramics

S13- Defects and Transport in Ceramics II

Room: Colorado H
Session Chairs: Till Frömling; Di Chen, Tsinghua University

2:00 PM

(EMA-S13-008-2025) Electric Field Effects on Defects Transport and Microstructural Evolution (Invited)

J. Luo*[1]

1. University of California, San Diego, USA

In a series of our earier studies, we have investigated the mechanisms of flash sintering and ultrahigh heating rates, on the order of ~100 K/s, can enable ultrafast sintering with and without applied electric fields. Although we have demonstrated that ultrafast sintering can be achieved without an electric field, we have observed a spectrum of electric field induced defects transport and microstructural evolution phenomena in flash-sintered specimens. Subsequently, we conducted controlled experiments to investigate how applied electric fields alter defects and microstructures at high temperatures. Notably, we observed an electrochemically induced grain boundary disorder-to-order transition in Bi_2O_3-doped ZnO to trigger abnormal grain growth, along with a spectrum of other defect transport phenomena. A more recent study created continuously graded microstructures in ZnO via polarizing the point defects distributions from the anode to the cathode and electrochemically altering grain boundary complexions. Other unpublished results on $SrTiO_3$ and $BaTiO_3$ will also be presented and discussed.

2:30 PM

(EMA-S13-009-2025) Characterization of Interfaces in Ceramics- From "Conventional" Hard Ceramics to Sensitive and Softer Systems (Invited)

H. Sternlicht*[1]; A. M. Minor[3]; N. P. Padture[2]

1. The Pennsylvania State University Department of Materials Science and Engineering, USA
2. Brown University, School of Engineering, USA
3. University of California, Berkeley, Department of Materials Science and Engineering, USA

Characterization of interfaces via direct measures, such as electron microscopy, plays an important role in gaining an ability to alter properties according to demand. For example, understanding the mechanism of grain boundary motion is important for both fundamental and applied issues related to microstructural evolution of materials, such as the role of grain boundary atomistic structure on growth, and controlling the grain size of polycrystalline material systems in order to optimize their engineering properties. Recently anisotropic disconnections (line defects with a step and/ or a dislocation component) were detected at general grain-boundaries in $SrTiO_3$ and ß-$Yb_2Si_2O_7$, and disconnection motion was experimentally shown to be the mechanism of grain growth at general and high symmetry grain-boundaries. However, when addressing sensitive ceramic systems, similar or equivalent characterization is not always possible. In this talk I will highlight challenges associated with the characterization of sensitive ceramic systems using electron microscopy, as well as recent progress in addressing those challenges. Systems such as hybrid halide perovskites for solar cells and Li-ion batteries will be addressed.

3:00 PM

(EMA-S13-010-2025) Evolution of defects and disorder at epitaxial Fe_3O_4 / Cr_2O_3 and Fe_2O_3 / Cr_2O_3 interfaces under irradiation

T. Kaspar*[6]; M. Liedke[2]; K. Yano[1]; J. Christudasjustus[6]; B. Matthews[1]; M. Bowden[6]; C. Ophus[3]; H. Kim[4]; Y. Wang[4]; G. Sterbinsky[5]; D. Schreiber[1]

1. Pacific Northwest National Laboratory, Energy and Environment Directorate, USA
2. Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, Germany
3. E O Lawrence Berkeley National Laboratory, NSEM, Molecular Foundry, USA
4. Los Alamos National Laboratory, Materials Science and Technology Division, USA
5. Argonne National Laboratory, Advanced Photon Source, USA
6. Pacific Northwest National Laboratory, Physical and Computational Sciences Directorate, USA

Disordering processes in oxide materials are complicated by the presence of interfaces, which can serve as either point defect sinks or accumulation sites; the response depends on factors such as interfacial structure, chemistry, and termination. We have characterized the point defect evolution and disordering of epitaxial $Fe_3O_4(111)$ / $Cr_2O_3(0001)$ and $Fe_2O_3(0001)$ / $Cr_2O_3(0001)$ thin film heterostructures after ion irradiation at room temperature. The density of misfit dislocations in both the Fe_3O_4 and Cr_2O_3 layers are varied by changing the thickness of Cr_2O_3 to be pseudomorphically strained to the Al_2O_3 (0001) substrate (5 nm thick), or partially relaxed (20 nm thick). In both cases, irradiation leads to damage accumulation on the Fe_3O_4 side of the heterointerface, and the interface with more misfit dislocations exhibits faster disordering and Fe reduction compared to the less-defective interface. Positron annihilation spectroscopy (PAS) of heterostructures after irradiation reveals different defect evolution pathways in Fe_3O_4 compared to Cr_2O_3, impacting lattice strain. PAS of Fe_2O_3 / Cr_2O_3 and Cr_2O_3 / Fe_2O_3 heterostructures after irradiation of the top film facilitates the investigation of point defects crossing the interface.

3:15 PM

(EMA-S13-011-2025) Effects of Electronic Energy Loss on Defect Production and Evolution in Oxide Perovskites under Ion Irradiation

W. J. Weber*[1]

1. University of Tennessee, Materials Science & Engineering, USA

Oxide perovskites (ABO_3) exhibit fascinating properties that identify them as key materials for the next generation of multifunctional devices, and ion-beam modification can be used to tune their functionality. Further, these devices may be exposed to extreme irradiation environments. It is well-established that atomic-level defects are created by elastic energy transfer (nuclear energy loss), S_n, from charged particles to atomic nuclei; however, the effects of inelastic electronic energy loss, S_e, to target electrons are more complicated. At low energies, where S_n dominates, radiation damage by elastic collision processes often leads to phase transformations, such as amorphization. When S_e is comparable to S_n, ionization-induced annealing can occur along the ion trajectory, reducing the rate of defect accumulation. High-energy ions with S_e values above a threshold can form amorphous nanotracks due to melt-quenching along the ion trajectory. In the presence of pre-existing defects, amorphous tracks are formed at much lower values of S_e, and the track size increases with S_e and the density of pre-existing defects. Below the threshold for amorphous track formation, ionization-induced annealing of defects is observed. Experimental and molecular dynamics results on $SrTiO_3$, $KTaO_3$ and $LiTaO_3$ will be presented to demonstrate these phenomena.

S13- Defects and Transport in Ceramics III

Room: Colorado H

Session Chairs: Tiffany Kaspar, Pacific Northwest National Lab; Hadas Sternlicht, The Pennsylvania State University Department of Materials Science and Engineering

4:00 PM

(EMA-S13-012-2025) Optoionics – A New Opportunity for Ionic Conduction-Based Radiation Detection (Invited)

T. Defferriere*[1]; C. Gilgenbach[1]; M. Muller[2]; J. F. Christian[2]; J. LeBeau[1]; H. L. Tuller[1]

1. Massachusetts Institute of Technology, Material Science and Engineering, USA
2. Radiation Monitoring Devices Inc, USA

We recently showed that photogenerated charge carriers could modulate the grain boundary resistance of a model oxygen conducting solid electrolyte (Gd-doped CeO_2). These findings were inspired by the recognition that above-bandgap light is known to reduce band bending at interfaces by providing additional charge carriers that screen potential barriers. While initially demonstrated on thin films, we then showed that we could reproduce a similar optoionic effect in a bulk pellet (1 mm thick) and achieve reversible resistance modulations on the order of ~1000 near room temperature. In this talk, I will discuss how our findings demonstrate a new radiation detection concept that relies on the modulation of ionic currents at grain boundaries in solid electrolytes instead of the collection of photogenerated charge carriers in single crystalline semiconductors. This paves the way for new, inexpensive, low-power, and miniaturizable solid-state detection devices that can operate in harsh environments. I will discuss our approaches for engineering impedance, radiation sensitivity, and response time with the aim of achieving high-performance detection. This phenomenon is an example of the rapidly developing field of Opto-ionics and is expected to apply to other kinds of ion-conducting solid electrolytes (Li^+ or H^+), thus opening opportunities for a broad new class of radiation detecting materials.

4:30 PM

(EMA-S13-013-2025) Light-Driven Stoichiometry Changes in a Non-Dilute, Mixed Conducting Perovskite Thin Film

E. J. Skiba[1]; H. Buckner[1]; C. Lee[1]; G. E. McKnight[1]; R. Wallick[1]; R. van der Veen[2]; E. Ertekin[1]; N. H. Perry*[1]

1. University of Illinois Urbana-Champaign, USA
2. Helmholtz Zentrum Berlin, Germany

The emerging field of photo-ionics offers the potential to direct ions with high spatial and temporal resolution using light. However, effects have been demonstrated in only limited prototype materials. E.g., intermediate-temperature UV-driven oxygen fluxes in single-crystal $SrTiO_3$ have been reported, but there are challenges in isolating mechanisms in that geometry with non-uniform light absorption. To clarify mechanisms and identify technologically-relevant, non-dilute responsive materials, we grew thin-film, mixed-conducting $SrTi_{1-x}Fe_xO_{3-d}$ (STF), x=0.07 and 0.35, using PLD. Films exhibited visible optical transmission relaxations at low-intermediate temperatures when exposed to either steps in pO_2 or steps in UV fluence (on/off), with equal time constants, suggesting UV-driven oxygen incorporation from the gas phase with surface-exchange-limited kinetics. Films capped with UV-transparent but O_2-blocking coatings exhibited no response to UV nor pO_2 steps. DFT simulations showed that oxygen vacancies and vacancy associates are more difficult to form when light excitation splits the Fermi level into quasi Fermi levels. Ultrafast pump-probe spectroscopy revealed long excited state lifetimes in these compositions, with the longer lifetime of x=0.07 corresponding to larger relative changes in hole and oxygen concentrations. Considerations for composition selection will be addressed.

4:45 PM

(EMA-S13-014-2025) Dynamic thermo-chemical interactions in Ni-rich layered cathodes for Li-ion batteries (Invited)

D. Hou*[1]

1. Clemson University, Materials Science and Engineering, USA

A long pursuit in developing high-energy batteries is the prognosis and improvement of thermal stability. Here, we report new understandings of the thermo-chemical transformation mechanism of delithiated Ni-rich cathodes. Our in situ measurements resolve the dynamic thermo-chemical interactions inside delithiated particles, illustrating the correlation between thermal performance and spatial distribution of various thermo-chemical interactions. Statistical analyses of thermally active and sluggish regions in cathode particles show that these minority regions govern thermal stability. We propose effective strategies to manipulate thermo-chemical interaction dynamics and to minimize the propagation of thermally active regions in these battery materials.

5:15 PM

(EMA-S13-015-2025) First principles investigations of the electronic properties of defects and impurities in 3C-, 4H-, and 6H-SiC

M. N. Huda*[1]; S. R. Jhilik[1]; N. D. Alkhaldi[2]

1. The University of Texas at Arlington, Physics, USA
2. ndawasalkhaldi@uhb.edu.sa, Department of Science and Technology, Saudi Arabia

Defects and impurities significantly impact semiconductors' electrical, thermal, optical, and transport properties. Unintentional impurities and defects, such as vacancies and impurities, can significantly impact the performance and reliability of semiconductor devices. Silicon carbide (SiC) is a wide-bandgap semiconductor known for superior properties like high breakdown electric field strength, carrier mobility, and thermal conductivity. Its applications can be found in, for example, power semiconductor devices, quantum technologies, photoconductive switches, radiation detectors, and optical detectors. SiC has over 200 polymorphs, among them 3C-, 4H-, and 6H-SiC being the most used polymorphs for device applications. A comprehensive understanding of impurities and defects is crucial for achieving the full potential of SiC semiconductors. Intentional doping is common, like using nitrogen (N) and aluminum (Al) for n-type and p-type doping in SiC, respectively. We will present our study of defects, such as combinations of vacancies, substitutional, anti-site defects, etc. in these three polymorphs of SiC. Charge density localizations, calculated with post-density functional theories will be presented. Changes in electronic transport properties due to these defects and impurities will be discussed as well.

S15 High-Performance computational design and discovery of electronic materials

S15- Computational Material Design and Discovery

Room: Matchless
Session Chairs: Christian Carbogno, Fritz-Haber-Institut der Max-Planck-Gesellschaft; Kayahan Saritas

2:00 PM

(EMA-S15-001-2025) From BIG-data to HOT-extreme-properties of high-entropy carbides, carbo-nitrides and borides (Invited)

S. Curtarolo*[1]

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

The need for improved functionalities in extreme environments is fueling interest in high-entropy ceramics. While resilient compositions can be stabilized by maximizing entropy, still the search for new systems is mostly performed with trial-and-error and phenomenological 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 disordered systems. In this presentation I will address many of the problems/solutions in the discovery of disordered ceramics, offer some data-based effective solutions, and discuss the avenues opened by the latter, especially for plasmonic-hyperbolic applications – ripe for ultra-high temperature photocatalysis discoveries.

2:30 PM

(EMA-S15-002-2025) Finding Signal in Noisy Data-Sets: Optimizing Feature Space for Small or Lower-Quality Data (Invited)

Y. Yao[1]; R. Anjum[2]; L. M. Ghiringhelli[3]; C. Carbogno[4]; M. Scheffler[1]; T. A. Purcell*[2]

1. Fritz-Haber-Institut der Max-Planck-Gesellschaft, NOMAD LAB, Germany
2. The University of Arizona College of Science, Chemistry and Biochemistry, USA
3. University of Erlangen-Nuremberg Department of Materials Science, Institute of Materials Simulation (WW8), Germany
4. Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

Artificial intelligence (AI) creates models that can accelerate the discovery of functional materials. An open question is selecting the relevant materials features (descriptive parameters that characterize the material, that should be used to represent the material's function of interest, especially when there is a paucity of good-quality data. Here we present an approach that combines symbolic regression, with feature importance methods such as SHAP to select an optimal subset of primary features from a large pool of candidate inputs for a given dataset. We then test the approach on two different problems: thermal conductivity, κ, and electron mobility, μ_e. For κ we use a set of primary features comprised of different structural and vibrational properties and use the models and importance metrics to learn the conditions needed for a hierarchical workflow. We then supplement this dataset with information about the DFT calculated electronic bandstructure to learn the experimentally measured μ_e of 64 materials. For this example, the reduced dataset not only preserves the main signal found by AI, but also significantly enhances the model performance. The presented approach highlights how explainable AI techniques can not only act as a post hoc explanation generator for machine learning, but also improve the training of models for smaller datasets.

3:00 PM

(EMA-S15-003-2025) Gated Active Learning for Scientific Exploration with Expert Knowledge in Autonomous Microscopy (Invited)

Y. Liu*[1]

1. Oak Ridge National Lab, USA

Recent advancements in autonomous experiment and machine learning have revolutionized the study of material properties, enabling comprehensive and systematic investigations. However, the current frameworks for autonomous experiment are often limited in their ability to accommodate vast variability of material responses and dynamic adaptation of reward functions that human expertise provides. In this talk, I will introduce a gated active learning framework for scientific exploration with expert knowledge, an approach designed to overcome these limitations by incorporating prior knowledge and human interest into the active learning-driven experiment workflow. This approach transitions from simple discovery loops to multi-stage decision-making processes, refining the exploration space and enhancing the discovery of intriguing functionalities. We demonstrate the application of this approach in both materials synthesis and characterization including autonomous pulsed laser deposition, hybrid perovskite synthesis, and autonomous scanning probe microscopy experiments. However, this approach is broadly applicable across general Bayesian Optimization autonomous experiments, making it a versatile tool for advancing research in materials science. Acknowledgments: This work was performed at the Center for Nanophase Materials Sciences, a US Department of Energy Office of Science User Facility.

4:00 PM

(EMA-S15-004-2025) Extending first-principles materials science across time and length scales via machine learning (Invited)

C. Lee*[1]

1. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA

Developing accurate models of material responses to intense radiation is crucial for creating radiation-resistant materials and precise materials manipulation at the atomic level, including in the excited electronic state. These models must account for rapid quantum interactions immediately post-irradiation, linking initial excited states to longer-term radiation effects. In this talk I will present my group's work on generalizing accurate quantum mechanical modeling of electronic stopping using real-time time-dependent density functional theory towards a cost-effective computational description of electronic stopping as ions travel through materials: With little loss of accuracy, we train a machine learning model on high-fidelity quantum mechanical simulation data of electronic stopping. With this approach we aim for multi-scale ion beam modification modeling and show that the million-fold reduced computational cost allows for first-principles Bragg peak simulations. Similarly, machine-learning can help with understanding disorder in materials that is induced by finite lattice temperature. I will present a model that connects atomic disorder with temperature dependent dielectric functions as well as with sampling the potential energy surface of hydrogen diffusion through disordered atomic configurations of amorphous materials.

4:30 PM

(EMA-S15-005-2025) Inorganic and Organic-Inorganic Semiconductors for Optoelectronics and Spin Control from Large-Scale Hybrid DFT (Invited)

V. Blum*[1]

1. Duke University, USA

This talk focuses on discovery and understanding of novel semiconductors using large-scale spin-orbit coupled hybrid DFT. The work is based on a highly efficient implementation of hybrid DFT in the FHI-aims code, making system sizes of thousands of atoms accessible in production simulations without precision compromises. For a group of multinary chalcogenide semiconductors I_2-II-IV-X_4 (I=Cu, Ag, Li; II=Eu; IV=Si, Ge, Sn; X=S,Se), hybrid DFT is used to predict stability and energy gaps. A resulting candidate material for photovoltaics, $Cu_2EuSnSe_4$, was subsequently verified experimentally. In layered hybrid organic-inorganic perovskites, fine-tuning of the organic component enables key refinements of the semiconducting properties of the inorganic components. Inversion-asymmetric and chiral hybrid perovskites show drastic selectivity towards spin-polarized currents and spin-polarized light emission and absorption. Spin-orbit coupled hybrid DFT reveals very large energy splittings (up to several 100s of meV) in the band structures of tailored layered hybrid perovskites, which can be traced to a simple structural parameter, tunable by careful selection of the organic molecules in the crystal structures. This understanding enabled the rational design of materials with previously inaccessible properties for spintronics.

S16 Controlling grain boundary structure, chemistry, and their network as a function of material processing

S16- Interface structure and chemistry

Room: Colorado C
Session Chairs: James Wollmershauser, U.S. Naval Research Laboratory; Amanda Krause, Carnegie Mellon University

2:00 PM

(EMA-S16-008-2025) Grain Boundary Space Charge Engineering in Model Ion Conducting Ceramic Thin Films (Invited)

T. Defferriere*[1]; Y. Kim[2]; C. Gilgenbach[1]; J. LeBeau[1]; W. Jung[2]; H. L. Tuller[1]

1. Massachusetts Institute of Technology, Material Science and Engineering, USA
2. Korea Advanced Institute of Science and Technology, Materials Science and Engineering, Republic of Korea

Grain boundaries in polycrystalline materials significantly influence electrical behavior, particularly in ion-conducting systems like those used in electrochemical cells. In those cases, these interfaces can lead to ohmic losses and long-term performance degradation. Space charge barriers, caused by trapped charges at grain boundaries, are often used to explain this behavior, though the exact source of the core charge remains debated. In this study, I will discuss our work on controlling the potential barriers at the grain boundaries in model oxygen ion conducting Gd-doped CeO_2 thin films. We build on previous studies that noted the ability to diffuse dopants into films selectively via grain boundaries at reduced temperatures (~ 700°C) and extend such concepts to control the space charge barrier properties. By growing our films on insulating substrates containing the appropriate in-diffusion elements and by exposing them to thermal anneals, we can achieve either non-blocking grain boundaries with essentially zero space charge or highly blocking grain boundaries with orders of magnitude higher resistivities. To the best of our knowledge, this is the first clear demonstration of successful and systematic space charge engineering of grain boundaries in ion-conducting solid electrolytes, which may pave the way to a more complete understanding of space charge physics at these interfaces.

2:30 PM

(EMA-S16-009-2025) Atomic Layer Deposition for Interfacial Engineering: Achieving Nano-to-Macroscale Ceramic Materials (Invited)

A. J. Cendejas*[1]; B. L. Greenberg[1]; K. Anderson[2]; B. N. Feigelson[1]

1. US Naval Research Laboratory, Electronics Science and Technology, USA
2. US Naval Research Laboratory, USA

Interfaces between two or more phases in multicomponent systems play a significant role in determining both the microstructure and the ultimate properties of materials. Atomic layer deposition (ALD) provides a means of intentionally designing conformal interfaces with sub-nanometer precision and scalability from nanometer to centimeter scale substrates. In this talk, we highlight three examples of ALD-enabled ceramic materials at the nanometer, micron, and centimeter scale. First, ALD Al_2O_3 is grown on free-standing Cr_2O_3 nanocrystals, allowing access to bottom-up synthesis of nanorubies between 20-50 nm in the bulk miscibility gap. The precise control over coating thickness offered by ALD allowed complete tunability of nanoruby composition and played a crucial role in the progression of crystallization. Subsequent discussion will surround efforts to broaden the accessible materials enabled by ALD starting with micron-thick films and scaling up to millimeter-thick porous compacts comprised of nanoparticles. Specifically, a new approach to infilling macroscopic nanoporous solids will be discussed in which pressure gradients on the order 10-100 Torr are employed to force precursor flow directly through the nanoporous network. This method was utilized to deposit conductive ZnO films on the internal surface of ~2 mm thick nanoparticle compacts comprised of 200 nm SiO_2 nanoparticles.

3:00 PM

(EMA-S16-010-2025) Co-design and Interface Control During Semiconductor Manufacturing of On-Wafer Solid-state Li^+ and Na^+ Microbatteries and Supercapacitors (Invited)

K. E. Gregorczyk*[1]; D. Fontecha[1]; K. Ahuja[1]; R. Nuwayhid[3]; D. Long[5]; A. Kozen[2]; D. Stewart[1]; S. Lee[4]; G. Rubloff[1]

1. University of Maryland, Materials Science & Engineering, USA
2. University of Vermont, Physics, USA
3. US Naval Research Laboratory, USA
4. University of Maryland, Chemistry, USA
5. Center for Integrated Nanotechnologies, USA

Over the past 15 years, our group has pursued an alternative approach to fabricating solid-state Li^+ and Na^+ microbatteries (SSMBS) and supercapacitors (SCs) by adapting semiconductor processes with high-aspect ratio substrates. This approach decouples energy and power, allowing for increased energy density while maintaining high power densities, particularly in SSMB and capacitors SC. To achieve this, we developed alkali-metal-containing thin films using atomic layer deposition (ALD), such as lithium phosphate (Li_3PO_4), lithium phosphorous oxynitride (LiPON), and sodium phosphorous oxynitride (NaPON). Challenges in device fabrication arise from the mobile alkali-metal ions and the time and temperature required for fabrication. This presentation will highlight three cases: (1) successful SSMB arrays fabricated in silicon micropores with a Ru/LiV_2O_5/LiPON/SnN_x/Ru stack; (2) challenges with Na^+ SSMBs, where intermixing of NaPON and NaV_2O_5 layers occurred; and (3) issues with a capacitor system using TiO_xNy/LiPON/TiO_xN_y, where lithiation of the TiN layer affected device performance. Throughout, we will compare the benefits of semiconductor methods in ion-storing and conducting films with the difficulties posed by alkali metal ions, and discuss techniques to study buried interfaces and internal modifications.

4:00 PM

(EMA-S16-011-2025) Using a Novel Spectro-electrochemical Set-up to Study Extrinsic Poisoning of the Metal-oxide Gas Interface (Invited)

K. F. Valeti[1]; S. Astle[1]; K. Rafiq[1]; A. F. Staerz*[1]

1. Colorado School of Mines, USA

The degradation of the metal oxide surface due to extrinsic poisons, e.g S- or Si-species, is problematic across different application fields including fuel cells and gas sensors. The influence of these poisons is a combination of electronic effects and altered surface chemistry. We have developed a novel set-up that allows us to probe the chemical changes using diffuse reflectance infrared Fourier transform spectroscopy while simultaneously gaining insights into charge transfer processes using impedance spectroscopy. With this versatile set-up, the degradation of oxide based electrochemical systems operated at elevated temperatures (< 800 °C) in different gaseous environments is possible. Specifically, we will present results on the degradation of metal oxide based gas sensors and symmetric solid oxide fuel cell electrodes during exposure to gaseous poisons. With this insights, we will clarify the degradation mechanism and identify pathways to intentionally design more robust systems.

4:30 PM

(EMA-S16-012-2025) Experimental Measurements of Grain Boundary Chemistry and Electrical Potentials in Electronic Oxides (Invited)

E. Dickey*[1]

1. Carnegie Mellon University, USA

Oxides ceramics comprise an important class of dielectric and electronic materials, where electrical properties are determined not only by the material's intrinsic band structure but also but its point-defect chemistry. In polycrystalline materials, the macroscopic conductivity may be significantly affected by grain boundaries, where gradients in point defect concentrations are correlated with gradients in the local and the local electrical potential. Consequently, the electrical conductivity of grain boundaries can differ by several orders of magnitude relative to the bulk. This talk will discuss experimental approaches to measuring grain boundary electrical potentials and their contribution to the macroscopic conductivity and degradation behavior of polycrystalline electronic oxides, with focus on dielectric materials for capacitor applications. The experimental approach employs complementary impedance spectroscopy and scanning transmission electron microscopy to develop a holistic understanding of the local grain boundary chemistry and potential profiles. This research was funded by AFOSR under grant FA9550-19-1-0222.

5:00 PM

(EMA-S16-013-2025) Investigation of grain boundaries in SrTiO$_3$: Correlation of Space charge, grain growth and non-Arrhenius grain growth

P. Zahler*[1]; D. Jennings[2]; O. Guillon[2]; W. Rheinheimer[1]

1. Universitat Stuttgart, Institute for Manufacturing Technologies of Ceramic Components and Composites, Germany
2. Forschungszentrum Julich GmbH, Germany

Space charge layers at GBs are known to decrease the conductivity of ceramics. Beyond electric properties, space charge is also impacting microstructure evolution: Strontium titanate is known for its non-Arrhenius grain growth behavior which results from solute drag that drives a transition from normal to abnormal grain growth. This study focuses on the correlation between non-Arrhenius grain growth and the electrochemical properties of GBs in SrTiO$_3$. The GBs electrochemistry is analyzed using STEM-EDS and EIS. The results are compared to predictions from different space charge models. Two GB impedance signals attributed to different space charge potentials were identified. Also, a dependence of space charge potential and width on the annealing temperature was identified. The data indicate huge scattering in GB properties or a co-existence of multiple GB types with distinct electrochemistry.

5:15 PM

(EMA-S16-014-2025) Modeling Charged Interfaces, Linear, and Point Defects in Ionic Ceramics (Invited)

R. Garcia*[1]

1. Purdue University, Materials Engineering, USA

The properties of ionic solids enable the development of a wide variety of applications that range from sensors and actuators to energy storage technologies. For all these applications, a wide variety of processing routes exist to consolidate an initial granular powder that will be later used as a starting point for the fabrication of carefully thought out layers and multifunctional architectures. Sintering of ceramics, in particular, is a processing methodology that is a result of the underlying contributions from individual point (vacancies and interstitials) line defects (dislocations), and surfaces and interfaces, as they interact in a local microstructural, mechanical, chemical, and electrical field induced through local or external stimuli. The spatial extent of these effects spans anywhere from a few angstroms to entire grains, greatly impact equilibrium and transport properties. In this presentation, a thermodynamically consistent variational framework is presented to understand the effects of ionic point and line defects on the stability of interfaces in polycrystalline ceramics as they pertain to their associated processing and properties. Applications to practical systems, such as Al$_2$O$_3$, 3YSZ, and TiO2 will be presented.

S17 Emerging semiconductor materials and interfaces

S17- Wide bandap (WBG) and ultra-wide bandgap (UWBG) materials

Room: Colorado I
Session Chairs: Hari Nair, Cornell University; Nidhin Kalarickal, Arizona State University

2:00 PM

(EMA-S17-007-2025) III-Nitride Heterojunction Bipolar Transistors for mm-wave Applications (Invited)

C. Joishi*[1]; S. Rahman[1]; Z. Xia[1]; A. Xie[2]; S. H. Sohel[1]; S. Rajan[1]

1. The Ohio State University, Electrical and Computer Engineering, USA
2. Qorvo Inc Richardson, USA

This presentation will give an overview of the current status and future prospects of III-Nitride HBTs. While III-Nitride HBTs offer intrinsic advantages over HEMTs- such as operation near theoretical breakdown limits, negligible surface state dispersion, and volumetric current injection, their experimentally demonstrated performance has lagged for several reasons, primarily related to high resistance associated with the p-type base layer. To date, III-Nitride HBTs have yet to achieve their full potential, with demonstrated output currents < 150 kA/cm^2 (pulsed) and < 100 kA/cm^2 (DC), cutoff frequency (f_T) < 8 GHz, and maximum oscillation frequency (f_{max}) < 2 GHz. We will present two innovative device designs aimed at addressing the long-standing base resistance vs. performance tradeoffs in III-Nitride HBTs: (a) the selective injection HBT and (b) the tunnel junction HBT with all n-type contacts. For the selective injection HBT, we will discuss two fabrication approaches—base contact regrowth and emitter regrowth (with state-of-the-art current density ~275 kA/cm^2). Additionally, we will highlight our tunnel junction HBTs, which can effectively mitigate challenges associated with p-type base contacts. Our current results demonstrate promising improvements in current densities, emphasizing the importance of continued research on III-Nitride HBTs to unlock new capabilities in high-power and RF device design.

2:30 PM

(EMA-S17-008-2025) Ultrawide Bandgap Aluminum Nitride Power Electronics (Invited)

D. Herath Mudiyanselage*[1]; B. Da[1]; H. Fu[1]

1. Arizona State University, School of Electrical, Computer and Energy Engineering, USA

Aluminum Nitride (AlN) is an ultra-wide bandgap (UWBG) semiconductor with a high bandgap of 6.2 eV and a critical electric field of 12–15 MV/cm. Based on Baliga's Figure of Merit (BFOM), AlN has the potential to outperform other wide bandgap semiconductors like GaN, SiC, and Ga_2O_3. However, AlN-based devices are still in their early stages, facing several challenges such as achieving high-quality epitaxial growth, establishing reliable ohmic and Schottky contacts, and understanding the current transport mechanisms in Schottky barrier diodes (SBDs). Recently, we demonstrated AlN-on-AlN lateral SBDs with breakdown voltages exceeding 3 kV, utilizing Pt/Au Schottky contacts and Ti/Al/Ni/Au ohmic contacts. Furthermore, we have demonstrated ultra-low ideality factor SBDs with over 600 V breakdown voltages. The devices show excellent rectification (ON/OFF ratio of 10^7), low η (1.65), and high φ_B (1.94 eV). These results indicate that the device operates mainly through TE. For passivation, we are investigating UWBG boron nitride (BN) and have demonstrated BN/AlN metal-insulator-semiconductor (MIS) diodes. To extend these results to transistors, we have developed high-voltage, kV-class AlN MESFETs on single-crystal bulk substrates. This work provides a valuable foundation for the development of high-voltage and high-temperature AlN devices.

3:00 PM

(EMA-S17-009-2025) Visualizing and Quantifying Thermal Conductance and Strain at Compression Bonded GaN-Diamond Interfaces (Invited)

L. Yates*[1]; W. Delmas[1]; A. Jarzembski[1]; M. Bahr[1]; Z. Piontkowski[1]; W. Hodges[1]; A. McDonald[1]; J. Steinfeldt[1]; R. Kaplar[1]

1. Sandia National Laboratories, USA

Exceptionally high-power densities during the operation of vertical GaN power devices impacts reliability, lifetime, and electrical performance. Here, the heterogeneous integration of diamond with vertical GaN devices is pursued as an effective means of heat removal. This work expands on previous diamond incorporation with lateral devices to include a metal compression bonding interface that allows for backside electrical contact. This necessary requirement precludes the ability to perform a direct GaN/diamond bond. We will discuss current efforts that have demonstrated a GaN/diamond intermetallic bonding process. Investigation of the GaN/diamond bond quality/interface is performed via hyperspectral frequency domain thermoreflectance imaging. A K-means clustering algorithm is used to allow for quick identification of bond quality. The interfaces are compared to confocal scanning acoustic microscopy (CSAM) and vibrational spectroscopy maps to obtain additional thermomechanical information. It is shown that partially bonded regions cannot be quantified via traditional CSAM approaches, and thermal/optical methods allow for higher fidelity and quantification of these regions. Substantial changes in the GaN/diamond thermal boundary conductance are identified on the same scale as a would-be power device. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

4:00 PM

(EMA-S17-010-2025) Epitaxial Growth of c-BN on Diamond for Electronic Applications (Invited)

R. Nemanich*[1]; A. Ebadi Yekta[1]; A. Patel[1]; S. Vishwakarma[1]; J. Brown[1]; D. Smith[1]

1. Arizona State University, USA

Cubic boron nitride (c-BN) is an ultra-wide bandgap semiconductor with properties appropriate for high power and high frequency electronics which operate in extreme environments (high temperature, high radiation, and corrosive environments). The 6.4 eV bandgap of c-BN projects a breakdown field > 12 MV/cm. Moreover, n-type doping with S and Si (~0.3eV) and p-type doping with Be and Mg (~0.24 eV) have been demonstrated. In this talk, I will discuss our recent research efforts on epitaxial c-BN on diamond using ECR plasma enhanced CVD with a fluorine-based chemistry. Our research established relations between the precursor chemistry and the growth modes. By varying the ratio of the hydrogen and fluorine species nucleation of c-BN on diamond can be achieved, which can then be evolved into growth at moderate rates of 50 nm/hr or more. In addition, we show that applied bias and nitrogen concentration are interrelated to achieve preference for cubic over hexagonal BN. The band alignment of c-BN on diamond is projected to depend on the interface bonding, and we describe our efforts to control the interface structure to optimize the c-BN-diamond band alignment. We describe how c-BN / diamond heterostructures could enable different electronic devices from transistors to radiation detectors. Acknowledgement: Financial support provided by DOE through the ULTRA EFRC DE-SC0021230 and the NSF DMR-2003567.

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(EMA-S17-011-2025) Sub-nanometer RMS roughness of thick homoepitaxial growth on miscut (100) β-Ga_2O_3 substrates by MOCVD

J. Buontempo*[1]; C. Gorsak[1]; S. Hellyer[1]; K. Gann[1]; M. Thompson[1]; H. Nair[1]

1. Cornell University, USA

β-Ga_2O_3 is an ultra-wide bandgap (~4.8 eV) semiconductor with high breakdown field (~8 MV/cm), ease of n-type doping, and melt-grown substrates. Previous work has shown homoepitaxial growth on (010) β-Ga_2O_3 substrates induces surface faceting due to surface energy minimization, typically resulting in RMS roughness > 1 nm when films are grown thicker than ~500 nm. To achieve smooth thick epitaxial layers needed for vertical devices, growth on a lower surface energy is desired. On-axis growth on (100) β-Ga_2O_3 substrates often leads to 2D island nucleation, resulting in poor structural quality and degraded electron mobility. However, growth on (100)-oriented β-Ga_2O_3 substrates with miscuts ≥ 4° transitions the growth mode from islanding to step-flow. We investigate the growth and surface morphology of ≥ 5 μm homoepitaxial layers on miscut (100) substrates grown by MOCVD. The substrates have miscut angles of ~1.8°, ~3.5°, and ~5.8° toward [00-1]. The structure of the films is characterized by AFM and X-ray diffraction and electrical characterization by Hall effect measurements. Films grown on the 1.8° substrates exhibit surface morphology consistent with 2D island nucleation and an RMS greater than 1 nm. Films grown on the 3.5° and 5.8° substrates have an RMS of ~0.22 nm, whereas a co-loaded (010)-orientated sample displayed an RMS of ~2.2 nm—an order of magnitude improvement!

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(EMA-S17-012-2025) Activation of Ge in β-Ga_2O_3: Role of capping layer, ambient, and defect formation

T. Luo*[2]; K. Gann[2]; C. Gorsak[2]; P. Evans[1]; H. Nair[2]; M. Thompson[2]

1. Air Force Research Laboratory, USA
2. Cornell University, Materials Science and Engineering, USA

We report on thermal annealing of ion-implanted Ge in β-Ga_2O_3, with control over annealing ambient, capping layers, time and temperature. At optimized conditions, we demonstrate over 40% activation for implant concentration of 3 to 5 * 10^{19} cm^{-3} with mobilities greater 60 cm^2/V-s. This is the highest reported activation for Ge-doped Ga_2O_3. Homoepitaxial films of β-Ga_2O_3 were grown by MOCVD on Fe-doped (010) substrates. Before ion implantation, samples were capped with a 20 nm SiO_2 by ALD to ensure uniform doping to the surface during implantation. Four implant energies are used to yield 100 and 50 nm box profile. Samples were annealed under high purity N_2 from 100 to 1050C for 5 to 20 min w/ or w/o the SiO_2 layer. Measurements conducted w/ Hall measuremnt, SIMS, XRD. Samples show γ phase after the implant and begin to recover at 100 C. Loss of γ phase begin at 600 C. Samples anneal at 950C 10 min w/o capping layer shows 15% activation and 74 mobility. Annealing w/ cap on at same temperature and time shows 40% and 60. Subsequent annealing without cap shows loss of activation to 20% and increased mobility. We believed the cap reduces the formation of compensating Ga vacancies. SIMS diffusion show redistribution of Ge with concentation dependant diffusivity, and 25% Ge immobile and trapped at damage peak, providing understanding of dopant diffusion and activation.

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(EMA-S17-013-2025) Shubnikov-de Haas Oscillations in MOCVD Grown β-(Al, Ga)$_2$O$_3$ 2DEG

P. Tripathi*[1]; C. Gorsak[1]; D. Jena[1]; H. Nair[1]

1. Cornell University, Materials Science and Engineering, USA

Devices based on β-Ga_2O_3, an ultra-wide bandgap (~4.8 eV) semiconductor, has promise for power and RF electronics. A key drawback is the relatively low intrinsic electron mobility at room temperature, primarily limited by polar optical phonon scattering, with further suppression from ionized impurity scattering. A pathway to increase the mobility is to mitigate the scattering from ionized impurities by spatially separating the ionized impurities from the carriers using an β-(Al, Ga)$_2$O$_3$ /β-Ga_2O_3 heterostructure, resulting in the formation of a two-dimensional electron gas (2DEG) at the heterointerface. The observation of Shubnikov-de Haas (SdH) oscillations in 2DEG structures indicates high purity. Prior to this study, only MBE-grown β-Ga_2O_3 2DEGs showed SdH oscillations. This study presents the first evidence of SdH oscillations in MOCVD-grown structures. Analysis of SdH oscillations is excellent for determining the electron's effective mass and quantum scattering time. This work investigates these parameters for 2DEGs in modulation-doped β-(Al ,Ga)$_2$O$_3$/Ga_2O_3, creating a quantum well with one sub-band occupation at the interface. We fit the temperature-dependent transport of the 2DEG including phonon, interface, and defect-based scattering to determine interface roughness as the dominant limiting factor. Analysing SdH oscillations and transport mechanisms enables 2DEG optimization and improves device performance.

5:15 PM

(EMA-S17-014-2025) Investigation of BC_3 vs Cl_2 ICP-RIE etching for fabrication of 3-D structures on (001) β-Ga2O3

N. Das*[1]; A. Gilankar[1]; N. Kalarickal[1]

1. Arizona State University, ECEE, USA

We study the impact of Cl2/BCl3 ratio on sidewall morphology, sidewall angle, and electrical properties. Dry etching experiments were carried on (001) HVPE grown Sn-doped β-Ga2O3 substrates using a bilayer hard mask (200 nm SiO2 & 250 nm Ni). Dry etching was carried out in a PlasmaTherm Apex ICP system with 20 sccm gas flow, 5 mTorr pressure, 600 W ICP power, and 75 W RF power. Three gas mixtures were tested by varying the Cl2/BCl3 ratio (0, 0.5, and 1) to assess their effects on sidewall morphology and angle. Ni Schottky diodes were fabricated post-etch to evaluate the impact of etching on electrical characteristics. Results show that increasing Cl2 content decreases the etch rate from 126 nm/min (100% BCl3) to 86 nm/min (100% Cl2) producing smooth surfaces without micro-masking effects. Sidewall roughness reduced with increasing Cl2, particularly for [010]-oriented fins. The sidewall angle decreases with increase in Cl2, dropping from 85° (100% BCl3) to 80° (100% Cl2). Schottky diodes fabricated post-etch displayed reduced leakage currents and forward current density, indicating sub-surface etch damage as compared to unetched HVPE samples. A slight reduction in Schottky barrier height (~0.16 V) with differing barrier inhomogeneity and possible dopant depletion near the etched surface was observed.

S18 Characterization of struture-property relationships in functional ceramics

S18- Addressing open questions in functional ceramics

Room: Colorado J
Session Chair: Megan Holtz, Colorado School of Mines

2:00 PM

(EMA-S18-007-2025) Correlations among polar nanoregions in $PbMg_{1/3}Nb_{2/3}O_3$-$PbTiO_3$

M. Eremenko[1]; V. Krayzman[2]; S. Gorfman[3]; A. Bosak[4]; H. Playford[5]; B. Ravel[2]; Z. Ye[6]; M. Tucker[1]; I. Levin*[2]

1. Oak Ridge National Laboratory, USA
2. National Institute of Standards and Technology, USA
3. Tel Aviv University, Israel
4. ESRF, France
5. Rutherford Appleton Laboratory, ISIS Facility, United Kingdom
6. Simon Fraser University, Canada

The exact nature of polar correlations and their relation to the local chemistry in relaxor ferroelectrics, exemplified by the $PbMg_{1/3}Nb_{2/3}O_3$-$PbTiO_3$ (PMN-PT) solid solutions, remains elusive. Recent studies of this system suggested that the relaxor state is characterized by ice-slush-like polar nanoregions (PNRs) separated by low-angle boundaries displaying a gradual change in the direction of the local polarization. Structural refinements using large atomic configurations to simultaneously fit the room-temperature powder X-ray and neutron total scattering, EXAFS, and single-crystal diffuse scattering data in PMN revealed the PNRs to form hierarchical assemblages. However, the type of correlations responsible for this hierarchy and a comprehensive understanding of the origins of the observed diffuse scattering remained uncertain. In this presentation, we will discuss our recent developments in the treatment of single-crystal diffuse scattering in such refinements, which significantly improved the fidelity of the recovered interatomic correlations and the scope of information captured by the refined models compared to the previous work. We will focus on using this methodology to study the nanoscale structures in PMN-PT, which permitted us to uncover the principal features of the polar correlations and their link to the chemical disorder, answering several outstanding questions about the polar ordering in relaxors.

2:15 PM

(EMA-S18-008-2025) Engineering nanostructured ceramics using eutectoid transformations (Invited)

A. Johnston-Peck*[1]; R. Maier[1]

1. National Institute of Standards and Technology, USA

Nanostructured (grain or microstructural feature size less than 100 nm) ceramics exhibit improved properties and can demonstrate unique function not possessed by materials with traditional (micron and larger) grain sizes. However, producing fully-dense nanostructured ceramics is difficult. We address this challenge by revisiting a classic phase transformation; specifically, the eutectoid transformation in cerium-based oxides. In these materials, oxidation, typically in the form of Ce^{+3} reacting to Ce^{+4}, is the catalyst for the phase transformation. For example, the perovskite cerium aluminate transforms into cerium oxide and aluminum oxide when heated to sufficiently high temperatures in air. Using thermogravimetric analysis we identify a relationship between the crystal chemistry of these materials and the onset temperature of the phase transformation. Various electron microscopy techniques were used to study the microstructure of these materials. Both cooperative (lamellar microstructure) and non-cooperative (non-lamellar microstructure) growth modes were exhibited in these eutectoid transformations. Origins of these different growth modes will be discussed. Mechanical properties of these materials were measured, and those results will be related to the microstructural observations to form structure-property relationships.

2:45 PM

(EMA-S18-009-2025) Phase formation Anomalies in Mixed-Oxide Aluminates *WITHDRAWN*

Y. Akyol[1]; Y. Yilmaz[1]; G. Sanli[1]; S. Semsari Parapari[2]; S. Sturm[2]; C. Ow-Yang[1]; M. A. Gulgun*[1]

1. Sabanci University, FENS MatSE and NanoEng, Turkey
2. Josef Stefan Institute, Department for Nanostructured Materials, Slovenia

Aluminates present phase formation anomalies irrespective of the initial stoichiometry of the oxide powder mixes. Multiples of phases form at different cation to aluminum (Me^{x+}/Al) ratios. We observed that the first forming phase in strontium, calcium and yttrium aluminate systems is 1:1 oxide compound SA ($SrAl_2O_4$), CA ($CaAl_2O_4$), and YAP ($YAlO_3$) irrespective of the starting Me^{x+}/Al^{3+}. This study claims that the Me^{x+}/Al ratio at the reaction interface determines the incipient phase. It also appeared that having a single type of Al-O coordination is facilitating the phase formation in aluminate systems. SrO-Al_2O_3, model binary system has 6 compounds: $Sr_4Al_2O_7$, $Sr_3Al_2O_6$, $SrAl_2O_4$, $Sr_4Al_{14}O_{25}$, $SrAl_4O_7$, and $SrAl_{12}O_{19}$. Phase pure powders were synthesized using Pechini and/or TEA-EG method. Crystallization temperatures were determined with thermal analysis. Evolution of phases were followed with XRD at 50-100 °C temperature increments. These powders were used to acquire Al-$L_{2,3}$ and O-K ELNES edges of compounds with different stoichiometry to be used as a fingerprint of the compound. Precursors having different Sr/Al ratio were deposited on sapphire substrates. The interphase forming at the interface of the reaction couple was characterized with high-resolution TEM (HRTEM), HR-STEM, and EELS-ELNES. ELNES signal from the interphase between reaction couples were compared orwith ELNES fingerprint of each pure aluminate compound.

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(EMA-S18-010-2025) Solution-deposited epitaxial thin films: Bilayer $La_xSr_{1-x}MnO_3$/$Ba_xSr_{1-x}TiO_3$ heterostructures

D. Piper*[1]; J. Vukmirović[1]; M. Milanović[1]; I. Stijepović[1]; X. Guo[2]; B. Rodriguez[3]; W. Wani[3]; D. Pajić[4]; I. Toković[1]; S. Armaković[5]; V. Srdić[1]

1. Univerzitet u Novom Sadu Tehnoloski fakultet, Department of Materials Engineering, Serbia
2. The University of Dublin Trinity College, Ireland
3. University College Dublin Conway Institute of Biomolecular and Biomedical Research, Ireland
4. Sveuciliste u Zagrebu Prirodoslovno-matematicki fakultet, Croatia
5. Univerzitet u Novom Sadu Prirodno-Matematicki fakultet, Serbia

The development of novel electronic devices requires materials with unique properties. Epitaxial thin films, due to their size and structure, offer such properties, allowing for strain engineering to tailor their characteristics. This work focuses on fabricating multifunctional thin films as heterostructures with ferromagnetic and ferroelectric layers deposited on $SrTiO_3$ (001). LaxSr1-xMnO3 was chosen for the ferromagnetic layer due to its room-temperature ferromagnetism and colossal magnetoresistance, while BaxSr1-xTiO3 was selected for the ferroelectric layer because of its electric properties and lattice compatibility. Films were deposited using solution methods and treated up to 900 °C. Structural properties were investigated by X-ray diffraction, TEM, and AFM. Electronic properties were measured by the four-point probe method, while magnetic properties were assessed via SQUID and VSM methods. Density functional theory (DFT) was used for theoretical studies. Acknowledgments: This research was supported by the Science Fund of the Republic of Serbia, grant No. 7383, "PROMTEH," The Ministry of Science, Technological Development, and Innovation under project No. 451-03-66/2024-03/200358, The OPERA COST Action CA20116: "EurOPean NEtwork foR Innovative and Advanced Epitaxy" and EU HORIZON-MSCA-2021-SE-01 project MX-MAP (Project Number: 101086184).

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(EMA-S18-011-2025) Use of X-ray and Neutron Scattering to Inform the Science of Additively Manufactured Soft Magnetics

C. Fancher*[1]; L. DeBeer-Schmitt[2]

1. Oak Ridge National Lab, USA
2. ORNL, Neutron Scattering Division, USA

Additive Manufacturing (AM), often called 3D printing, offers the unique opportunity to transform how materials are consolidated into bulk 3D structures. The localized melt strategies in metal AM introduce non-equilibrium thermal conditions that can affect the microstructure and phase evolution in as-fabricated parts. Steep thermal gradients (~10^{3-5} K/s) can lead the presence of metastable phase in Fe-Co and Fe-Si alloys, ubiquitous soft-magnetic materials. Despite these promising results about the improved processability, there remains a notable knowledge gap in the process-structure-mechanical relationships at the atomic scale for AM processed Fe-Co and FeSi alloys. This talk will discuss the implications of the effects of metastable phase formation and their thermal stability on the macroscopic magnetic characteristics.

S18- Advances in connecting local and global structure to properties

Room: Colorado J
Session Chairs: Igor Levin, NIST; Chris Fancher, Oak Ridge National Lab

4:00 PM

(EMA-S18-012-2025) Compositional Effects on Proton and Oxygen Ionic Transport of $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_{3-\delta}$

K. Agyekum*[1]; Z. Jiang[2]; B. Cladek[1]; Y. Shin[3]; S. M. Haile[2]; R. O'Hayre[4]; C. Wolverton[2]; J. Liu[5]; K. Page[1]

1. The University of Tennessee Knoxville, Materials Science and Engineering, USA
2. Northwestern University, Materials Science and Engineering, USA
3. Colorado School of Mines, Materials Science, USA
4. Colorado School of Mines, Metallurgical and Materials Engineering, USA
5. Oak Ridge National Laboratory, Spallation Neutron Source, USA

$BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-\delta}$ (BCFZY4411) has garnered heightened interest due to its triple conducting capability, convenient synthesis, and stability. Recent studies suggest that the electrocatalytic activity and H^+/O^{2-} transport behavior of BCFZY4411 can be tailored through the Co/Fe composition. We present a structural and H^+/O^{2-} transport study of the BCFZY solid solution series ($BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_{3-\delta}$; x = 0.1, 0.2, 0.4, 0.6, 0.7) using neutron diffraction and high-throughput density functional theory (HT-DFT) calculations. Rietveld refinements with associated Fourier difference maps and bond valence sum analyses, as well as HT-DFT calculations, were applied to quantify lattice vacancies, locate proton positions, and calculate O^{2-}/H^+ transport pathways and energy barriers for migration. In all compositions, the cubic perovskite structure forms with Co/Fe substitution on the B-site and hydration. Increasing Co content is correlated with an increase in oxygen vacancy concentration and lowered O^{2-} diffusion barriers. Protons surround oxygen ions, promoting rotational and hopping diffusion mechanisms with consistent activation energies across the series. While oxygen ion dynamics are closely linked to Co/Fe concentration, proton dynamics appear to be more complex, prompting further exploration.

4:15 PM

(EMA-S18-013-2025) Investigating the local structure and chemical nuances in High Entropy Oxides using Scanning/Transmission Electron Microscope

S. Ayyagari*[1]; D. Mukherjee[2]; K. M. Roccapriore[4]; S. S. Almishal[3]; J. Maria[3]; N. Alem[3]

1. The Pennsylvania State University, USA
2. Oak Ridge National Lab, Computational Sciences & Engineering Division, USA
3. Pennsylvania State University, Department of Materials Science and Engineering, USA
4. Oak Ridge National Laboratory, USA

High Entropy Oxides (HEOs) have gained much attention due to their tunable functional properties. The functional properties in these materials can be tailored without changing the composition due to the presence of different cations that can adapt to multiple oxidation states. In this study, we investigate a six-component HEO ($(Mg_{1/6}Ni_{1/6}Co_{1/6}Cu_{1/6}Zn_{1/6}Sc_{1/6})O$) stacked thin film, where the thin films grown at different growth conditions are stacked on top of each other. We observed that the thin films of the same composition grown at different conditions exhibit different out-of-plane lattice parameters. Due to the presence of aliovalent cations, the role of elemental distribution and synthesis conditions is not completely understood yet. Scanning Transmission Electron Microscopy (STEM) along with EELS and EDS, is an ideal characterization technique to investigate the local crystal structure, variation in oxidation states of elements, and overall compositional mapping of various elements present in the HEO system. As properties are directly correlated to their structure and chemical bonding, this study provides insight into the structure-process-property correlation of HEOs. This work is supported by the NSF through the Pennsylvania State University Materials Research Science and Engineering Center (MRSEC) DMR-2011839 (2020 - 2026).

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(EMA-S18-014-2025) Chemical and Structural Changes in HZO Ferroelectric Films on TaN and W Electrodes: An EELS Study

E. Gunay*[1]; B. L. Aronson[2]; J. Ihlefeld[2]; E. C. Dickey[1]

1. Carnegie Mellon University, Materials Science and Engineering, USA
2. University of Virginia, Department of Materials Science and Engineering, USA

Hafnium zirconium oxide (HZO) ferroelectrics have emerged as a promising class of materials for non-volatile memory applications due to their CMOS compatibility, robust ferroelectric properties, and scalability to nanometer dimensions. In this study, we investigate the interfaces between HZO and TaN vs W electrodes and their impact on the retention capacity of HZO films. Samples are prepared via atomic layer deposition (ALD) and characterized by aberration-corrected scanning transmission electron microscopy (STEM) couple with electron energy loss spectroscopy (EELS). The EELS analyses focus on changes in energy loss near-edge structure (ELNES) and low-loss features before and after retention tests, which provide insight into the stability and performance of the films. By comparing the interface evolution between different electrode materials, TaN and W, we aim to understand the effects the electrode interface on the retention and degradation mechanisms. This material is based upon work supported by the center for 3D Ferroelectric Microelectronics (3DFeM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE-SC0021118. The authors acknowledge use of the Materials Characterization Facility at Carnegie Mellon University supported by grant MCF-677785.

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(EMA-S18-016-2025) Simple Method to Determine Image-Diffraction Pattern Rotations in TEM

A. Roshko*[1]; G. Burton[1]; R. Geiss[2]

1. National Institute of Standards and Technology, USA
2. Colorado State University, ARC, OVPR, USA

All magnetic lenses produce a rotation between the sample and the image and/or diffraction pattern. Accurate knowledge of the diffraction pattern orientation with respect to the corresponding TEM image is essential for transferring crystallographic information between the two, e.g. for identifying crystallite orientation, indexing dislocations, and determining polarity. In modern microscopes the lens induced rotations and inversions are usually electronically "corrected" by the manufacturer, and the diffraction pattern is electronically rotated to align with the image. However, this diffraction pattern correction can be (and frequently is) 180 ° off, which is difficult to detect due to the symmetry of zone axis diffraction patterns, even of noncentrosymmetric materials. We present a novel method to determine the correct orientation of the diffraction pattern relative to the sample image, which can also be used to determine the rotation with any change of lens conditions. The technique utilizes the quasi-diffraction pattern that results from the out of focus image when the beam is focused in the object plane and the sample is shifted above the object plane. It does not rely on sample shape and can be used on any sample with a large enough crystalline area to obtain a diffraction pattern. The method will be illustrated with images of GaN nanowires and Si lamellae.

5:00 PM

(EMA-S18-015-2025) Structure-property Exploration in Compositionally Complex Rare Earth Titanate and Zirconate Families (Invited)

K. Page*[1]

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

In multicomponent ceramics there are a variety of factors that determine phase selection, stability, and thermomechanical properties, such as the ionic radii of the constituent cations, configurational entropy of the system, and the propensity for vacancies, antisite defects, and other types of crystalline disorder. We explore structure-property trends in two compositionally complex oxide families, titanate pyrochlores ($RE_2Ti_2O_7$) and zirconate fluorites ($RE_{0.5}Zr_{0.5}O_{2-x}$), taking advantage of the large diversity of ionic radii available in the Lanthanide series (RE=La to Lu, large to small). We present thermal conductivity and thermal expansion coefficient trends, and we examine corresponding average and local atomic structures using a combination of electron, X-ray, and neutron scattering probes. Mechanochemistry and sintering pathways are shown to influence cation chemical short-range order and microstructure in compositions with promising property combinations. Structural stability and select properties are examined at extreme temperatures (~2800 °C) using aerodynamic levitation and laser heating, evaluating suitability for thermal protection system applications. Challenges and opportunities for intrinsic property enhancements in these and other multicomponent complex ceramics are discussed.

S22 Advanced Electronic Materials- Processing structures and applications

S22- Advanced electronic materials, including ferroelectric, piezoelectric, dielectric, electrostrictive, and pyroelectric materials

Room: Colorado F
Session Chairs: Neamul Khansur, Case Western Reserve University; Lynette Keeney, Tyndall National Institute, University College Cork

2:00 PM

(EMA-S22-010-2025) Mechanistic aspects of the piezoelectric response of samarium-doped $Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ ceramics (Invited)

M. Arzensek[2]; U. Tos[2]; S. Drnovsek[2]; M. Dragomir[2]; H. Uršič[2]; M. Otonicar[2]; P. Jankauskas[1]; S. Svirskas[1]; M. Koblar[2]; T. Rojac*[2]

1. Vilniaus Universitetas, Lithuania
2. Institut Jozef Stefan, Slovenia

Lead-based relaxors ferroelectrics, represented by the solid solution of relaxor $Pb(Mg_{1/3}Nb_{2/3})O_3$ and ferroelectric $PbTiO_3$ (i.e., PMN–PT), are the most performant electromechanical materials among perovskites and beyond. Paradoxically (or ironically), as they exhibit superior functional properties, they are also extremely complex. It is thus of no surprise that still today, i.e., >60 years after their discovery, we are reading reports providing new (and often contradictory) explanations of their basic structure, local polarity and dielectric/piezoelectric properties. We are witnessing a similar trend also after the discovery of the large piezoelectricity (d_{33}~1500 pC/N) of Sm-doped PMN–PT ceramics. In fact, various mechanisms have been proposed, which are incompatible and contradictory. In this contribution, based on nonlinear harmonic piezoelectric characterization and multiscale structural analysis, we will present our view on this issue. By deconvoluting the total piezoelectric response into various contributions, we will try to show that the mechanisms so-far reported, when considered individually, fail to explain the totality of our data. The large response is thus more likely a result of combined contributions arising from the structural consequences of the Sm-dopant incorporation in terms of the local and average structure, as well as point defects.

2:30 PM

(EMA-S22-011-2025) Aliovalent Substitution of Pb with $(Li_{\frac{1}{2}}Bi_{\frac{1}{2}})$ in $PbZrO_3$ Model System

O. Taylor*[1]; A. Hoyt[1]; X. Tan[1]

1. Iowa State University, Materials Science and Engineering, USA

$PbZrO_3$-based antiferroelectric ceramics have been modified extensively with dopants which act as sintering aids or increase properties like energy density, energy efficiency, fatigue resistance, and relaxor characteristics. Replacing lead (Pb^{2+}) with equimolar Li^+ and Bi^{3+} has been shown to exhibit many benefits in complex solid solutions of $(Pb,Sr,La)(Zr,Sn,Ti)O_3$. To better understand the role of Li^+ and Bi^{3+} co-doping on crystal structure and dielectric behavior, this work studies the effect of increasing amounts of $Li_{\frac{1}{2}}Bi_{\frac{1}{2}}$ substitution in the model system of $PbZrO_3$. $[Pb_{1-x}(Li_{\frac{1}{2}}Bi_{\frac{1}{2}})_x]ZrO_3$ appears to be perovskite phase pure up to x=0.05, with a small amount of secondary phases up to x=0.15. At x=0.20 and beyond, significant impurities with a general degradation in properties occur. $(Li_{\frac{1}{2}}Bi_{\frac{1}{2}})O$ did perform as an effective sintering aid, reducing sintering temperature of 1210 °C at x=0.05 down to 1100 °C at x=0.20. Substitution caused little effect on dielectric properties: the temperature at dielectric maximum T_m only varied from 232.4 to 237.6 °C, the relaxation parameter γ showed minimal change, and the diffuseness of the phase transition δ slightly increased. Antiferroelectric-ferroelectric phase transitions were induced in all compositions at 160 °C with a field strength of 160 kV/cm, showing that Li^+-Bi^{3+} substitution reduced the critical field, increased energy storage density, and improved energy efficiency.

2:45 PM

(EMA-S22-012-2025) So Many Cations, So Little Time: A Structural Study of $(1-x)Bi(Fe_{2/3}Mg_{3/8}Ti_{3/8})O_3$ - $(x)PbTiO_3$ Using X-ray and Neutron Diffraction

M. Dolgos*[1]

1. Oak Ridge National Laboratory Neutron Sciences Directorate, USA

Piezoceramics have intricate crystallographic structures that play a crucial role in determining the material's properties. As such, understanding structure-property relationships is essential for designing high performance piezoelectric ceramics. Our recent work has found a novel lead-reduced piezoelectric system with enhanced properties at the morphotropic phase boundary (MPB) and a high Curie temperature (Tc = 650 degrees C). This system exists as a solid solution between a lead-free perovskite, $Bi(Fe_{2/3}Mg_{3/8}Ti_{3/8})O_3$, and $PbTiO_3$ (BFTM-PT). Of particular significance, the compositions within the MPB have a high piezoelectric response (d_{33} = 145 pC/N) compared to previous conventional high-Tc piezoelectric ceramics. This work presents a detailed structural investigation of the BFTM-PT solid solution using neutron and x-ray diffraction as well as in situ measurements. Neutron diffraction was crucial to providing an accurate description of the atomic structure in this system, so how this technique can help solve complex structural problems will be highlighted.

3:00 PM

(EMA-S22-013-2025) Understanding, design and control of electrical properties and defect chemistry in electroceramics

M. Li*[1]

1. University of Nottingham, Advanced Materials Research Group, Faculty of Engineering, United Kingdom

Electroceramics often exhibit complex electrical behaviours involving different types of charge carriers (e.g., electrons, holes, ions) and inhomogeneity in different regions (e.g., grains, grain boundaries, surface layers). Such complex electrical behaviours are often associated with defects and low levels of nonstoichiometry (typically < 1 at%) induced by impurities in raw materials, deliberate chemical doping or 'accidental' element loss/gain during sample processing. Measuring the electrical and dielectric properties, interpreting the data and understanding the electrical conduction mechanisms in electroceramics can be challenging. The ferroelectric perovskite $BaTiO_3$ has been extensively studied since the 1940s. The electrical properties of $BaTiO_3$ have been known to be highly sensitive to low levels of acceptor- and donor-doping, but the doping mechanisms remain to be clarified. This presentation will reveal how subtle differences in starting composition dramatically influences the electrical conduction mechanisms and electrical conductivity in La- and Mg-doped $BaTiO_3$. A new general doping mechanism is proposed to suppress both the oxide ion conductivity and electronic conductivity for dielectric applications.

3:15 PM

(EMA-S22-014-2025) Structural and electrical property relationship of Mn doped $BiFeO_3$-x$BaTiO_3$ ceramics

A. R. Marotta*[1]; G. Kamm[1]; S. Bishop[1]; E. Neuman[1]; D. Lowry[1]; T. C. Douglas[1]

1. Sandia National Laboratories, USA

$Pb(Zr/Ti)O_3$ (PZT) is known for its excellent piezoelectricity, and relatively high Curie temperature (T_c) (~350 °C). However, due to environmental and human hazards, strides have been made to develop alternative Pb-free piezoceramics. The high T_c of ~450 °C and competitive d_{31} for $BiFeO_3$-$BaTiO_3$ (BF-BT) solid solution makes it an attractive PZT replacement. BF-BT has a morphotropic phase boundary reported at ~30-35% $BaTiO_3$ content, where high d_{31} is reported. At low $BaTiO_3$ content (~10%), BF-BT has been shown to exhibit a large polarization release from poled samples at high strain, resulting in very high-power density. Though promising, there is limited understanding of structure-processing-properties for BF-BT in the literature. Moreover, the processing of BF-BT is difficult due the volatilization of Bi^{3+} and Fe^{3+} to Fe^{2+} transition, leading to low resistivity and thus high current leakage. To address current leakage, dopants are introduced to help stabilize the B-site oxidation state. Here, we investigate BF-xBT, doped with MnO_2, where x=10-35%. This study, aids to elucidate the structure-electrical property relationship of BF-BT. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2024-12491A

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(EMA-S22-015-2025) Insights into the Performance of Multifunctional Flexible Structures Fabricated by Deposition of Ferroelectric Oxide Films on Magnetic Metallic Foils (Invited)

M. Algueró*[1]; A. Barreto[1]; R. Jiménez[1]; H. Amorín[1]; I. Bretos[1]; P. Ramos[2]; L. Calzada[1]

1. Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Spain
2. Universidad de Alcala Escuela Politecnica Superior, Spain

Multifunctional flexible structures fabricated by deposition of ferroelectric perovskite films on magnetic metallic foils can provide a range of sensing, actuation and multisource harvesting capabilities. In addition to the piezoelectricity and magnetostriction of the components, magnetoelectricity is also obtained through their elastic coupling. Outstanding performances have been attained with $Pb(Zr,Ti)O_3$ layers deposited on nickel, though a large scatter of functional responses is also evident. (Poor) Quality of the interface is usually raised associated with the distinctive challenges of processing oxides and metals together. Interface control is especially difficult with lead-containing perovskites and Ni, because there is no processing window where the metal is not oxidized or the oxide reduced. At ICMM-CSIC, interfacial engineering approaches using low-temperature chemical solution deposition have been employed to kinetically limit interface reactions between Ni and an alternative high-sensitivity piezoelectric perovskite oxide, selected for its highly favourable down-scaling behaviour. Here, we review and update current on-going investigations, with emphasis on the gained insights into the factors that determine functional response. Funded with TED2021-130871B-C21, PID2022-136790OB-I00 and PID2021-122708OB.

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(EMA-S22-016-2025) Ceramics Nanocomposite Materials for Green Energy and Heat Management

Z. Hanani[2]; B. Rozic[1]; M. Spreitzer[2]; H. Uršič[3]; D. Mezzane[4]; M. El Marssi[5]; A. N. Morozovska[6]; S. Ivanchenko[7]; Z. Kutnjak*[1]

1. Jozef Stefan Institute, Slovenia
2. Jozef Stefan Institute, Advanced Materials, Slovenia
3. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia
4. Universite Cadi Ayyad, Morocco
5. Université de Picardie Jules Verne, LPMC, France
6. Nacional'na akademia nauk Ukraini, Institute of Physics, Ukraine
7. Nacional'na akademia nauk Ukraini, Institute for Problems of Materials Science, Ukraine

The quest for sustainable, greener energy through harvesting and heat-management technologies has recently developed a significant interest in new nanocomposite ceramics with large electromechanical, triboelectric, pyrocatalytic, and electrocaloric (EC) effects. An overview of the large EC, piezoelectric, and triboelectric response in flexible ceramic nanocomposites exploiting enhanced multiferroic properties of lead-free BCZT and BaTiO3-based nanoparticles will be presented in this contribution, including flexible polymer composites' large energy harvesting potential. The impact of filler's dielectric permittivity and size of nanoparticles on enhanced properties of flexible nanocomposites will be discussed. In addition, the catalytic potential of ceramic nanoparticles in hydrogen evolution will be presented.

4:45 PM

(EMA-S22-017-2025) Aerosol Deposition of Nano-structured Mixed Composite Thick Films

E. Patterson*[1]; S. C. Mills[1]; J. Wollmershauser[1]; E. Gorzkowski[1]

1. U.S. Naval Research Laboratory, Materials Science & Technology Division, USA

Aerosol Deposition has been established as a reliable method to deposit thick-film that enables rapid, room temperature depositions of thick layers of ceramic materials entirely at room temperature. Due to the impact-based consolidation of the precursor materials, the resulting microns-thick films consistently have a crystallite size on the order of 10-20 nm and with a direct match the starting powders stoichiometry. Previously, ferroelectric and ferromagnetic materials, such as barium titanate (BT), bismuth sodium titanate-based phases (BNT-based), barium hexaferrite (BAM), yttrium iron garnet (YIG), and many more, have been demonstrated. This work, therefore, aims to deposit multiple combinations of ferromagnetic-ferromagnetic and ferroelectric-ferromagnetic in mixed 0-3 or 2-2 type composites. Films were deposited onto alumina, glass, gold-coated glass or thin foil metal substrates (copper or aluminum) to facilitate their electrical and magnetic characterization. The resulting films' processing, deposition, structural, dielectric, ferromagnetic, and ferroelectric properties are presented.

5:00 PM

(EMA-S22-018-2025) Piezoelectric and energy-storage properties of $0.5BaZr_{0.2}Ti_{0.8}O_3–0.5Ba_{0.7}Ca_{0.3}TiO_3$ films prepared by the aerosol deposition

S. Merselmiz[1]; I. Goričan[1]; V. Regis[1]; B. Kmet[1]; A. Bencan Golob[1]; T. Rojac[1]; A. Debevec[1]; B. Malic[1]; H. Uršič*[1]

1. Institut Jozef Stefan, Slovenia

$0.5Ba(Zr_{0.2}Ti_{0.8})O_3–0.5(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT–BCT) have been investigated for their excellent ferroelectric and piezoelectric properties. BZT–BCT thick films deposited on platinum substrates by screen-printing and electrophoretic methods have already been reported. However, the use of platinum, an expensive metal, limits the industrial integration of BZT–BCT films. Accordingly, the use of a low-cost substrate such as stainless steel could encourage applications. In this work, BZT–BCT films were deposited on stainless steel substrates using the aerosol-deposition method, resulting in a dense and homogeneous microstructure. The films annealed at 800 °C exhibit a high dielectric breakdown strength of more than 1500 $kVcm^{-1}$, making them promising for energy storage applications. The recovered energy density and energy efficiency of these films reach 9.5 Jcm^{-3} and 84%, respectively, at 1500 $kVcm^{-1}$. The films also exhibit excellent stability to electric fields with up to 100 million cycles and thermal stability from −50 to 200 °C. The strain versus electric field measurements of these films demonstrated piezoelectric performance, with an effective piezoelectric coefficient d_{33}^{eff*} of 41.5 pmV^{-1}. The functional properties of the BZT–BCT thick films will be discussed in correlation with their structural and microstructural properties.

Poster Session

Room: Penrose Ballroom

5:30 PM

(EMA-P001-2025) Mechanical Characterization of Kaolin Clays for Microporous Membrane Reactors

R. McGinnis*[1]; S. Ricote[3]; G. Coors[4]; I. Reimanis[2]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA
2. Colorado School of Mines, USA
3. Colorado School of Mines, Mechanical Engineering, USA
4. Hydrogen Helix, LLC, USA

The naturally occurring kaolin family of clays exhibits nano-pores and ideal reactor channel morphology. These high-porosity ceramics have great potential as microporous membrane reactors (MMR) for hydrogen reforming of hydrocarbons and gas separation. This ongoing investigation seeks to characterize and optimize the mechanical strength while maintaining porosity levels to maximize refinement efficiency while ensuring mechanical resiliency. Previous efforts utilized a factorial design of experiments approach (DOE) to characterize the relationship between firing temperature and porosity for discs of Edgar Plastic Kaolin (EPK). Using ASTM C20-00 for apparent porosity testing, it was found that temperatures between 1000°C and 1100°C did not have a significant effect on porosity. Current and ongoing work uses these results to characterize mechanical strength and flaws following the ASTM C1684-18 and ASTM C1899-21 standards for 4-point bend tests of tubes and rods. Using optimized EPK as the reference material, a new DOE is being applied to investigate a range of factors (including clay composition, geometry, and firing curve) to find ideal candidates for MMRs. Additional ongoing work measures single gas permeabilities of the candidates to quantify separation and diffusion mechanisms.

(EMA-P002-2025) Insights into the electrode-electrolyte interface of protonic ceramic electrochemical cells using thin film nanostructures

P. Chery*[1]; E. Griffin[1]; G. Trindade dos Santos[1]; Y. Cheng[1]; R. dos Reis[1]; V. Dravid[1]; S. M. Haile[1]

1. Northwestern University, Materials Science and Engineering, USA

Protonic ceramic electrochemical cells (PCECs) employ proton-conducting electrolytes with mixed electronic and ionically conducting (MIEC) electrodes. Recent research efforts have produced breathtaking advances in the power output and electrolysis efficiency of such cells through the compositional optimization of the positrode. A growing body of evidence suggests that the cell performance is limited by high interfacial impedance at the interface between the electrolyte and positrode components. Yet, a fundamental understanding of the interfaces between these materials is lacking. Thin film structures, which can be used to create precisely-defined features and coherent interfaces, are uniquely suited to the study of interfacial phenomena. In this work, the chemical, electrical, and crystallographic features of the interface formed between the triple-conducting electrode PrBa0.5Sr0.5Co1.5Fe0.5O5+ε (PBSCF) and the proton-conducting electrolyte BaZr0.8Y0.2O3-δ are characterized. Multilayer structures of oriented, single-crystal thin films are grown via pulsed laser deposition onto the substrate SrTiO3. X-ray diffraction and transmission electron microscopy reveal the chemical and crystallographic features of the interfaces. Through-plane A.C. impedance spectroscopy measurements are used to assess the interfacial impedance.

(EMA-P003-2025) Materials Selection Principles for Designing Electro-thermal Neurons

F. Jardali[1]; J. Chong*[1]; Y. Yu[1]; M. Altvater[2]; T. Nguyen[1]; Y. Lin[1]; R. S. Williams[4]; S. Kumar[3]; P. Shamberger[1]; T. D. Brown[3]

1. Texas A&M University System, Materials Science and Engineering, USA
2. Air Force Research Laboratory, USA
3. Sandia National Laboratories California, USA
4. Texas A&M University System, Electrical & Computer Engineering, USA

Screening materials for brain-inspired neuromorphic hardware can be streamlined by exploiting the electro-thermal nonlinearities of a diverse set of electronic materials. Neuronal dynamics can be modeled through physics-based reduced order models, resulting in a predictive tool to optimize artificial neuron-like devices for high dynamical reconfigurability, high frequency, and low power designs. We apply governing electrical and thermal transport relationships, along with constraints imposed by external circuitry across a wide range of well-known semiconductors, oxides, and chalcogenides. We predict that more materials are viable than previously recognized, and this prediction is largely supported by the available literature. For a particular design constraint, we develop uniform simulation and meaningful evaluation of materials with properties varying by orders of magnitude and predict typical MHz response at mW power for micron devices. From these predictions, we have down-selected molybdenum disulfide (MoS_2) from the list of viable materials for growth and subsequent measurement of its temperature-dependent electrical and thermal transport properties in order to validate this model and its predictions. Here, we will describe the overall model and its predictions, as well as progress in experimental validation of those predictions.

(EMA-P005-2025) Chemical Contributions in Functionality of Energy and Electronic Materials

A. V. Levlev*[1]

1. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA

The functionality of energy and electronic devices are governed by a complex coupling between electrical properties and charge carrier dynamics at the nanoscale. While the physical mechanisms underlying this behavior have been intensively studied, the chemical contributions remain largely elusive. This gap in understanding is mainly due to the lack of techniques capable of resolving chemical changes at the nanoscale. Recently, time-of-flight secondary ion mass spectrometry (ToF-SIMS) has emerged as effective tool for characterizing static chemical states across a wide range of systems. ToF-SIMS offers high sensitivity to chemical composition and is capable of mapping chemical species with high spatial resolution, making it particularly suitable for nanoscale chemical analysis. The integration of ToF-SIMS with complementary AFM techniques could provide a comprehensive approach to studying both the physical and chemical dynamics in energy and electronic devices. Here, we demonstrate the application of a combined AFM/ToF-SIMS platform to reveal chemical contributions to the functionality of various energy and electronic materials, including ferroelectrics, photovoltaics, and memristors. This approach has proven effective in studying both static and dynamic chemical phenomena in devices under operando conditions, which is crucial for understanding the mechanisms that drive the functionality of these devices.

(EMA-P006-2025) Focused helium beam patterned nickelate synaptic device for neuromorphic computing *WITHDRAWN*

R. Basak*[1]; A. Frano[1]

1. University of California San Diego, Physics, USA

A neural network is an interconnected network of ever-evolving synapses through which information passes as well as gets mathematically acted upon. We propose a device design using nickelates to mimic synaptic plasticity in neural networks, enhancing post-von Neumann architecture. This will be accomplished by using (i) the natural domain heterogeneity of a single device, (ii) manipulating the morphology with a static helium pattern, dynamical hydrogenation pattern, and the complex interplay between them, and (iii) developing a synaptic module to create an interplay of devices for an externally tunable, complex pulse correlation between input and output.

(EMA-P007-2025) Siloxane Poisoning of Semiconducting Metal Oxide Gas Sensors: Mechanism Elucidation and Material Design

S. Astle*[1]; A. F. Staerz[2]

1. Colorado School of Mines, USA
2. Colorado School of Mines, MME, USA

Semiconducting metal oxide (SMOX) gas sensors are a popular choice in the gas sensing field due to their quick response, sensitive detection rate, and inexpensive manufacture. However, they become irreversibly "poisoned" in the presence of siloxane vapor. This study investigates the mechanism of how SMOX sensors are poisoned. To do so, we use simultaneous, in-operando electrochemical impedance spectroscopy (EIS) and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS). With these techniques, we are able to probe both the electronic effects of siloxane (with EIS) and its chemical effects (with DRIFTS). Preliminary results show a decrease in hydroxyl groups as siloxane is flowed over our sensors. This leads us to believe that siloxane preferentially attacks hydroxyl groups on the surface.

(EMA-P008-2025) Dynamic Implementation of Metal Oxide Based Gas Sensors

K. Rafiq*[1]; A. F. Staerz[2]

1. Colorado School of Mines, Mechanical Engineering, USA
2. Colorado School of Mines, MME, USA

Semiconducting metal oxide (SMOX) gas sensors are widely used for their robustness, affordability, fast response, and sensitivity to various gases. These sensors, primarily based on n-type semiconductors such as tungsten, tin, and indium oxides, operate at elevated temperatures (around 300°C), where oxygen adsorbs onto the metal oxide surface. Oxygen adsorbs through chemisorption, trapping electrons and increasing resistance by raising the energy barrier between grains. When a reducing gas reacts with the surface oxygen, it releases electrons back into the bulk, lowering resistance. Traditional designs used ceramic beads over metal heaters, while modern designs employ planar structures with interdigitated electrodes and backside heaters, both of which have large thermal masses limiting them to steady-state operation. However, new generation micromachined sensors with lower thermal masses enable dynamic heating cycles and exhibit behaviors distinct from steady-state sensors. To study this mode of operation, our team will develop a novel testing protocol to evaluate the performance of these dynamically operated gas sensors under controlled conditions.

(EMA-P009-2025) Room-Temperature Thermal Rectification in Suspended Graphene: Asymmetric Channel Design via Electron Beam Lithography

R. Ali*[1]; M. Islam[2]

1. University of Kentucky, Department of Electrical and Computer Engineering, USA
2. Hokuriku Sentan Kagaku Gijutsu Daigakuin Daigaku, School of Material Science, Japan

This study explores thermal rectification in graphene-based devices, focusing on the thermal transport properties of asymmetric suspended graphene nanostructures. Previously, sub-10 nm periodic nanopore phononic crystal structures were patterned on one-half of the suspended graphene ribbons using HIBM. Results revealed significant thermal rectification ratios at temperatures below 250 K, with improvements linked to nanopore size and pitch adjustments. However, the rectification effect diminished at room temperature, attributed to insufficient asymmetry-induced differences in heat flow between the forward and reverse directions. To achieve thermal rectification at room temperature, we introduced a novel approach involving the fabrication of periodic parallel nanoribbons on one side of the suspended graphene ribbon using EBL followed by reactive ion etching. This approach yielded a thermal rectification ratio of approximately 45% at room temperature. The success of EBL over HIBM lies in its ability to introduce structural irregularities and point defects near the nanoribbon edges, acting as phonon scattering centers and manipulating phonon dynamics to enhance thermal rectification. EBL's cost-effectiveness and capability to manipulate phonon transport dynamics make it the preferred technique for achieving room-temperature thermal rectification in graphene.

(EMA-P010-2025) Additive manufacturing of architected battery components for fast charging batteries

A. Orhan*[1]; J. Ye[1]

1. Lawrence Livermore National Laboratory, USA

Fast charging batteries require facile Li+ ion transport through the porous electrodes. Demand for batteries with high energy and power density coupled with fast charging capability necessitates increasing active material mass loading, which results in thicker electrodes. Commonly used tape casted electrodes typically demonstrate sluggish ion transport with the increase of layer thickness due to the limited porosity and high tortuosity. Architecting the electrodes to introduce fast ion transport highways is a promising strategy to enhance the power density with limited sacrifice of energy density. In this work, we report our recent efforts in additive manufacturing (AM) of architected electrodes and separators. Two AM techniques are employed for the fabrication of electrodes and separators, including direct ink writing and projection micro stereolithography, respectively. A variety of geometries are designed, fabricated, and compared for the fast charging capabilities. The results show that optimized electrode and separator design achieved by AM as well as proper material chemistry selection enhances the performance and fast charging capabilities of batteries. The limitations, and future directions of AM application in batteries will also be discussed.

(EMA-P011-2025) Rapid Fabrication of Solid-State Batteries by Cold Spray Deposition

E. P. Ramos Guzman*[1]; A. Baker[1]; E. Kim[1]; J. Ye[2]; J. Roehling[1]

1. Lawrence Livermore National Laboratory, Material Science, USA
2. Lawrence Livermore National Laboratory, USA

Widespread adoption of electric vehicles and clean technologies demands significant advances in solid-state batteries, meeting needs for increased energy density and improved safety. The fabrication of electrode materials used in currently commercialized Li-ion batteries relies on wet coting processes that use environmentally harmful and toxic solvents such as N-methyl-2-pyrrolidone (NMP). Thus, the development of new cost-effective manufacturing alternatives to conventional wet electrode processing are required. Here we explore the use of the rapidly emerging cold spray deposition technology, which is a coating technique that entrains micron-scale particles in supersonic gas to direct impacts on substrates, producing dense deposits through mechanical interlocking. Cold spray is well-suited for battery fabrication due to its extremely high rate of deposition (>1mm/s under the nozzle), ability to bond dissimilar materials through the high kinetic energy of impact, and capability to coat non-planar surfaces. This research is supported by the development of DEM models of particle impact and CFD investigations of gas flow and particle velocity. This poster will present initial results from deposition trials, including fundamental studies of particle impact and demonstration of dry processing of NMC-based composite cathodes, as well as halide SSEs.

(EMA-P012-2025) Strain Engineering of NdNiO3 Thin Films with Substrate-implanted Helium

R. Glefke*[1]; A. Frano[1]

1. University of California San Diego, Physics, USA

Nickelates provide a platform for studying strongly correlated electron physics, where charge, spin, and structural degrees of freedom couple with each other. Small perturbations to the nickelates' perovskite structure can modify their electronic and magnetic properties. NdNiO3 in particular undergoes concomitant paramagnetic-metal to antiferromagnetic-insulator transitions at ~200K, and recently we have observed Helium ion implantation in NdNiO3 films changes strain uniaxially and suppresses these transitions. We have used various X-ray techniques to study the effects of Helium implantation in NdNiO3 films of different strain configurations. The results of this work will contribute to the development of ground-state property-tuning in oxides in general.

(EMA-P013-2025) Spin reorientation in Dy-based high-entropy oxide pervoskite thin films

M. Cocconcelli[2]; D. Miertschin*[1]; B. Regmi[1]; D. Crater[1]; F. Stramaglia[3]; L. Yao[4]; R. Bertacco[2]; C. Piamonteze[3]; S. van Dijken[5]; A. Farhan[1]

1. Baylor University, Physics, USA
2. Politecnico di Milano, Physics, Italy
3. Paul Scherrer Institut PSI, Physics, Switzerland
4. Aalto-yliopisto, OtaNano-Nanomicroscopy Center, Finland
5. Aalto-yliopisto, Applied Physics, Finland

High-entropy oxide perovskites (HEOPs) are a new class of material that have emerged from the general oxide perovskite formula, ABO_3, such that disorder is introduced by mixing elements in equiatomic proportions in either the B-sites or A-sites leading to entropy-driven stabilization. Here, we present a study of the magnetic and structural properties of the high-entropy oxide perovskite thin film $Dy(Fe_{0.2}Mn_{0.2}Co_{0.2}Cr_{0.2}\ Ni_{0.2})O_3$ (Dy5BO). Element-sensitive x-ray absorption spectroscopy measurements were performed employing x-ray magnetic circular and linear dichroism (XMCD and XMLD). The results reveal that the 3d transition metal ions and rare-earth Dy ions produce magnetization that are an order of magnitude larger than any previously studied high-entropy oxide perovskites. Furthermore, temperature dependent analysis of the XMLD measurements exhibit clear spin reorientation at around 18K for the Mn and Fe sites, which is likely caused by interactions with the corresponding transition metals and the rare-earth Dy.

(EMA-P014-2025) Apparent ferrimagnetism in $Sr(Fe_{0.2}Mn_{0.2}Co_{0.2}Ti_{0.2}V_{0.2})O_3$ high-entropy oxide perovskite thin films

B. Regmi[1]; D. Miertschin[1]; M. Cocconcelli[2]; C. Piamonteze*[3]; A. Farhan[1]

1. Baylor University, Physics, USA
2. Politecnico di Milano, Dipartimento di Fisica, Italy
3. Paul Scherrer Institut PSI, Switzerland

High-entropy oxide perovskites (HEOPs) have recently gained an appealing avenue for creating novel functionalities by mixing multiple cations in equatomic proportions to stabilize in a single-phase structure. Herein, we explore the structural and magnetic properties of $Sr(Fe_{0.2}Mn_{0.2}Co_{0.2}Ti_{0.2}V_{0.2})O_3$ (S5BO) thin film deposited on $SrTiO_3$ substrate. In depth structural, compositional, and magnetic characterization was performed by utilizing x-ray diffraction (XRD), scanning transmission electron microscope (STEM), and element-sensitive synchrotron-based x-ray absorption spectroscopy (XAS) employing x-ray magnetic circular dichroism (XMCD). XRD, and STEM show that the thin film achieves very good crystalline quality and coherent growth of S5BO. XAS and XMCD data revealed a ferrimagnetic order, marked by the dominant presence of high spin Co^{2+} ion featuring a magnetic response which opposes that of other transition metal elements like Fe and Mn. This unique magnetic ordering in S5BO highlights the potential insights into tuning the magnetic properties through strategic element introduction in the B-site of the HEOPs.

(EMA-P015-2025) Effect of Argon Ion Bombardment During Growth on Phase Stabilization of Hafnium Zirconium Oxide Thin Films

N. Lam*[1]; L. Shvilberg[1]; M. K. Lenox[1]; B. L. Aronson[1]; Y. Choi[1]; I. A. Brummel[1]; J. Ihlefeld[1]

1. University of Virginia, Material Science and Engineering, USA

Hafnium zirconium oxide (HZO) has potential applications in a variety of technologies, particularly in non-volatile memory. This is largely due to HZO's ability to display ferroelectricity in size scales below 10nm, incorporation in already existing mass production infrastructure, and complementary metal oxide semiconductor compatibility. However, the widespread implementation of HZO as a memory material is hindered by a variety of problems, such as wake-up, imprint, and retention. A major issue is the inability to make phase pure ferroelectric HZO partially due to a phase transformation from the antiferroelectric phase. The effect of argon ion bombardment on HZO has been investigated as a possible means to circumvent the formation the antiferroelectric phase. In this work, thin films of HZO were grown using plasma-enhanced atomic layer deposition by varying the DC bias applied to the substrate during growth. The films were evaluated using grazing-incidence X-ray diffraction and Fourier transform infrared spectroscopy to determine the structure of the phases present. The electrical properties were evaluated using polarization electric field, capacitance-voltage, and positive up negative down measurements.

(EMA-P016-2025) Ordering in Sr_2CoTaO_6 Double Perovskites Grown Via Hybrid Molecular Beam Epitaxy

B. Opatosky*[1]; J. Ahammad[2]; R. Comes[1]

1. University of Delaware, Astronomy & Physics, USA
2. Auburn University, Physics, USA

$AA'CoB'O_6$, double perovskites exhibit a multitude of application-based effects, including photocatalysis, multiferroicity, and thermoelectricity as well as exotic unexplained physics, largely due to the complexity of the Co ion states. However, stabilization of these double perovskites has been historically challenging, due to the Co ions' ability to form multiple valence and spin states.

A common issue is the formation of Co^{2+} ions, rather than the ideal Co^{3+}. The less stable valence difference between the Co^{2+} and B ions is compensated for by the larger Co^{2+} radii. This has been shown in bulk materials such as $Sr_{2-x}La_xCoNbO_6$ (x=0-1), where higher La concentrations were found to stabilize the B-site ordering through increased Co^{2+} formation. Similar results were found in thin films of Sr_2CoNbO_6, where substrate selection showed varied $Co^{3+}/Co^{2+}/Co^{4+}$ formation. To date, only a few papers have been published on Nb^{5+} isovalent Sr_2CoTaO_6, with syntheses focusing exclusively on bulk materials. We fabricate Sr_2CoTaO_6 thin films via hybrid molecular beam epitaxy, allowing precise epitaxial growth of the material on various substrates. Grow is monitored in situ via RHEED to monitor cation ordering, while stoichiometry and oxidation states are evaluated in vacuo by x ray photoelectron spectroscopy. Further characterization was conducted via HXRD and transport.

(EMA-P017-2025) Doping regulated room-temperature dislocation plasticity in oxides: A scale bridging study on $SrTiO_3$

C. K. Okafor*[1]; S. Bruns[2]; I. Huck[3]; K. Takahara[4]; Y. Li[4]; A. Nakamura[4]; K. Durst[2]; X. Fang[1]

1. Karlsruher Institut fur Technologie, Mechanical Engineering, Germany
2. Technical University Darmstadt, Physical Metallurgy, Germany
3. Technische Universitat Darmstadt, Department of Chemistry, Germany
4. Osaka University, Department of Mechanical Science and Bioengineering, Japan

Doping plays a crucial role in determining the physical properties of metal oxides, which have a wide range of scientific and technological applications. However, the impact of doping on the mechanical compliance of oxides during service has been explored less. We present a detailed study of the mechanical behavior of undoped and donor(Nb)-doped single-crystal $SrTiO_3$ across the length scale, via nanoindentation (nano-/microscale), Brinell cyclic indentation (mesoscale), and bulk uniaxial compression (macroscale) focusing on dislocation mechanisms. Contrasting Nb-doped, higher oxygen vacancy concentrations (>10^{16} cm^{-3}) in undoped $SrTiO_3$ promote dislocation nucleation, as evidenced by the maximum shear stress for dislocation nucleation at the nano-/microscale. Mesoscale Brinell indentation (2.5 mm indenter diameter), shows a discrete density of slip traces (evidence of dislocation activity) with Nb-doping indicating a hindered dislocation mobility and multiplication. An ~ 50% increase in the yield stress during macroscale deformation (strain rate ~ 10^{-5} s^{-1}) of Nb-doped $SrTiO_3$ reflects on the hindered dislocation multiplication and mobility analogous to mesoscale deformation. Overall, these findings provide new insight into the impact of defect chemistry on the mechanical compliance of doped $SrTiO_3$ across the length scale, with the potential to be extended to other oxides.

(EMA-P018-2025) He-Doping Induced Symmetry Breaking and Metal-Insulator Transition in Correlated Electron Materials

C. L. Jacobson*[1]; A. Georgescu[1]

1. Indiana University, Department of Chemistry, USA

Correlated electron materials that exhibit a metal-insulator transition (MIT) are key to a wide array of practical applications, ranging from novel transistors to neuron-mimicking devices. While MITs are often induced by a change in temperature, pressure, electric field, doping, or disorder, in this study, we explore the effects of He-doping to induce an insulating state in transition metal compounds without altering the valence of the transition metal site. We use first principles (DFT+U) calculations to model doping of the metallic perovskite $SrVO_3$ (SVO) with He in epitaxially constrained thin film form. We find that He doping not only increases the out-of-plane lattice parameter of the material but induces symmetry lowering lattice distortions, including octahedral rotations and Jahn-Teller like local distortions in the vanadium environment. These distortions localize the electrons on the V d-orbitals, causing a metal-insulator transition. We discuss the implications of magnetic order, crystal structure symmetry, and the Hubbard U parameters on the resulting electronic structure of SVO doped with He. Acknowledgement: This work is partially supported by the Lilly Endowment, Inc., through its support for the Indiana University Pervasive Technology Institute Indiana University.

(EMA-P019-2025) Automating $Hf_{0.5}Zr_{0.5}O_2$ Phase Identification from 4D-STEM Data with Hybrid Machine Learning

T. J. Yoo[1]; S. Gandhi*[1]; G. Baucom[1]; H. Kim[1]

1. University of Florida, USA

$Hf_{0.5}Zr_{0.5}O_2$ (HZO) is a widely studied ferroelectric material sought for a range of applications in next-generation memory and transistor technologies, owing to its scalability and compatibility with current semiconductor fabrication technology. A major materials design crux, however, is that the metastable orthorhombic phase exhibits ferroelectricity, thus phase-pure ferroelectric HZO thin films have not yet been realized. Conventional phase characterization of HZO films has been hindered due to polycrystallinity, structurally similar coexisting phases, and nanosized grains. Here, we employ four-dimensional scanning transmission electron microscopy (4D-STEM) and a hybrid machine learning model to analyze the phase distribution in HZO thin films across micron length scales. This hybrid model utilizes an unsupervised clustering algorithm – involving cepstral analysis, nonnegative matrix factorization, and K-means clustering – to identify unique grains. Then, it determines the phases of grain-averaged patterns using an ensemble of five ResNet8 models, trained on the full range of crystallographic orientations of tetragonal, monoclinic, and orthorhombic HZO. While training all five models takes roughly 24 hours, the full hybrid model application on experimental 4D-STEM datasets takes under five minutes.

(EMA-P020-2025) Accelerating Discovery of Atomistic Defects via Machine Learning

G. Guinan*[1]; M. A. Smeaton[1]; B. Wyatt[2]; H. Egan[1]; B. Anasori[2]; S. R. Spurgeon[1]

1. National Renewable Energy Laboratory, USA
2. Purdue University, USA

The quantification of defects such as vacancies in crystalline structures is a cornerstone of materials science research. Traditional efforts often rely on manual detection, a process that is time-intensive, prone to human error, and challenging to scale. Here we leverage machine learning (ML) methods to identify and quantify vacancies within a crystalline lattice, aiming to expedite detection while improving accuracy. Additionally, we explore the transferability of these ML techniques, identifying characteristics of atomistic imaging data that complicate this task. We show how the integration of ML can drive innovation, providing a powerful tool that will play an increasingly crucial role in the future of materials science.

(EMA-P021-2025) Modeling Surface Structure by Broken Bond Density

A. Loew*[1]; V. Stevanovic[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA

Surface science is often introduced through the concept of the breaking of chemical bonds. However, it is largely understood that there is much more to the structure and energy of surfaces than can be explained by bond breaking alone. To understand the limits of estimating surfaces solely with breaking bonds, we conducted a quantitative study comparing the results with known structures. The results are quite surprising. The structure of both simple and complex ionic systems can be nearly fully reproduced through the geometric minimization of the surface density of broken bonds. We can also distinguish between different chemical bonds and account for differing bonding strengths. Because of the limited knowledge of surface structures in crystals, the results were also qualitatively validated by comparing Wulff shapes created using the surface density of broken bonds as the proxy for surface energies with naturally occurring crystals.

(EMA-P022-2025) Tracking Grain Growth Behavior in Polycrystalline Alumina using 3D X-ray Diffraction Microscopy

H. Hall*[1]; D. P. DeLellis[1]; M. S. Kesler[2]; A. Krause[1]

1. Carnegie Mellon University, Materials Science and Engineering, USA
2. Oak Ridge National Laboratory, USA

Classical models for grain growth use topological features such as curvature to predict growth while assuming isotropic grain boundary energy and mobility. Recent studies suggest that grain boundary energy anisotropy introduces energy minimization mechanisms aside from area reduction that cause local deviations from classically predicted growth. Though current simulations attempt to account for anisotropy, both contemporary and classical models remain ineffective at replicating grain growth observed experimentally. As such, a better mechanistic understanding of grain growth in polycrystals is required to build more precise models. Here, alumina is used as a model ceramic material to investigate the impacts of anisotropy on growth behavior. Both textured and untextured undoped alumina are studied in 3D using laboratory diffraction contrast tomography. Individual grains are tracked over time to determine their velocities, grain boundary character, and local growth changes at various heat treatment intervals. This approach enables us to discern the role of anisotropy on local growth in polycrystals to improve upon predictive grain growth models.

(EMA-P023-2025) Magnetic field-driven grain boundary mobility measurements in doped metal oxides

M. C. Dursun*[1]; M. S. Kesler[2]; A. Krause[1]

1. Carnegie Mellon University, Materials Science and Engineering, USA
2. Oak Ridge National Laboratory Physical Sciences Directorate, USA

Controlling grain growth enables designing materials with superior mechanical, and electronic properties. To control grain growth, grain boundary (GB) migration must be understood well. GB migration is described by the driving force and its mobility. However, the mobility of individual GBs are unknown, resulting in inaccurate grain growth predictions. Mobility is unknown because the driving force for growth in a polycrystal is difficult to control due to contributions from both GB energy and curvature. Therefore, GB mobility cannot be isolated. Instead, the reduced mobility, product of mobility and the GB energy, is typically measured and used to understand the influence of dopants on grain growth. This work focuses on measuring the true mobility of GBs in alumina with and without dopants, and correlating them to the GB structure to elucidate the migration mechanisms. Specifically, a magnetic field is used as the driving force to move a synthetic flat GB, thus isolating the mobility from the driving force. The measurements are done in doped aluminum oxide bicrystals with different misorientations. GB migration is tracked by transmission electron microscopy (TEM), and the GBs are characterized at the atomic-scale before and after motion with scanning TEM. This work aims to elucidate the effect of GB segregants on mobility to control grain growth and, thus design materials with superior properties.

(EMA-P024-2025) Structure–Property Relationships in Electrospun $Ba_{1-x}Sr_xTiO_3$ Nanofibers for Dielectric Applications

B. X. Ekdahl*[1]; A. S. Padgett[2]; S. Bishop[3]; J. Andrew[1]

1. University of Florida, Materials Science and Engineering, USA
2. Sandia National Laboratories, High Voltage Sciences, USA
3. Sandia National Laboratories, Materials, USA

Dielectric materials find widespread use in electronics and computing technologies, where Sr-substituted $BaTiO_3$ ($Ba_xSr_{1-x}TiO_3$) is of note due to its high dielectric constant across a wide temperature range. This makes it suitable for applications such as storage capacitors, sensors, and transducers. To expand its application potential, we have developed a method to synthesize high-κ dielectric $Ba_xSr_{1-x}TiO_3$ nanofibers. Here, we demonstrate the reproducible synthesis of $Ba_xSr_{1-x}TiO_3$ nanofibers using electrospinning of sol-gel precursors followed by calcination. The resulting nanofibers maintain a consistent diameter of 227.75 ± 52.5 nm across different compositions. Additionally, we investigate the effect of Sr substitution on the crystal structure using x-ray diffraction (XRD) for average structure analysis and Raman spectroscopy to examine local structural variations. This method provides a reliable way to produce $Ba_xSr_{1-x}TiO_3$ nanofibers with tunable crystal structures, enabling their integration into smaller, more intricate device geometries that require robust dielectric properties for advanced applications.

(EMA-P025-2025) Tight-Binding Models for Complex Materials and Applications to Lone Pair, Heteroanionic Solids

E. G. Ward*[1]; A. Georgescu[1]

1. Indiana University Bloomington, USA

We have developed a methodology to understand complex bonding and symmetry in solids, and here we discuss its application to BiOCl and Bi_2YO_4Cl, two complex heteroanionic, lone pair materials investigated for photocatalytic or photoluminescent applications. Our methodology builds a tight-binding model based on Wannier functions fit to density functional theory results to generate a basis set of atomic orbitals, which are then symmetrized using a unitary transformation. By connecting and disconnecting these orbitals from the model, we can quantify the contribution each orbital plays in the electronic structure and properties of the materials studied. For example, we show how this allows us to investigate the bonding interaction between Bismuth lone pairs and Oxygen and Chlorine p-orbitals, critical to both photoluminescence and photocatalysis mechanisms– even though the Bi lone pairs are ~10eV below the Fermi level. These results and methodology are generalizable to the theoretical study of solids with complex bonding.

(EMA-P026-2025) Elucidating the Coupling in Inorganic-Organic Magnetoelectric Materials

A. Hope*[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA

Magnetoelectric materials, which exhibit coupled dielectric and magnetic properties, are of research interest for applications in multistate digital storage and field sensors. These materials generate electric polarization in response to a magnetic field and vice versa. However, few materials exhibit this behavior because magnetism typically requires partially filled d- or f- orbitals, while dielectric responses require closed-shell electron configurations. These conflicting requirements make it challenging to find materials where both properties coexist effectively. Hybrid inorganic-organic materials offer an alternative, where the inorganic component provides magnetism, and the organic component contributes the dielectric response. Our goal is to systematically engineer such materials by correlating their crystal structures with their magnetic and dielectric properties. To achieve this, we will synthesize a series of candidate materials and characterize their structure to examine how different components affect magnetoelectric responses. We will then correlate structural trends to functional properties using dielectric spectroscopy and magnetometry and investigate local electronic and magnetic environments through nuclear magnetic resonance spectroscopies. This approach will elucidate the structural features that influence magnetoelectric behavior, guiding the design of new multifunctional materials.

(EMA-P027-2025) Enhanced dielectric and energy storage properties in $(Na_{0.5}Bi_{0.5})TiO_3$-$Ba(Ti_{0.98}Zr_{0.02})O_3$ piezoceramics

E. Kumari*[1] ***WITHDRAWN***

1. Indian Institute of Technology Patna, Metallurgical and materials engineering, India

$(Na_{0.5}Bi_{0.5})TiO_3$-based ferroelectric systems have attracted researchers' attention for energy storage applications because of their antiferroelectric characteristics and high transition temperature. However, challenges arise due to high dielectric loss and a large coercive field.

In our study, a critical composition of (1-x)($Na_{0.5}Bi_{0.5}$)TiO_3-xBa($Ti_{0.98}Zr_{0.02}$)O_3 (NBT-BZT) solid solutions show an enhanced dielectric permittivity of ~3000, with minimum dielectric loss of ~0.02 & a high transition temperature of ~295 °C. A large energy storage properties (storage density ~ 1.25 J/cm^3, discharge efficiency ~ 80.4%) at a nominal low E-field of ~65kV/cm at room temperature is observed. Enhanced response has been associated with the morphotropic phase boundary and the dielectric maxima (T_m) observed at room temperature. This results in the existence of nanodomains of much smaller size and ii) the coexistence of multiple phases (AFE/F).

(EMA-P028-2025) Design, Fabrication, and Characterization of UHF Ferrite Hybrid Absorbers

A. S. Padgett[1]; D. Bosomtwi[1]; A. Peretti*[2]; S. Bishop[2]; D. Lowry[2]; M. Blea-Kirby[2]; C. A. Sahasrabudhe[2]

1. Sandia National Laboratories, Electrical Sciences, USA
2. Sandia National Laboratories, Ceramics and Materials Physics, USA

As 5G technology becomes ubiquitous, sources of UHF electromagnetic (EM) interference are rapidly increasing, and the threat of coupling into susceptible electronics grows in tandem. Mitigating this threat requires compact, lightweight broadband EM absorbers. Magnetite, MnZn-, and NiZn-ferrite, hybrid absorbers have the potential to meet the weight and EM attenuation needs. Optimizing absorption loss requires improved understanding of the role of particle size and volume fraction on the complex permittivity and permeability of these materials and the accuracy of mixing rules to predict EM properties. This work discusses investigation of the particle size and volume fraction on the absorption and return loss of ferrite composites with respect to sintered crystal properties as well as their effects on loading volume fraction limits for high quality samples. We present a possible explanation of our results in the context of resonance and relaxation mechanisms and the mixing rules which most accurately capture these results. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(EMA-P030-2025) Oxygen Doping of Ferroelectric $Al_{0.73}Sc_{0.27}N$ Thin Films

M. Brown*[1]; M. Islam[2]; N. Wolff[2]; T. Kreutzer[3]; G. Schoenweger[2]; M. Gremmel[2]; S. Fichtner[3]; L. Kienle[2]; G. Brennecka[4]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA
2. Christian-Albrechts-Universitat zu Kiel, Institute for Materials Science, Germany
3. Fraunhofer-Institut fur Siliziumtechnologie ISIT, Germany
4. Colorado School of Mines, USA

In 2019 ferroelectricity of $Al_{1-x}Sc_xN$ was first measured, opening substantial opportunities for non-volatile, high density memory storage. Significant efforts have been made in investigating the electrical properties of this material, but outstanding questions regarding the role of oxygen defects persist. Here, textured thin films of $Al_{0.73}Sc_{0.27}N$ grown via reactive sputtering were performed with oxygen doping varying from approximately 2 to 7 at. %. These films showed a reduced leakage current, a reduced optical band gap, and a polarization switch in the as-grown state while maintaining structural quality. This work demonstrates the electrical impacts of oxygen incorporation into $Al_{0.73}Sc_{0.27}N$ and the potential benefits of such doping.

(EMA-P031-2025) Exploration of the $(AlN)_x(SiC)_{1-x}$ system for enhanced piezoelectricity & increased elastic modulus

W. Yeo*[1]; G. Brennecka[1]; V. Stevanovic[1]; L. Wolf[1]

1. Colorado School of Mines, Metallurgical & Materials Engineering, USA

There is strong interest in exploring aluminum nitride (AlN)-based alloys for piezoelectric applications. This project seeks to develop a piezoelectric material with higher elastic modulus to operate in higher frequency ranges via alloying with silicon carbide (SiC). This work explores the compositional space of $(AlN)_x(SiC)_{1-x}$ via combinatorial RF magnetron co-sputtering of Al & SiC in mixed Ar & N_2 ambience. One of the challenges of the synthesis of this system is the high temperatures (> 700 °C) required for the SiC to crystallize via sputter deposition in an in-house assembled sputter chamber. Computational guidance suggests the use of AlN to stabilize the overall wurtzite structure. We report here on the relationships between sputtering parameters and the crystal quality, surface morphology, stiffness and piezoelectric response of the alloyed thin films.

(EMA-P032-2025) Electrical and thermal properties of $Al_{0.5}Sc_{1.5}W_3O_{12}$, a zero thermal expansion insulator

S. Bishop*[1]; A. S. Padgett[2]; R. R. Martin[1]; M. Blea-Kirby[1]; P. A. Salinas[1]; D. Lowry[1]; A. Peretti[1]

1. Sandia National Laboratories, Materials, USA
2. Sandia National Laboratories, High Voltage Sciences, USA

Thermal expansion mismatch during thermal cycling between electronic components can lead to mechanical degradation and ultimately failure. Larger temperatures generated by higher power electronics will only exacerbate thermal cycling stresses. Tuning thermal expansion of functional components can aid in extending device lifetime. Examples are low thermal expansion fillers in polymer encapsulants or optimized thermal expansion substrates. In this presentation, the electrical and thermal properties of an insulating zero thermal expansion ceramic, $Al_{0.5}Sc_{1.5}W_3O_{12}$, are discussed. The electrical conductivity at room temperature is estimated to be $>10^{13}\Omega$cm and permittivity is similar to alumina. High frequency (GHz) dielectric properties are also presented. Thermal conductivity is shown to be similar or lower than glass. Lastly, different fabrication processes including thermal spray for dielectric coatings, and polymer and metal ceramic composites are discussed. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(EMA-P033-2025) Structure and Thermoelectric Properties of Hydrothermally Grown $Bi_2Te_{3-x}Se_x$ Nanocrystals

M. Isram*[1]; D. Pankratova[2]; V. Demontis[3]; A. Vomiero[4]; F. Rossella[1]

1. Universita degli Studi di Modena e Reggio Emilia, Physics and Nanoscience, Italy
2. Lulea tekniska universitet, Department of Engineering Sciences and Mathematics, Sweden
3. Universita degli Studi di Cagliari, Physics, Italy
4. Lulea University of Technology, Engineering Sciences & Mathematics, Sweden

N-type bismuth telluride materials are ideal for generating TE power at low temperatures. The electrical characteristics of a semiconductor material can be precisely tuned to enhance TE functionality by doping it with impurities. Hydrothermal technique used to synthesize nanostructured TE $Bi_2Te_{3-x}Se_x$ (x = 0, 0.4, 0.8, 1.2, and 1.6) nanocrystals. By manipulating the concentration of NaOH, which has a significant impact on the synthesis mechanism of Bi2Te3, the particle size and morphology can be regulated. We investigated the structures and morphologies of the materials by using XRD, SEM, EDX, and Raman spectroscopy. XRD result indicates that the crystal structure exhibits a hexagonal geometry, with a preferred growth

along the (015) plane. Additionally, the positions of the diffraction peaks gradually move towards the lower angle side as the Se concentration increased, which is attributed to the substitution of Te atoms by Se atoms in the crystal structure, SEM results indicated that the size of the nanocrystals decreased with an increase in the Se concentration. PF of the best-performing material, Bi2Te1.4Se1.6, was enhanced to 156 μWm-1°C-2 at 350 °C (the highest reported for Bi2Te3-xSex nanocrystals up to now), compared to the undoped sample (23 μWm-1°C-2), indicating its potential for developing novel materials and devices for TE applications.

(EMA-P034-2025) The Effect of Sintering on the Dielectric and Polarization Properties of PZT 65/35 Ceramics

E. Neuman*[1]; W. Dong[1]; S. Bishop[1]; W. Bachman[1]; C. Bailey[1]; S. Ehlers[1]; J. Nikkel[1]; R. Trujillo[1]

1. Sandia National Laboratories, USA

Lead zirconate titanate near the zirconium rich morphotropic phase boundary (PZT 95/5) finds use as explosive electric transducers through the pressure induced FE to AFE phase transition. PZT 65/35 also finds using in EETs but works through pressure induced suppression of the FE to P transformation temperature. This work examines the impact of sintering condition on microstructure, phase, dielectric, polarization, and temperature induced phase transformations of $Pb_{0.9875}(Zr_{0.65}Ti_{0.35})_{0.984}Nb_{0.025}O_3$. The ceramic is sintered between 1100 and 1300 °C for between 1 and 45 hours. Increasing sintering temperature and time results in reduced density and increased grain size. Remnant polarization and coercive field are found to increase with decreasing grain size. The temperature dependence of dielectric and polarization behavior is also presented. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(EMA-P035-2025) Marine energy harvesting through piezoelectric fluttering flags

H. Chavez*[1]; A. Marotta[1]; X. S. Bishop[1]; D. Kim[1]; B. Gunawan[1]

1. Sandia National Laboratories, Albuquerque, USA

Mechanical energy is an abundant renewable energy source in the environment. Due to the positive piezoelectric effect, piezoelectric materials are advantageous towards harvesting the mechanical energy and converting it directly to electrical power. From the simple working mechanisms inherent to piezoelectric energy harvesters (PEHs), these devices are self-powered and have reduced maintenance cost. Low-cost piezoelectric sheets will generate electricity in response to wind or water stimuli. However, state of the art designs for water energy PEHs yield low output power. This research, focuses on the design and development of a piezoelectric (Pb(Zr/Ti)O3) fluttering flag, that may permit higher output power from marine energy. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This manuscript describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Thursday, February 27, 2025

Plenary Sessions

Plenary Speaker- Sergei V. Kalinin

Room: Colorado E
Session Chairs: Mina Yoon, Oak Ridge National Laboratory; Reeja Jayan, Carnegie Mellon University

8:30 AM

(EMA-PLEN 01-002-2025) Closing the Materials Discovery Loop via ML-Assisted Characterization: Building Optimized Rewards

S. Kalinin*[1]

1. The University of Tennessee Knoxville Tickle College of Engineering, USA

Over the last two decades, we've learned that scaling computation or synthesis alone does not accelerate materials discovery. Progress invariably relies on the iterative loop between theory, hypothesis formation, experiment planning, synthesis, and characterization. Theory scales universally across materials classes. Synthesis scaling is possible within specific material classes or methods, and can now handle thousands of compositions daily. However structural, functional, and chemical analysis can still take hours or days. This lag in characterization is also tied to the interpretability bottleneck—integrating multidimensional measurements back into theoretical frameworks. To address this, we developed an approach to build single- and multi-instrument workflows connecting synthesis and characterization using reward functions. For autonomous electron and scanning probe microscopies, we define several reward function categories: fundamental physical discoveries, structure-property relationships, and microstructure optimization. These support integrated optimization workflows across shared chemical spaces, balancing costly experiments and models that address uncertainties. This research opens opportunities for using LLMs to generate probabilistic reward functions, propelling autonomous materials discovery forward.

S2 Electronic and Ionic Materials for Energy Storage and Conversion Systems

S2- Characterizations, mechanics, and development of advanced electrodes, electrolytes, and interfaces

Room: Colorado I
Session Chairs: Hua Zhou, Argonne National Lab; Hui Xiong, Boise State University

10:00 AM

(EMA-S2-001-2025) Insights into Na-ion Battery Operation through X-ray Scattering (Invited)

M. Toney*[1]

1. Univeristy of Colorado, USA

Electrochemical energy storage is an enabling technology as humanity transitions to a carbon neutral economy. While Li-ion batteries are presently the dominant technology, a diversity of energy storage needs demands a diversity of storage technologies. My research group is focused on helping to enable these types of batteries through an understanding of their operation and degradation modes, using operando X-ray based methodologies coupled to electrochemistry. In this talk I will discuss our use of X-ray scattering to understand the Na storage mechanisms and heterogeneous nanopore filling and defect assisted intercalation in hard-carbon anodes for Na-ion batteries. L. Kitsu Iglesias et al., Adv. Energy Mater. 13, 2302171 (2023). L. Kitsu Iglesias et al., in preparation.

10:30 AM

(EMA-S2-002-2025) Impacts of the conductive networks on solid-state battery operation (Invited)

Y. Liu*[1]

1. The University of Texas at Austin, Walker Department of Mechanical Engineering, USA

The micromorphology of composite solid-state battery cathodes plays a crucial role in shaping battery performance. However, much of our current knowledge remains rooted in empirical observations. The fundamental "rocking chair" battery chemistry concept underscores the necessity of preserving charge neutrality at both the cathode and anode, pointing to the importance of analyzing electrode micromorphology through the framework of conductive networks. In this talk, I will discuss our recent work on the design and construction of model solid-state batteries to thoroughly investigate this relationship. Our findings demonstrate that the composite cathode structure significantly impacts the balance and efficiency of electron and lithium-ion transport pathways, influencing electrochemical heterogeneity and polarization across various scales. Based on these results, we propose several practical strategies to enhance the performance and lifespan of next-generation solid-state batteries. We highlight the powerful integration of synchrotron characterization and data mining methods in the presented research.

11:00 AM

(EMA-S2-003-2025) Morphology and Crystallinity Effects of Nanochanneled Niobium Oxide Electrodes for Na-Ion Batteries

C. A. Koroni*[1]; K. Dixon[1]; P. Barnes[2]; D. Hou[3]; L. Landsberg[1]; Z. Wang[1]; G. Grbic'[1]; S. Pooley[1]; S. Frisone[1]; T. Olsen[1]; A. Muenzer[1]; D. Nguyen[1]; B. Bernal[1]; H. Xiong[1]

1. Boise State University, Materials Science and Engineering, USA
2. Idaho National Laboratory, Energy Storage and Electric Vehicle Department, USA
3. Argonne National Laboratory, Center for Nanoscale Materials, USA

Niobium pentoxide (Nb_2O_5) is a promising negative electrode for sodium ion batteries (SIBs). By engineering the morphology and crystallinity of nanochanneled niobium oxides (NCNOs) the kinetic behavior and charge storage mechanism of Nb_2O_5 electrodes were investigated. Amorphous and crystalline NCNO samples were made by modulating anodization conditions (20 - 40V and 140 - 180 °C) to synthesize nanostructures of differing pore sizes and wall thicknesses with identical chemical composition. The electrochemical energy storage properties of the NCNOs were studied with the amorphous samples showing better overall rate performance than the crystalline samples. The enhanced rate performance of the amorphous samples is attributed to the higher capacitive contributions and Na-ion diffusivity analyzed from cyclic voltammetry (CV) and galvanostatic intermittent titration technique (GITT). It was found that the amorphous samples with smaller wall thicknesses facilitated improved kinetics. Among samples with similar pore size and wall thickness, the difference in their power performance stems from crystallinity effect, which plays a more significant role in the resulting kinetics of the materials for Na-ion batteries.

11:15 AM

(EMA-S2-004-2025) Pressure Gradient-Driven Preferential Lithium Plating in All-Solid-State Batteries for Enhanced Stability

D. Shin*[1]; J. Jung[1]; Y. Roh[1]; C. Park[1]; I. Kim[1]; H. Kwon[1]; J. Baek[1]; W. Oh[1]; J. Kim[1]; S. Jeong[1]; J. Hwang[1]; Y. Kim[1]; D. Yoon[2]; H. Kim[1]

1. Korea Advanced Institute of Science and Technology, Chemical and Biomolecular Engineering, Republic of Korea
2. Samsung SDI Co Ltd, Republic of Korea

This study investigates the morphological instability of lithium (Li) plating in all-solid-state batteries (ASSBs), a critical issue that hinders their practical application due to dendrite-induced short circuits. By introducing a pressure gradient at the interface between the solid electrolyte and structured electrodes, we demonstrate controlled Li plating behavior. Using sulfide-based solid electrolytes and square hole-patterned electrodes, simulations reveal that the pressure gradient drives Li-ion flux toward interfacial voids, leading to preferential Li deposition in these regions. Experimental validation confirms that Li plating primarily occurs in the void areas under increased stack pressure, mitigating dendritic growth and enhancing the stability of ASSBs. This pressure-driven mechanism offers a promising strategy for improving battery performance, providing new insights into the control of interfacial phenomena in ASSBs and contributing to the development of safer and more reliable energy storage systems.

11:30 AM

(EMA-S2-005-2025) Defect Structure, Ionic Transport, and Surface Exchange Kinetics in the $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_{3-d}$ (BCFZY, $0.1 \leq x \leq 0.7$) Triple-Conducting Oxide System (Invited)

R. O'Hayre*[1]; Y. Shin[1]; M. Sanders[1]; Z. Jiang[2]; C. Wolverton[2]; S. M. Haile[2]; K. Ageyekum[3]; B. Cladek[4]; K. Page[4]; J. Liu[5]; B. Ogbolu[6]; E. Truong[6]; Y. Hu[6]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA
2. Northwestern University, Materials Science and Engineering, USA
3. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science and Engineering, USA
4. University of Tennessee, Materials Science and Engineering, USA
5. Oak Ridge National Laboratory, USA
6. Florida State University, Chemistry, USA

Triple-conducting oxides enable simultaneous transport of three charge carriers ($h^+/O^{2-}/H^+$), making them highly effective electrodes in various electrochemical devices. Among these, $BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-\delta}$ has garnered great interest in recent years. Defect transport and electrocatalytic activity in BCFZY might be further optimized by tuning the Co/Fe ratio. This can modulate ionic/electronic conduction behavior and can also enhance the catalytic activity for oxygen reduction/oxygen evolution. Here, we explore the defect structure, surface exchange kinetics, and bulk transport of oxygen ions and protons vs. Co/Fe ratio in $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_{3-\delta}$ (BCFZY, $0.1 \leq x \leq 0.7$). We use isotope exchange to decouple and quantify oxygen ion and proton transport in selected BCFZY compositions, yielding bulk diffusivity (D^*) and surface exchange (k^*). These results are coupled to symmetric cell and full cell performance along with neutron diffraction, density-functional theory super-cell modeling, and solid-state nuclear magnetic resonance as an extension of this structure and transport study of the BCFZY system. This work supported by the Hydrogen in Energy and Information Sciences (HEISs) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under award no. DE-SC0023450.

12:00 PM

(EMA-S2-006-2025) Dynamics and heterogeneity of particle network in composite electrodes (Invited)

K. Zhao*[1]

1. Purdue University System, USA

We use a data-driven approach to assess the heterogeneous electrochemistry and mechanics in composite cathodes. We visualize the morphological defects at multi-scales ranging from the macroscopic composite, particle ensembles, to individual single particles. Particle fracture and interfacial debonding are identified in a large set of tomographic data. The mechanical damage of active particles is highly heterogeneous. The difference originates from the polarization of the electrolyte potential, various local conducting environments, and thus the non-uniform distribution of the activation energy for the charge transfer reaction. We model the kinetics of intergranular fracture and interfacial degradation to assess the heterogeneous mechanical damage in composite electrodes using microstructure-informed mechanics modeling. We quantify the influence of the mechanical damage on the metrics of battery performance. More interestingly, the interfacial failure reconstructs the conductive network and redistribute the electrochemical activities that render a dynamic nature of electrochemistry and mechanics evolving over time in the composite electrodes.

12:30 PM

(EMA-S2-007-2025) Electrochemically-Driven Orthorhombic-to-Cubic Phase Transition in Ta2O5 Electrode Materials

S. Pooley*[1]; C. A. Koroni[1]; T. Merrell[1]; K. Dixon[1]; P. Barnes[2]; D. Hou[3]; H. Xiong[1]

1. Boise State University, Micron School of Materials Science & Engineering, USA
2. Idaho National Laboratory, USA
3. Argonne National Laboratory, USA

Electrochemically driven phase transition can play a key role in stability and rate performance of electrode materials for rechargeable batteries. Amorphous-to-crystalline transformations have been previously reported to improve capacity and rate performance in TiO2 and Nb2O5 negative electrode materials for lithium-ion batteries. It is critical to understand the mechanisms behind electrochemically-driven phase transition and its role in electrode performance and stability. In this work, we report orthorhombic-to-cubic phase transition in tantalum pentoxide particles as a result of cycling as the negative electrode of a Li-ion battery.

S3 Nano4Neuro-Mechanisms and Materials for Next Generation Computing

S3- Materials that compute

Room: Colorado C
Session Chair: Petro Maksymovych, Clemson University

10:00 AM

(EMA-S3-001-2025) Low-Dimensional Neuromorphic Electronic Materials and Applications (Invited)

M. C. Hersam*[1]

1. Northwestern University, Materials Science and Engineering, USA

The exponentially improving performance of digital computers has recently slowed due to power consumption issues resulting from the von Neumann bottleneck. In contrast, neuromorphic computing circumvents these limitations by spatially co-locating logic and memory in a manner analogous to biological neuronal networks. This talk will explore how low-dimensional nanoelectronic materials enable gate-tunable neuromorphic devices. For example, by utilizing self-aligned, atomically thin heterojunctions, dual-gated Gaussian transistors have been realized, which show tunable anti-ambipolarity for artificial spiking neurons and mixed-kernel support vector machines. In addition, field-driven defect motion in polycrystalline monolayer MoS_2 enables gate-tunable memristive phenomena for memtransistors that concurrently provide logic and memory functions. The planar geometry of memtransistors further allows multiple contacts that mimic the behavior of biological systems such as heterosynaptic responses. Moreover, control over polycrystalline grain structure enhances the tunability of potentiation and depression for unsupervised continuous learning in spiking neural networks. Finally, the moiré potential in asymmetric twisted bilayer graphene/hexagonal boron nitride heterostructures gives rise to robust room-temperature electronic ratchet states that underlie diverse bio-realistic neuromorphic functionalities.

10:30 AM

(EMA-S3-002-2025) Electrochemical memory for robust analog computing systems (Invited)

A. A. Talin*[1]

1. Sandia National Laboratories, USA

Compared to digital, analog encoding and processing of information employ quasi-continuous states defined by non-equilibrium thermodynamics and kinetics and separated by small energy barriers. Additionally, instead of using only electrons to encode information, analog electronics can use electrical, thermal and electrochemical gradients to move electrons, ions, and domains. Understanding these complex, frequently coupled mechanisms is difficult, resulting in few reliable physics-based models that can be used by circuit and chip designers. These aspects of emerging analog devices also present increased sensitivity to variability, noise, and poorly controlled kinetic processes. Current device and circuit design models, which guide manufacturing of digital CMOS are overly simplistic and provide limited guidance for exploiting the features or mitigating the issues of analog electronics. Thus, despite decades of research knowledge gaps in the features of analog electronics have led to their consistent failures to meet the stringent requirements needed for their commercialization. In my presentation, I will discuss our recent work to address this challenge using 3-terminal electrochemical random access memory (ECRAM) that encodes information in three dimensional volumes, rather than 2-dimensions channels or 1-dimensional filaments and combines thermodynamic and kinetic mechanisms to stabilize a high density of analog states.

11:00 AM

(EMA-S3-003-2025) Proton migration in mixed conducting oxides for fast conductivity modulation in neuromorphic devices

M. Siebenhofer*[1]; P. Zguns[2]; B. Yildiz[2]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria
2. Massachusetts Institute of Technology, USA

Mixed ionic and electronic conducting oxides, such as WO_3, MoO_3, V_2O_5 are suitable candidates for programmable resistors in crossbar arrays, one of the most promising novel computing architectures for implementing artificial neural networks with high energy efficiency. By intercalation and distribution of mobile ions, such as H^+, the electronic conductivity of these materials can be finely tuned over a wide range, hence facilitating a high degree of control over the resistance state of each device. To reach target values for the operation speed of these so-called electrochemical ionic synapses, fast proton redistribution, and thus fast proton migration in these mixed conducting oxides is a key requirement. In this contribution, we present our recent results from computational investigations of proton migration in these mixed conducting oxides with density functional theory (DFT) methods. We investigated the most favorable migration pathways with a particular focus on the effect of polarons on the proton mobility, which are the predominant type of mobile electronic charge carriers in these materials at low degrees of ion intercalation. Building on our results for this selection of materials, we identify and discuss geometric and electronic material characteristics that promise to yield fast proton diffusion through the crystal lattice.

11:15 AM

(EMA-S3-004-2025) High-temperature electrochemical memory based on phase separation of Tantalum Suboxide

A. J. Jalbert*[1]; Y. Li[1]

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

One limitation of conventional Si-based memory is its temperature limits to below 150°C. Electrochemical random-access memory (ECRAM) based on oxygen vacancies offers one promising solution to such extreme environments. In this work, we demonstrate stable switching and retention behavior of Tantalum Suboxide ECRAM at high temperatures of 300°C to 600°C. We also quantify the transport of Oxygen Vacancies in thin film TaOx ECRAM and show its ability to scale to micron-sized dimensions.

11:30 AM

(EMA-S3-005-2025) Materials and Device Engineering of Resistive Non-volatile Memory for Next Generation Computing (Invited)

N. Cady*[1]

1. University at Albany, Nanoscale Science & Engineering, USA

Non-volatile memory devices such as resistive random access memory (RRAM) and ferroelectric tunnel junctions (FTJs) have strong potential for use as analog memory cells for in-memory computing, and synaptic devices for neuromorphic computing and AI hardware. RRAM and FTJs can be implemented using multiple approaches, with transition metal oxide based devices being the most readily integrated with current state-of-the-art CMOS chip fabrication technology. Key challenges for successful implementation of these devices for next generation computing is to control stochastic switching behavior, minimize variability in device resistance or conductance levels, maximize the memory window (highest vs. lowest resistance or conductance state) and to demonstrate device endurance (number of switching cycles). Our research group has successfully implemented hafnium oxide and tantalum oxide based RRAM, and hafnium zirconium oxide (HZO) ferroelectric memory cells in exploratory small wafer platforms and with advanced CMOS on 300mm wafers. This presentation will review materials development approaches, and design/testing of in-memory computing and neuromorphic hardware with these devices, and will include examples of vertical profiling of metal oxide stoichiometry in the switching layer, the effects of doping of the switching layer, and implementation of barrier layers and interface engineering.

12:00 PM

(EMA-S3-006-2025) Recent Progress on Phase Change Memory for Analog In-Memory Computing (Invited)

N. Li*[1]

1. The Pennsylvania State University, USA

Among the emerging approaches for deep neural network (DNN) acceleration, compute-in-memory (CIM) in crossbar arrays using non-volatile memories (NVMs) is very promising for achieving high execution speeds and high energy efficiency. Phase change memory (PCM) is one of the most promising candidates for analog CIM – particularly for inference using previously-trained DNN weights. However, when NVMs are used in analog mode, devices will exhibit nonidealities compared to a perfect analog resistor, limiting the computing accuracy. These nonidealities for PCM devices include resistance drift, read noise, limited memory window, and various device failures due to fabrication yield. We will talk about the recent status of using PCM for analog computing in memory. We discuss the device level improvement and system level schemes for overcoming these challenges. We then summarize the projected energy efficiency and discuss the recent chip demonstrations.

S4 Oxide Quantum Materials: Synthesis, Properties and Application

S4- Quantum Electromagnetism

Room: Colorado B
Session Chairs: Ho Nyung Lee, Oak Ridge National Lab;
Seung Sae Hong, University of California, Davis

10:00 AM

(EMA-S4-013-2025) Spin and Topological Phenomena in Low Loss Ferromagnetic Insulator Thin Films (Invited)

S. Channa[4]; C. Zheng[4]; H. Sabri[2]; H. Ren[1]; T. Chen[1]; Z. Galazka[3]; Y. Li[4]; A. Kent[1]; J. Zang[2]; Y. Suzuki*[4]

1. New York University, USA
2. University of New Hampshire, USA
3. Leibniz-Institut fur Kristallzuchtung im Forschungsverbund Berlin eV, Germany
4. Stanford University, USA

Ultra-thin ferromagnetic insulators with perpendicular magnetic anisotropy and low damping provide new opportunities for inducing emergent magnetic and topological phenomena at interfaces and efficiently sourcing, controlling and detecting pure spin currents, thereby changing the landscape of spin wave devices. We have developed a new class of nanometer thick low loss spinel ferrite thin films with Gilbert damping parameter as low as a ~ 0.0006 and negligible inhomogeneous linewidth broadening, resulting in narrow half-width half-maximum linewidths. When combined with a Pt overlayer, we have also demonstrated efficient spin pumping from these spinel ferrites into the adjacent heavy metal layer through measurement of the spin-mixing conductance, Gilbert damping enhancement and electrical voltage peaks that appear at ferromagnetic resonance. These bilayers are also an excellent model system for the demonstration of fluctuation driven topology. The large spin-orbit coupling and breaking of inversion symmetry from the Pt layer leads to an interfacial DMI. In these bilayers, we observe electrical transport signatures of fluctuation driven topology by analyzing the scaling relation between the topological Hall effect and the magnetic field and comparing with Monte Carlo simulations. Our results provide insight into the origins of fluctuation driven topology and analysis of topological transport data.

10:30 AM

(EMA-S4-014-2025) Model-Based Quantum Materials Realized in Oxide Heterostructures and Superlattices (Invited)

J. Liu*[1]

1. University of Tennessee, USA

The complex interplay between the quantum degrees of freedom in oxides is known to cause intriguing emergent states. While the underlying physics is usually captured by model Hamiltonian, most of the known models, such as the Hubbard Hamiltonian, are difficult to resolve theoretical. This challenge calls for toy-model-based design and synthesis of novel structures for complex oxide materials synthesis. In this talk, I will discuss our recent work on experimental realization of Hubbard-like iridate thin films and superlattices that simulate the correlation-topology interplay with engineered complex hopping. While the electronic correlation stabilizes an antiferromagnetic Mott insulating ground state, its intermediate coupling strength allows the SU(2) symmetry-preserving and breaking components of the complex hopping to induce anomalous charge transport through significant longitudinal spin fluctuations. I will also discuss another example in pyrochlore heterostructures which simulate charge transport due to fluctuations in model systems of spin ice physics.

11:00 AM

(EMA-S4-015-2025) Insight on Two-Dimensional Electron Gas Systems at $KTaO_3$ (001) and (111) Surfaces (Invited)

K. Zou*[1]

1. The University of British Columbia, Physics and Astronomy, Canada

Two-dimensional electron gas systems (2DEGs) formed at oxide interfaces have opened new avenues in oxide-based electronics, photonics, and spintronics due to their rich physical phenomena. Among these, $KTaO_3$ (KTO) has emerged as a remarkable platform for exploring the interplay between electronic and spin degrees of freedom, particularly after the recent discovery of superconductivity and strong spin-orbit coupling within 2DEGs on its surfaces. We have significantly contributed to the understanding of 2DEGs at KTO surfaces, focusing on both nonsuperconducting (001) and superconducting (111) orientations. On the (001) KTO surface, we investigated the electronic transport properties of 2DEGs in proximity to strongly correlated oxides with nontrivial topological nodes. Our findings revealed that the proximity effect induces electronic reconstruction, leading to anomalous behaviors in transport properties. Furthermore, our research on the superconducting (111) KTO surface involved comprehensive magnetotransport experiments, which uncovered features consistent with the Berezinskii-Kosterlitz-Thouless (BKT) transition—a key indicator of 2D superconductivity—further changed by strong spin-orbit coupling. These investigations have substantially advanced our understanding of 2DEGs at KTO surfaces, underscoring the immense potential of these materials for future quantum technologies and beyond.

11:30 AM

(EMA-S4-016-2025) Nonsymmorphic symmetry induced correlated topological states in 4d perovskite oxide thin films (Invited)

Y. Park*[1]; S. Kang[1]; J. Song[1]; S. Lin[1]; H. Zhou[2]; M. Yoon[1]; S. Yoon[5]; J. Ok[4]; S. Okamoto[1]; H. Lee[3]

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Argonne National Lab, Advanced Photon Source, USA
3. Oak Ridge National Laboratory, USA
4. Pusan National University, Republic of Korea
5. Gachon University, Republic of Korea

Quantum materials (QMs) with strong correlation and nontrivial topology are indispensable to next-generation information and computing technologies and microelectronics. Exploiting topological band structure is an ideal starting point to realize correlated topological QMs. Despite its potential, observation of such topological band structure to enable quantum transport in oxide materials remains challenging. Our recent findings indicate that manipulating oxygen octahedral symmetry (OOS) is one of the key approaches in creating topological band structures near the Fermi level. In this work, we synthesize 4d niobate thin films (e.g., $SrNbO_3$ and $CaNbO_3$) and manipulate crystal symmetry by epitaxial strain to induce the nonsymmorphic crystal symmetry, yielding the topological band structure and related physical properties. The 4d niobate thin films exhibited extremely high electron mobility and non-saturated extreme magnetoresistance due to the linear band dispersion near the Fermi level. Moreover, quantum oscillation from the magnetotransport measurements and the corresponding Landau-Fan diagram confirm a non-zero Berry phase. Therefore, the deliberate control of the octahedral symmetry provides a novel mechanism to host topological band structures in the strongly correlated oxide systems, which is an important step toward developing correlated topological quantum materials.

12:00 PM

(EMA-S4-017-2025) Anisotropic magnetoresistance and planar Hall effect in $NiCo_2O_4$ thin films and membranes

Q. Wu*[1]; Y. Zhang[1]; T. Li[1]; X. Chen[1]; X. Hong[1]

1. University of Nebraska-Lincoln, Department of Physics and Astronomy, USA

Due to the high Curie temperature and spin polarization, epitaxial $NiCo_2O_4$ (NCO) films are promising candidates for spintronic applications. We report the studies of anisotropic magnetoresistance (AMR) and planar Hall effect (PHE) in 30 nm ferrimagnetic NCO thin films and membranes. Epitaxial NCO thin films are deposited on (001) $LaAlO_3$ (LAO) and $Sr_3Al_2O_6$ (SAO) buffered LAO substrates via off-axis RF magnetron sputtering. Free-standing NCO membranes are achieved by water etching of the SAO buffer layer. All samples exhibit T_C above 300 K. Above 200 K, the AMR of NCO films on LAO exhibit $\cos 2\theta$ dependence on the angle θ between current and in-plane magnetic field direction, consistent with the coherent rotation model. Below 200 K, an additional $\cos 4\theta$ term emerges and increases with decreasing temperature. Similar transistion has been observed on NCO films on SAO buffered LAO, while the $\cos 4\theta$ term emerges at 50 K. After etching of SAO, the NCO membranes exhibit qualitative similar AMR and PHE behaviors. At low magnetic fields, both the AMR and PHE show hysteresis behaviors in the angular dependence till the variation of resistivity is dominated by the magnetoresistance. We also compare the magnetoresistance of these systems. Our results highlight the complex interplay of epitaxial strain, disorder, and interfacial epitaxy in determining the magnetotransport properties of $NiCo_2O_4$.

12:15 PM

(EMA-S4-018-2025) Electronic Phenomena in Doped $SrIrO_3$ Films and $SrIrO_3/SrNbO_3$ Superlattices Grown by Hybrid Molecular Beam Epitaxy

T. Tasnim*[1]; G. Rimal[3]; B. Opatosky[4]; R. Comes[2]

1. University of Delaware College of Arts & Sciences, Physics, USA
2. University of Delaware College of Engineering, Material Science and Engineering, USA
3. Western Michigan University, Physics, USA
4. University of Delaware, Astronomy & Physics, USA

Semi-metallic $SrIrO_3$ is a compelling candidate for electron doping, with the potential to induce phenomena such as Kondo scattering through the manipulation of donor concentrations. We previously showed that the Kondo effect can be tuned via strain-induced differences in oxygen vacancy concentrations, suggesting that electron doping is a viable route to emergent phenomena in $SrIrO_3$. $SrNbO_3$ is promising as a donor material and is expected to donate electrons to $SrIrO_3$, filling hole-like pockets in the Fermi surface. To probe interfacial phenomena in such a system, we synthesized $(SrNbO_3)_m/(SrIrO_3)_n$ superlattices with different thicknesses by using a hybrid MBE system. The growth and crystallinity of the superlattices were monitored via in-situ reflected high-energy electron diffraction (RHEED), followed by XRD. Temperature-dependent electrical transport measurements were carried out to probe the electronic nature of the superlattices after electron doping. To observe the chemical states of the constituent elements and the charge transfer phenomena we did in-vacuo X-ray photoelectron spectroscopy (XPS) and synchrotron-based polarization-dependent hard X-ray absorption spectroscopy (XAS). In addition, we also successfully synthesized Nb-doped $SrIrO_3$ with different Nb concentrations to probe the Kondo effect and other electronic phenomena.

S7 Additive manufacturing for power sources in electronics

S7 - AM for Lithium Batteries I

Room: Colorado E
Session Chair: Jianchao Ye, Lawrence Livermore National Laboratory

10:00 AM

(EMA-S7-001-2025) Manufacturing RD&D Needs for Power Sources: From the Perspective of the U.S. DOE's Advanced Materials and Manufacturing Technologies Office (Invited)

C. Suh*[1]

1. US Department of Energy, USA

The Department of Energy's (DOE) Advanced Materials and Manufacturing Technologies Office (AMMTO) works with stakeholders to innovate in parallel to accelerate the development and adoption of transformative manufacturing technologies for power sources such as energy storage and batteries. AMMTO continues to invest in research, development, and demonstration (RD&D) of manufacturing platform technologies, enabling improved performance, manufacturability, and scalability of energy storage. Such platform technologies include additive manufacturing, power electronics, smart manufacturing, characterization, and/or computational approaches. Despite recent promising advances, continued manufacturing capability improvements remain necessary to meet the expected demand for power sources as we move towards a clean energy economy. Strengthening the domestic manufacturing supply chains are a crucial task to tackle simultaneously. AMMTO recognizes that a multi-pronged approach is required to strengthen domestic power source manufacturing and to reduce time-to-commercialization. In this session, the status and impacts of AMMTO projects will be highlighted. In addition, there will be a discussion of a wide variety of AMMTO's efforts mentioned above in the context of technical, manufacturing, and supply chain challenges.

11:00 AM

(EMA-S7-002-2025) Reinventing Manufacturing For Better Batteries (Invited) *WITHDRAWN*

A. Niestroj*[1]

1. Sakuu Corporation, Commercialization, USA

The US battery manufacturing industry is crucial in maintaining America's economic prosperity, standard of living, and national security. However, in 2024 and beyond, manufacturers are expected to face economic uncertainty, ongoing shortages of skilled labor, lingering and targeted supply chain disruptions, and new challenges spurred by the need for product innovation to meet market demand and emissions goals. It's no secret a fundamental shift is needed to improve both profits and carbon footprints. We need a better way to make better batteries. The old way of manufacturing isn't agile — to change the design of a part, significant amounts of today's factory equipment have to change. This is an unsustainable process that takes too much time, impedes innovation, and wastes resources. The future of battery production is dry process additive manufac-turing. Incorporating electrode printing technology in factories improves resilience and reduces both risk and material cost, while increasing sustainability and enabling new electrochemistries and safer batteries with a building block approach. Adopting improved production technology is the only viable way to scale a new wave of manufacturing capability, with a platform that brings dry printing capability to battery manufacturers — and it is available today. Learn how dry process additive manufacturing improves performance and reduces carbon footprint and required resources.

11:30 AM

(EMA-S7-003-2025) Electrodeposition of dense monolithic cathodes for small and large format conventional and solid-state batteries (Invited)

P. V. Braun*[1]; B. Zahiri[1]; H. Yang[2]

1. University of Illinois Urbana-Champaign, Materials Science and Engineering, USA
2. Xerion Advanced Battery Corp, USA

Conventional batteries contain composite cathodes cast as a mixture of active material, solid electrolyte, and usually conductive additives on a current collector. Such composite electrodes exhibit energy densities below the theoretical limit of an active material only cathode (a single-component cathode) due to the volume and mass of the additives and are limited to planar form factors. Via electrodeposition, we have realized nearly dense crystallographically oriented cathodes within the families of $LiCoO_2$, $NaCoO_2$, $LiMn_2O_4$, and Al-doped $LiCoO_2$ which provide near-theoretical capacities and attractive rate performances. Two unique aspects of electrodeposition are that 1) the electrode can be formed on a wide range of size and shape of current collectors, and 2) the electrodeposition process provides control of the crystallographic orientation of the deposited film which is important to enable good rate performance. We will discuss the scalability of the process, as well as microbatteries, unique form factor batteries, and solid-state batteries built using electrodeposited cathodes.

12:00 PM

(EMA-S7-004-2025) Developing Methods to Additively Manufacture Energy Storage Electrodes (Invited)

M. Worsley*[1]

1. Lawrence Livermore National Laboratory Physical and Life Sciences Directorate, USA

Electrode materials discovery and development is a popular strategy as the charge storage mechanism and electrode resistance play a key role in kinetics of the device. Within electrode materials development, engineering of the electrode pore architecture is an extremely effective strategy to decrease the diffusive transport lengths and electrode resistances. This pore engineering can be achieved through synthetic chemistry for small pores (e.g. <10 um) and via additive manufacturing for larger pores (> 10 um). Here we show how electrode materials development can be used to overcome sluggish transport in aerogel-inspired electrodes. Particular focus will be given to the use of synthetic means to tune to the properties of electrode material (e.g. surface area, pore size, mechanical properties) and 3D printing to define the larger pore structure to improve the ultimate performance of the device. We explore a number of additive manufacturing techniques (e.g. direct ink write, projection microstereolithography, etc.) to print a variety of simple and complex structures to determine the optimal electrode architecture. The impact of these different methods on both aerogel properties and device function will be discussed. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

S6 Two-Dimensional Quantum Materials-Synthesis, theories, properties and applications

S6- Two dimensional quantum materials: Synthesis, theories, properties & applications

Room: Colorado G
Session Chair: Haozhe Wang, Duke University

10:00 AM

(EMA-S6-006-2025) Atomic layer etching of lithium niobate for quantum photonics (Invited)

A. Minnich*[1]

1. California Institute of Technology, USA

Lithium niobate (LiNbO3, LN) is a ferroelectric crystal of interest for integrated photonics owing to its large second-order optical nonlinearity and the ability to impart periodic poling via an external electric field. However, on-chip device performance based on thin-film lithium niobate (TFLN) is presently limited by propagation losses arising from surface roughness on the nano- and micro-scale. Atomic layer etching (ALE) could potentially smooth these features and thereby increase photonic performance, but no ALE process has been reported for LN. Here, we report an isotropic ALE process for x-cut MgO-doped LN using sequential exposures of H2 and SF6/Ar plasmas. We observe an etch rate of 1.59 +/- 0.02 nm/cycle with a synergy of 96.9%. We also demonstrate ALE can be achieved with SF6/O2 or Cl2/BCl3 plasma exposures in place of the SF6/Ar plasma step with synergies of 99.5% and 91.5% respectively. The process is found to decrease the sidewall surface roughness of TFLN waveguides etched by physical Ar+ milling by 30% without additional wet processing. Our ALE process could be used to smooth sidewall surfaces of TFLN waveguides as a post-processing treatment, thereby increasing the performance of TFLN nanophotonic devices and enabling new integrated photonic device capabilities.

10:30 AM

(EMA-S6-007-2025) Semimetal Device Technology for 2D Semiconductor Electronics (Invited)

Y. Lin*[1]

1. Texas A&M University, Department of Materials Science and Engineering, USA

2D semiconductor has emerged as promising candidates for the channel materials in a future ultimately scaled transistor technology. A number of challenges still remain both in terms of material processing and device technologies. The weak interlayer coupling and the unique mesoscopic physics of semimetal/2D semiconductor heterostructures have shown great promises to address some of these fundamental challenges and have demonstrated viable pathways towards scalable and high-performance electronic device technologies based on 2D semiconductors. This talk will summarize our recent research efforts on the material processing and device technologies for semimetal/2D semiconductor electronics. First, I will discuss a wafer-scale semi-automated dry transfer process for monolayer CVD transition-metal dichalcogenides (TMDs) utilizing the weakly coupled interface between semimetal (Bi) and TMDs. Second, our recent progress of semimetal contacts (Bi, Sb) to 2D TMDs for high performance n-type field effect transistor (nFET) technologies will be covered. The thermal stability of these contact technologies will also be evaluated. Finally, I will talk about our computational efforts on the searching of pinning free semimetallic p-type contacts to 2D TMDs.

11:00 AM

(EMA-S6-008-2025) The Resurrection of Tellurium as an Elemental van der Waals Semiconductor (Invited)

P. Ye*[1]

1. Purdue University, USA

The graphene boom has triggered a widespread search for novel elemental van der Waals materials thanks to their simplicity for theoretical modelling and easy access for material growth. Group VI element tellurium is an unintentionally p-type doped narrow band gap semiconductor featuring a one-dimensional chiral atomic structure which holds great promise for next-generation electronic, optoelectronic, and piezoelectric applications. In this talk, we first review recent progress in synthesizing atomically thin Te two-dimensional (2D) films and one-dimensional (1D) nanowires. Its applications in field-effect transistors and potential for building ultra-scaled Complementary metal–oxide–semiconductor (CMOS) circuits are discussed. We will also overview the recent study on its quantum transport in the 2D limit and progress in exploring its topological features and chiral related physics. We envision that the breakthrough in obtaining high-quality 2D Te films will inspire a revisit of the fundamental properties of this long-forgotten material in the near future.

11:30 AM

(EMA-S6-009-2025) High-Throughput Search and Prediction of New Two-Dimensional 4f-Magnets

L. Hou*[1]; Y. Li[1]; C. Lane[2]

1. Los Alamos National Laboratory, USA
2. Los Alamos National Lab, Theoretical Division, USA

The development of next-generation microelectronics, signal processing, and data storage systems calls for the discovery of new two-dimensional (2D) materials with novel electronic functionalities that can be miniaturized and integrated with silicon. f-electron systems promote a rich set of novel phases of matter that emerge from the intertwining and competition of spin–orbit coupling, electron–electron interactions, and the hybridization between itinerant and local electrons, however, very little attention has been devoted to exploring the 4f compounds for new promising 2D materials. To address this gap in the field we employ a high-throughput search that combines first-principle and many-body perturbation theory calculations to identify and predict the properties of new 2D rare earth compounds. Specifically, we find 295 candidate 2D rare earth compounds that exhibit a spectrum of lattice symmetries, exfoliation energies, magnetic instabilities, and electronic properties that pave the way for innovative applications in advanced electronic devices. This study not only lays the groundwork for future systematic investigations into the correlation-driven properties of 4f systems, but also highlights the untapped potential of 4f compounds in the rapidly evolving field of 2D materials

11:45 AM

(EMA-S6-010-2025) Atomic substitution approach for non-vdW 2D materials (Invited)

X. Ling*[1]

1. Boston University, Department of Chemistry, USA

Atomically thin materials often exhibit extraordinary chemical, optical, electronic, and magnetic properties compared with their bulk 3D counterparts, enabling a variety of applications for next generation electronics and quantum information technologies. While extensive research has been conducted on 2D van der Waals (vdW) materials such as graphene, transition metal dichalcogenides (TMDs), and hexagonal boron nitride (hBN), little attention has been given to non-vdW materials, which make up the majority of materials in nature. One significant challenge is the lack of an effective synthesis method to access them. In this talk, I will introduce an atomic substitution approach that we have developed to convert vdW layered materials to ultrathin non-vdW materials. This approach is universal, enabling the synthesis of diverse unconventional 2D materials with tunable thicknesses, desired dimensions, and properties for fundamental physics investigations and nanodevices. As a model system, we will demonstrate the conversion of MoS_2 to MoN_x, investigate the conversion process and dynamics, and highlight the benefits of this approach in creating new 2D heterostructures as essential building blocks for 2D electronics.

12:15 PM

(EMA-S6-011-2025) Controlled Morphology and Crystallinity of (200) SnSe Grown by Pulsed Laser Deposition

M. Frye*[1]; J. R. Chin[1]; J. Knight[1]; V. Pozzi[1]; L. M. Garten[1]

1. Georgia Institute of Technology, School of Materials Science and Engineering, USA

SnSe has a thickness dependent band gap and carrier mobility, but unlike other 2D materials the interlayer binding energy limits the ability to use exfoliation for layer control. Thus, a direct growth method is needed to control the layering of SnSe. Pulsed laser deposition (PLD) is proposed as a route to deposit SnSe with precise layer control using the ability to tune adatom energy through laser fluence and substrate temperature. We systematically varied the laser fluence, substrate temperature, background gas, and throw distance during PLD growth of SnSe on (001) mica and (100) MgO to control the adatom energy and growth rate. The films grown across a wide range of deposition conditions formed in the Pnma phase of SnSe oriented (200) out-of-plane, determined by x-ray diffraction and Raman spectroscopy. The consistent orientation across different growth parameters indicates that the (200) is the energetically stable orientation of SnSe. Thickness control is maintained down to 2 nm, approximately 4 monolayers. Increasing throw distance reduced the surface roughness of the films from 1.4 nm to 0.4 nm while simultaneously decreasing the (400) rocking curve FWHM from ~3° to 0.18° for 15 nm films, indicating an increase in crystalline orientation. The methods developed in this work open new avenues to synthesize of a wide range of 2D layered materials with controlled thickness and crystallinity.

S11 Complex oxide thin films and heterostructures- from synthesis to strain/interface-engineered emergent properties

S11- Ferroelectric Oxide Thin Films and Heterostructures

Room: Colorado A
Session Chair: Shriram Ramanathan, Rutgers University

10:00 AM

(EMA-S11-008-2025) Highly tunable magnetocrystalline anisotropy energies in magnetically-doped ferroelectric oxides (Invited)

E. Nowadnick*[1]; B. Barker[2]; H. Ahmad[1]; N. Pokhrel[1]; M. Hossain[1]; K. Inzani[3]; S. Griffin[4]

1. University of California, Merced, USA
2. Florida Polytechnic University, USA
3. University of Nottingham, United Kingdom
4. E O Lawrence Berkeley National Laboratory, USA

Electric field control of single spins can probe the atomic-scale limits of multiferroic behavior. One platform to explore this scenario is to form isolated spin centers in ferroelectric materials via inclusion of dilute concentrations of magnetic dopants. The preferred orientation of a spin is connected to its local crystallographic environment via the spin-orbit interaction, and is described by the magnetocrystalline anisotropy energy (MCAE). In a ferroelectric material, structural changes that occur during polarization switching can modify the local crystalline environment of a magnetic dopant, which provides a path towards electric field control of spin directionality. This talk will present density functional theory calculations of the MCAE of isolated Fe^{3+} dopant atoms in the tetragonal, orthorhombic, and rhombohedral phases of the prototypical ferroelectric $BaTiO_3$. Our calculations reveal a highly tunable MCAE, which changes by an order of magnitude as $BaTiO_3$ traverses these structural phases of different symmetries. This evolution of the MCAE is linked to changes in the local crystal field environment of the Fe^{3+} dopant atom, which can be further tuned by application of epitaxial strain in thin films. We formulate design principles for achieving large and tunable MCAEs, and discuss extensions of these ideas to other ferroelectric hosts and magnetic dopant atoms.

10:30 AM

(EMA-S11-009-2025) Oxygen Transport During Electric Field Cycling and Retention Testing in Ferroelectric Hafnium Zirconium Oxide Thin Films

L. Shvilberg*[1]; F. J. Vega[4]; C. Zhou[3]; B. L. Aronson[2]; T. E. Beechem[4]; J. Ihlefeld[1]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. University of Virginia, USA
3. NC State University, USA
4. Purdue University, Mechanical Engineering, USA

The promise of hafnium oxide-based thin films for low-power nonvolatile memory applications has led to significant research interest in this material. Of the various ferroelectric hafnia compositions, hafnium zirconium oxide (HZO) is the most broadly studied due to its thermal compatibility with complementary metal oxide semiconductor device processing. Many phenomena observed in HZO films, such as wake-up, fatigue, retention loss, and imprint, are challenges that are, in part, linked to oxygen vacancies. Point defects, including oxygen vacancies and other charge carriers, are speculated causes for poor device performance. In this presentation, isotopic oxygen tracer studies using time-of-flight secondary ion mass spectrometry will reveal extremely low diffusion coefficients, indicating that electronic carriers may dominate the observed performance issues. Tracer diffusion studies on devices subjected to field cycling and retention tests will show that oxygen motion might not be the leading cause of the discussed performance issues. Rather, electronic carriers associated with oxygen vacancies will be shown to be more consistent with the performance degradations.

10:45 AM

(EMA-S11-010-2025) Effect of precursor purge time on plasma-enhanced atomic layer deposition-prepared ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ performance

Y. Choi*[1]; B. L. Aronson[1]; M. K. Lenox[1]; L. Shvilberg[1]; C. Zhou[2]; K. Holsgrove[3]; A. Kumar[3]; A. Watson[1]; S. McDonnell[1]; J. Ihlefeld[1]

1. University of Virginia, Materials Science and Engineering, USA
2. NC State University, Analytical Instrumentation Facility, USA
3. Queen's University Belfast, School of Mathematics and Physics, United Kingdom

Hafnium oxide (HfO_2) holds great promise for applications in non-volatile memory and energy harvesting. However, its monoclinic phase lacks polarization, making it unsuitable for ferroelectric applications. Alloying with ZrO_2 (HZO) in HfO_2 stabilizes a ferroelectric phase. The most common deposition technique is atomic layer deposition (ALD), which has superior thickness control and relatively low process temperatures. Previous studies have shown the effects of different metal precursors, oxidizer precursors, and process temperatures on the ferroelectric properties of HZO. However, no mechanism has been identified to describe different phase stabilities when the metal precursor purge time varies. This presentation discusses how HZO thin film properties change when the metal precursor purge time varies during plasma-enhanced ALD. Grazing-incidence X-ray diffraction, Fourier transform infrared spectroscopy, and scanning transmission electron microscopy were used to study the changes in the crystal structure of

HZO with variation of the metal precursor purge time during the ALD process. The observed phase changes correlate to polarization and relative permittivity responses with electric field. The resulting properties are linked to changes in composition as measured using time-of-flight secondary ion mass spectrometry and X-ray photoelectron spectroscopy.

11:00 AM

(EMA-S11-011-2025) Exploring Atomic Layer Deposition of Wurtzite-Structured Zinc Magnesium Oxide Thin Films for Ferroelectric Applications

B. L. Aronson*[1]; J. Maria[2]; J. Ihlefeld[1]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. The Pennsylvania State University, Department of Materials Science and Engineering, USA

Wurtzite ferroelectrics such as zinc magnesium oxide ($Zn_{1-x}Mg_xO$) show promise for integrated microelectronics; however, depositing these materials as thin films in 3D geometries remains a challenge. Atomic layer deposition may be useful in depositing these films conformally into 3D structures so long as the c-textured wurtzite structure and ferroelectric properties are maintained. In this work, the role of processing conditions on wurtzite phase stability is investigated for $Zn_{1-x}Mg_xO$ grown using atomic layer deposition. X-ray diffraction is utilized to assess the phase, texture quality, and lattice parameters in the deposited films. $Zn_{1-x}Mg_xO$ deposited in the composition range of x=0 to x=0.27 results in films exhibiting single phase c-textured wurtzite structure. Deposition plasma conditions including pressure and oxygen content progressively impact the wurtzite phase stability upon approaching the measured solubility limit of x=0.27. With increasing Mg content up to x=0.27, a plasma pressure and oxygen content of at most 220 mTorr and 15%, respectively, are necessary for wurtzite-structured $Zn_{1-x}Mg_xO$ formation. Wurtzite-favorable deposition plasma conditions were quantitatively studied using optical emission spectroscopy and a retarding field energy analyzer to understand the plasma species and corresponding energetics needed for wurtzite formation.

11:15 AM

(EMA-S11-012-2025) Electrode Elastic Modulus as the Dominant Factor in the Capping Effect in Ferroelectric Hafnium Zirconium Oxide Thin Films

M. K. Lenox*[1]; M. Islam[3]; M. Bin Hoque[3]; C. Skidmore[4]; A. Salanova Giampaoli[1]; S. Fields[2]; S. Jaszewski[5]; J. Maria[4]; P. Hopkins[3]; J. Ihlefeld[1]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. US Naval Research Laboratory, Materials Science and Technology, USA
3. University of Virginia, Mechanical and Aerospace Engineering, USA
4. Pennsylvania State University, Materials Science and Engineering, USA
5. Sandia National Laboratories, USA

Recent studies have revealed that several mechanisms, including a tensile biaxial stress, used to stabilize the ferroelectric phase (o-phase) of hafnium zirconium oxide (HZO), are impacted by electrode material selection when fabricated in conventional metal-ferroelectric-metal geometries. This work describes correlations between electrode and ferroelectric HZO remanent polarization (P_r) response through the lens of the elastic modulus (E) of the electrode material. TaN/HZO/TaN/M devices, where M is platinum, TaN, iridium, tungsten, and ruthenium, were fabricated. Two-dimensional X-ray diffraction, utilized to derive the $\sin^2(\psi)$ in-plane biaxial stress in the HZO, revealed a strong correlation between stress and E. Polarization-electric field (P(E)) measurements showed dependence of P_r on measured E. Increasing electrode E results in a greater resistance to deformation, which when deposited prior to annealing the HZO to crystallize from the amorphous state, restricts the out-of-plane expansion of the HZO, increasing biaxial stress and promoting the stabilization of the ferroelectric orthorhombic phase, in a phenomenon known as the "capping effect". This work further promotes the acceleration integration of HZO into MFM devices, such a non-volatile memory devices.

11:30 AM

(EMA-S11-013-2025) Active and dynamic photonic devices enabled by non-centrosymmetric oxide thin films (Invited)

D. Barton*[1]

1. Northwestern University, Materials Science and Engineering, USA

The lack of centrosymmetry in many crystals enables useful optical and photonic effects through a nonlinear contribution to the electronic polarizability tensor that underpin modern telecommunications. Specifically, optical frequency conversion and electric field-controlled changes to the refractive index (the Pockel's effect) enable the ability to control the propagation of light in space and time. Emerging platforms based on nanostructured thin films promise a new generation of photonic systems for efficient communications and computation. This presentation will highlight some device demonstrations only possible with nanofabricated thin films of high bandgap ferroelectrics. First, we will show how to create femtosecond pulses of light on a chip the size of a penny using microwave fields and nanostructured thin films of lithium niobate. We will discuss a few other device demonstrations enabled by this platform, and will end with a vision of future opportunities enabled by emerging high bandgap non-centrosymmetric oxide thin films. Notably, control of ferroelectric domain orientation at micron length scales can unlock new possibilities in computing and communications, while developing new thin film materials with enhanced optical properties can enable stronger light-matter interactions, promising dense scaling of electro-optic devices akin to the modern semiconductor revolution.

12:00 PM

(EMA-S11-014-2025) Tunable electrochemical activity in ferroionic CeO2/BTO thin films *WITHDRAWN*

M. Vasiljevic*[1]; V. Esposito[1]

1. Danmarks Tekniske Universitet, DTU Energy, Denmark

This study investigates the potential of combining multifunctional materials to develop artificial catalysts that may outperform traditional noble metals in catalysis. We employed ferroionic heterostructures, grown by Pulsed Laser Deposition (PLD), integrating defective cerium oxide (CeO2-δ) with ferroelectric barium titanate (BaTiO3, BTO), to explore how the polarization of the BTO layer influences charge concentration and catalytic activity of ceria. By engineering BTO films with controlled polarization directions, confirmed by Piezoresponse Force Microscopy (PFM), and examining the defect chemistry of the ceria layer through Kelvin Probe Force Microscopy (KPFM), we observed significant changes in the reduction and oxidation states at the interface. Our results indicate that the ceria termination dynamically responds to the polarization at the BTO layer, enabling effective modulation of water adsorption-desorption dynamics and redox overpotentials within ±400 mV at room temperature. These findings demonstrate that the polarization-driven properties of the ferroionic design can be harnessed to tune the catalytic performance of ceria thin films, offering a promising approach to reducing reliance on rare noble metals in catalytic processes.

12:15 PM

(EMA-S11-015-2025) Nano-volumetric Characterization of BCT-BZT Ferroelectric Superlattice with Tomographic PFM

K. Lizu*[2]; A. Chen[1]; B. Huey[2]

1. Los Alamos National Laboratory, Center for Integrated Nanotechnologies (CINT), USA
2. University of Connecticut College of Engineering, Materials Science & Engineering, USA

Ferroelectric materials have garnered significant interest due to their compatibility with CMOS technology, with potential impact on next-gen memory storage devices, quantum computing, and smart energy solutions. Piezoresponse Force Microscopy (PFM) has emerged as a powerful tool with exceptional nanoscale resolution for the characterization of ferroelectric materials. In this study, we investigate BCT-BZT superlattice with our novel tomographic Atomic Force Microscopy (T-AFM) technique. When combined with PFM, it circumvents the limitation of traditional AFM as a surface characterization tool by instead enabling nano-volumetric piezoelectricity mapping. Applied to heteroepitaxial superlattices of BCT-BZT, with layer thicknesses and strain tuned to investigate and optimize ferroelectricity, reveals layer dependent piezoelectricity and even interfacial strength with depth resolution better than 5 nm. Our T-AFM analysis of this Pb-free ferroelectric system thus provides new insights into fundamental mechanisms for these materials, especially the effects of local strain coupling, contributing to the eventual implementation of sustainable ferroelectric and piezoelectric device applications.

S13 Defects and transport in ceramics

S13- Defects and Transport in Ceramics IV

Room: Colorado H
Session Chairs: Nicola Perry, University of Illinois at Urbana-Champaign; Thomas Defferriere, Massachusetts Institute of Technology

10:00 AM

(EMA-S13-016-2025) Exploring Oxygen-Ion Transport Kinetics via In Situ Isotope Exchange Raman Spectroscopy (IERS) (Invited)

M. Burriel*[1]

1. Centre National de la Recherche Scientifique, LMGP, France

The Isotope Exchange Raman Spectroscopy (IERS) technique is based on the continuous measurement of a specific Raman mode of a given material (such as an oxide) while it is exposed to an isotope-enriched atmosphere (e.g. ^{18}O) within a temperature-controlled environment. It allows for estimating the isotopic concentration as a function of time (and/or position), facilitating the measurement of ion transport kinetics, including oxygen surface exchange and diffusion coefficients, in functional materials. This innovative approach was first developed for gadolinium-doped ceria (CGO), a well-known ionic conducting oxide typically used as an electrolyte in solid oxide cells.[1] For thin films, we demonstrated that employing various sample configurations allows for the in situ measurement of both in-plane and out-of-plane kinetic coefficients. In addition, the IERS technique has been further developed and expanded to the study of several mixed ionic electronic perovskites thin films, but also bulk materials and composites. During my presentation, I will discuss the latest findings, as well as the advantages and limitations of the technique. [1] A. Stangl, et al, Adv. Mater. 2023, 35, 1.

10:30 AM

(EMA-S13-017-2025) Leveraging defects for optimal stability-activity tradeoff in mixed conductors

F. Baiutti*[1]; J. Sirvent[1]; F. Chiabrera[2]; A. Morata[1]; A. Tarancon[3]

1. IREC, Spain
2. Institut de Recerca en Energia de Catalunya, Spain
3. ICREA/IREC, Spain

In this contribution, we present specific examples demonstrating how defect engineering can be effectively utilized to enhance the electrochemical performance and long-term stability of thin-film perovskites for high-temperature applications. For 0-dimensional defects (cationic substitution), we explored co-doped materials within the La,Sr(Co,Mn,Fe)O_3 family using combinatorial thin-film synthesis and advanced characterization techniques, including high-throughput methods. The results provide a map of structural and electrochemical properties that directly correlate with the B-site cation composition. Interestingly, while Fe- and Co-rich compositions exhibit the highest electrochemical performance, the presence of Mn plays a crucial role in stabilizing the material at high temperatures by minimizing the formation of Sr-rich secondary phases. In another example focusing on high-dimensional defects, we present recent progress in studying oxygen transport properties at grain boundaries. Special attention is given to the local chemical characterization of fast-conducting boundaries, using advanced techniques like high-resolution TEM and isotope-APT. Specifically, for Sr-doped lanthanum chromite, our analyses revealed a four-order-of-magnitude increase in oxygen diffusivity compared to the bulk. Comparative analyses with other systems will also be discussed.

10:45 AM

(EMA-S13-018-2025) Oxygen diffusion in amorphous metal oxides for resistive memory and other microelectronic applications (Invited)

Y. Li*[1]

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

Amorphous thin-film metal oxides are used in many microelectronics devices due to their low-temperature deposition and conformal coating. Understanding oxygen diffusion rates is critical in determining the speed, retention, and endurance of these microelectronic devices. We present our recent reserach on oxygen diffusion in amorphous tantalum and hafnium oxide. Our key findings are that the density of amorphous thin films can be tuned by tens of degrees based on the processsing conditions without composition changes, and that this difference in density can tune the ionic conductivity by over two orders of magnitude. Furthermore, we show how nonideal oxygen diffusion as a result of phase separation controls oxygen diffusion kinetics in resistive memory and enable such devices to store information over long periods of time.

11:15 AM

(EMA-S13-019-2025) Revealing the surface termination effect of (La,Sr)FeO_{3-X} for oxygen exchange reaction (Invited)

D. Chen*[1]

1. Tsinghua University, China

Surface termination structure plays a critical role in the activity and reaction mechanism of solid/gas interface reactions. However, precise control of uniform single termination for electrochemical solid/gas reactions remains challenging. In this study, we developed an atomically flat epitaxial (La,Sr)FeO_{3-x} thin film (Figure 1) to understand how a single atomic termination influences oxygen exchange activity and the corresponding reaction mechanism. Specially, the oxygen exchange activity exhibited a typical volcano-shaped relationship with surface termination. A single terminated LSF demonstrated the highest activity compared to other counterparts under both equilibrium and polarization conditions, showing up to more than 30-fold enhancement. A framework combining experimental micro-kinetic analysis through electrochemical and operando spectroscopic measurements with density functional theory calculation reveals that single termination induces a switch in the rate-determining step from a sole oxygen dissociation step to two comparable steps by significantly reducing the energy barriers for oxygen dissociation. This study emphasizes the critical role of the top surface termination in regulating oxygen exchange kinetics and reaction mechanisms. Furthermore, this work provides a new framework applicable to extensive structure-activity studies on diverse solid/gas interface reaction systems.

11:45 AM

(EMA-S13-020-2025) Modeling surface atomic structure of perovskite oxide $La_{0.6}Sr_{0.4}FeO_3$ under realistic thermodynamic conditions

B. Liu*[1]; B. Yildiz[2]

1. Massachusetts Institute of Technology, DMSE, USA
2. Massachusetts Institute of Technology, USA

$La_{0.6}Sr_{0.4}FeO_3$ (LSF) is recognized as a leading perovskite oxygen electrode, widely used in energy applications. Though catalytic reactions primarily occur on the surface, the specific interface atomic structures remain unclear. This talk will thoroughly analyze the bulk and surface thermodynamics of LSF perovskite oxides through a combination of quantum chemistry calculations and Grand Canonical Monte Carlo (GCMC). The chemical potentials are determined by choosing a physically meaningful path within the multi-component chemical potential space. These potentials are calculated based on equilibrium conditions with relevant reference states, and are derived as functions of oxygen partial pressure, oxygen/cation vacancy concentration, and the bulk composition of the system. Bulk thermodynamic calculations show the LSF phase diagram regarding decomposition reactions. Within LSF's stable regime, the stable phases under varying oxygen chemical potentials serve as reasonable initial structure guesses for GCMC simulations. GCMC simulations provide insights into the realistic surface and interface structures of LSF under different environmental conditions. Surface segregation of SrO_2, SrO, La_2O_3, and exsolution of Fe is observed at different oxygen chemical potentials. The resulting surface phase diagram highlights the predominance of SrO segregation under ambient conditions.

12:00 PM

(EMA-S13-021-2025) Predicting Point Defect Concentrations Upon Doping Using the Doping Factor Method

Y. Tsur*[1]

1. Technion Israel Institute of Technology, Chemical Engineering, Israel

The doping factor is the ratio between the concentration of quasi-free electrons in the doped state and their concentration in a reference, usually the undoped state. In binary compounds, as long as the Boltzmann statistics holds, the neutrality equation becomes a polynomial equation for the doping factor. Once the doping factor is found, all the concentrations of the native point defects are readily found. While other computational methods allow us to find those concentrations, it is healthy for the researcher to have such a simple tool for calculating the resulting new concentrations 'on the back of an envelope.' Furthermore, this method might be the only one available in cases with small deviations from stoichiometry. I will first demonstrate the method using a simple case and then discuss other examples as time permits.

S14 A1 in Materials research: from data analysis, autonomous experimentation, to human AI cooperation

S14- AI for data analysis and simulation

Room: Matchless
Session Chairs: Arpan Biswas, University of Tennessee Knoxville; Esther Tsai, Brookhaven National Laboratory

10:00 AM

(EMA-S14-001-2025) Specialized Data-Driven Framework for Predictive Synthesis of Compositionally Complex Ceramic Materials (Invited)

B. Ouyang*[1]

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.

10:30 AM

(EMA-S14-002-2025) Determining the structure and properties of defects at interfaces - a combined modeling, experiment, and AI/ML approach (Invited)

M. K. Chan*[1]

1. Argonne National Laboratory, USA

Defects including vacancies, impurities, and grain boundaries influence the properties of electronic and other materials. In some cases, the defects provide the functional properties of interest, such as in the case of defect qubits for quantum information science. The ability to determine the structure and electronic properties of defects is key to their understanding and manipulation. In this talk, we will discuss our work to use a combination of first principles modeling, spectroscopic and microscopic data, and artificial intelligence/machine learning approaches to determine the properties of defects for a variety of materials, including defects in CdTe solar cells, oxide battery materials, and hBN quantum emitters.

11:00 AM

(EMA-S14-003-2025) Seeing crystalline defects: whether magnetic frustration or structural factor is more sensitive? (Invited)

Y. Wang*[1]

1. The University of Tennessee Knoxville, Materials Science and Engineering, USA

X-ray and neutron diffraction are powerful techniques in resolving crystalline structures from the structural factors. However, for physical properties highly sensitive to crystalline imperfections, establishing a structure-property relationship requires a precision, in determining occupancy, interstitial defects, and thermal parameters, that exceed the state-of-art refinement resolution. One example of such defects-sensitive properties is magnetism in materials with competing interactions, known as magnetic frustration, where exotic states with topological ordering and/or quantum entanglement are expected to emerge. In contrast to pinning spin dynamics, as observed in spin glasses, local defects interacting with a many-body ground state potentially enhance spin dynamics thus push the system closer to the quantum regime, as suggested by our recent experiments in classical spin ice. To establish the quantitative description of such enhancement, we collected neutron and x-ray diffraction data in a series of single crystals demonstrating dynamic time scales across several decades. We compare refinement results from conventional GUI-based methods, customized Bayesian optimization, and Variational Autoencoder assisted Bayesian optimization. Using the spin ice materials for prototyping, we aim to establish the methodology to address materials defects in frustrated magnetism.

11:30 AM

(EMA-S14-004-2025) Big Data Analytics and Neural Networks for Prediction of Oxide Film Composition Using RHEED

P. Gemperline[2]; S. Harris[4]; R. K. Vasudevan[3]; R. B. Comes*[1]

1. University of Delaware, Dept. of Materials Science and Engineering, USA
2. Auburn University, Physics, USA
3. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
4. Oak Ridge National Lab, USA

Reflection high energy electron diffraction (RHEED) is a highly common form of real time analysis used in growth systems such as molecular beam epitaxy (MBE) and pulsed laser deposition (PLD). Traditional RHEED analysis focuses primarily on the intensity and shape of the diffraction pattern for a few still images taken during growth or on the intensity of a single diffraction peak in real time. While this information can be quite insightful, there is far more information that can be gleaned from RHEED, which is often qualitative and learned through many repeated trials by the film grower. In order to obtain greater insight from RHEED videos, we have developed new approaches for principal component analysis (PCA) and K-means clustering to analyze recordings of the RHEED taken during the MBE growth of epitaxial thin film perovskite oxides, including $LaFeO_3$ and $SrHfO_3$. To further enhance the utility of RHEED, we have developed a convolutional neural network that is trained on a series of $SrTiO_3$ homoepitaxial films grown via PLD. Film composition was measured via X-ray photoelectron spectroscopy (XPS) and the network was trained to estimate composition of samples grown outside of the training set. These methods yield more quantitative results from the RHEED with minimal time requirements and open the door for future real-time computer control of film growth for optimal growth conditions.

S18 Characterization of struture-property relationships in functional ceramics

S18- Advances in scattering, imaging, and analytical techniques

Room: Colorado J
Session Chair: Hadas Sternlicht, The Pennsylvania State University Department of Materials Science and Engineering

10:00 AM

(EMA-S18-017-2025) Imaging 3D crystallography down to atomic resolution using 4DSTEM (Invited)

I. MacLaren*[1]; A. Silinga[1]; C. Allen[3]; A. Kirkland[3]; J. Barthel[4]; J. MacManus-Driscoll[2]

1. University of Glasgow, School of Physics and Astronomy, United Kingdom
2. University of Cambridge, Dept. of Materials Science, United Kingdom
3. University of Oxford, Department of Materials, United Kingdom
4. Forschungszentrum Julich GmbH, Ernst Ruska Centrum für Mikroskopie und Spektroskopie mit Elektronen, Germany

Thin films have often been studied by either projection imaging using HAADF or possibly BF/ABF imaging in the STEM. But this misses all the action happening in the third dimension, and this can, at best, only be inferred from column shapes or modelling. In some cases, discrete tomography can be used to reveal more about the interface structures, but this depends on having specimens with the same kind of interface and different surface normals. In this talk I will show that the 3D crystallography is available from imaging along a single projection when the high angle scattering is included (which contains components parallel to the beam) and can be mapped right down to atomic resolution. The atomic resolution results reveal far more information than is available in any projection image and are interpretable with the aid of multislice simulations. This is applied to double perovskite thin films grown on perovskite substrates and reveals for the first time ever atomic resolution mapping of 3D atom displacements, the detailed reason why specific unit cell orientations are promoted by specific substrates, and gives unprecedented insights into the mechanism by which the B-site ordering can be maximised for optimum properties. This also shows the more complex domain structures that can be formed when a non-optimal substrate is chosen instead.

10:30 AM

(EMA-S18-018-2025) Towards In Situ Visualization of Nanoscale and Atomic-Level Dynamics and Transport in Electroceramics (Invited)

P. Crozier*[1]

1. Arizona State University, SEMTE, USA

The ability to design structures that can regulate and control the transport functionalities of electroceramics for applications in a wide range of devices requires a fundamental understanding of structural dynamics and migration. Elucidating the relationship between local structure and transport remains an ongoing challenge for both experimental and computational techniques. Modern transmission electron microscopy (TEM) allows the structure and composition of electroceramics to be characterized down to the atomic level. However, a goal of in situ electron microscopy is to characterize the transport variations and pathways with high spatial resolution. Can transport/diffusion processes be directly observed at the atomic level? Here we use aberration corrected in situ transmission electron microscopy and deep learning denoising techniques to explore oxygen ionic dynamics and diffusion in cerium dioxide. With in situ light illumination and electron holography, we also investigate variations in the induced electric fields at nanoparticle surfaces that can drive transport processes. We demonstrate local sensing of photo-induced electronic conductivity in nanoscale particles of strontium titanate. This presentation will discuss what is currently possible from in situ TEM approaches and how the field is likely to evolve over the near future.

11:00 AM

(EMA-S18-019-2025) Measuring Polar Displacement and Lattice Strain in Ferroelastic Specimens via Precession-Enhanced Cepstral Analysis

A. Mis*[1]; C. Brown[2]; S. Dahl[2]; M. Holtz[2]

1. NIST, Physical Measurement Laboratory, USA
2. Colorado School of Mines, Metallurgical and Materials Engineering, USA

In this work, we demonstrate a precise and robust method to measure polar displacement, lattice strain, and crystalline orientation of ferroelastic specimens on the nanometer length sale. Here we employ precession electron diffraction (PED) to enhance cepstral analysis techniques of 4-dimensional scanning transmission electron microscopy (4D-STEM) data. We first apply these techniques to a reference sample of GaN and demonstrate that the addition of PED reduces the standard deviation of the lattice parameter measurement 0.56 pm to 0.32 pm. We also measure the length of the vector associated with the non-centrosymmetric nature of the unit cell, and see that its standard deviation is reduced from 3.5 pm to 1.9 pm. Computational work shows that adding precession also increases the robustness of these measurements to specimen mistilt. We then apply these techniques to study polar domains in a sample of PMN-PT, and observe domains on the 100 nm length scale.

11:15 AM

(EMA-S18-020-2025) Probing Nanoscale Optical Excitations in Low Symmetry Ceramics with Monochromated Electron Energy-Loss Spectroscopy (Invited)

J. A. Hachtel[1]; S. Woo*[1]

1. Oak Ridge National Laboratory, USA

Much of the interest in ceramics centers around their unique thermal, electronic, and magnetic properties. However, many ceramic materials also play host to a range of novel optical phenomena that have applications in nanotechnology. One exciting prospects for nanoscale optics in ceramics is phonon polaritons, where electromagnetic waves couple directly into lattice vibrations, enabling infrared light with wavelengths of tens of microns to be confined effectively to nanoscale volumes and manipulated across massive length scales. As a result, there is a fundamental need to probe these polaritons directly at the length scale of the confinement and at the frequency of the mid-infrared light. Here, I will present experiments conducted with monochromated electron energy-loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM). This technique possesses the needed simultaneous spatial and spectral resolution to measure the nanoscale behavior of polaritons, and enables highly complementary experiments to the nanoscale optical techniques (such as scanning near-field optical microscopy). I will present results on hyperbolic phonon polaritons supported in low-symmetry materials such as h-BN and β-Ga_2O_3, and show how the spatial profile of polaritonic response can be used to extract critical information of the underly polariton dispersion.

11:45 AM

(EMA-S18-021-2025) In-situ characterization of the high-temperature spin-state transition in $LaCoO_3$ via STEM imaging and EELS (Invited)

M. A. Smeaton*[1]; E. Salagre[2]; E. J. Fuller[3]; K. L. Jungjohann[1]

1. National Renewable Energy Laboratory, USA
2. Sandia National Laboratories California, USA
3. Sandia National Laboratories California, Materials Physics, USA

In-situ measurements of switching behavior in neuromorphic devices provide crucial insights for the optimization of materials and device architectures. The combination of high spatial and energy resolution in scanning transmission electron microscopy (STEM) makes it a particularly powerful tool for simultaneously probing lattice, electronic, and spin degrees of freedom at the nanoscale. Transitions involving these degrees of freedom are core to neuromorphic functionality, which seeks to emulate neurons and synapses in the brain by controllably and reversibly tuning electrical conductivity. Here, we leverage in-situ STEM imaging and spectroscopy to track the intermediate-to-high spin transition in $LaCoO_3$, which is correlated with current-driven oscillatory behavior recently demonstrated in devices. We first investigate this transition through in-situ heating in the STEM and then extend the analyses to in-situ I/V measurements on a working device. These capabilities and the insights they generate will be instrumental in optimizing and developing materials for neuromorphic devices.

12:15 PM

(EMA-S18-022-2025) Electric field measurement in GaAs and GaInP solar cells using differential phase contrast and precession scanning transmission electron microscopy

E. Supple*[1]; K. Bertness[1]; A. Mis[1]; J. Geisz[2]; A. Roshko[1]

1. National Institute of Standards and Technology, USA
2. National Renewable Energy Laboratory, USA

Characterization of electric fields at interfaces in microelectronic devices is necessary to improve device design and to advance theoretical understanding of these interfaces. Differential phase contrast in the scanning transmission electron microscope measures the momentum shift of transmitted electrons due to electric field in the specimen. Unfortunately, signal is also generated by dynamical diffraction effects, limiting quantification of the electric field. Electric fields with variation on the scale of the electron probe also cause intensity redistribution within the direct beam that is not fully captured by segmented annular detectors. We use precession electron diffraction to reduce dynamical contributions to the diffraction pattern and a direct electron detector to measure the center of mass shift of the entire direct beam in an effort to improve accuracy and precision of the DPC measurement. We apply this technique to GaAs and InGaP solar cells to quantify electric field at interfaces in the device and analyze the effect of experimental conditions on measurement accuracy and precision. Experimental results are also compared with nanoscale modeling taking into account the TEM specimen geometry and resulting band structure.

S20 Magnetic and superconducting materials-from basic science to applications

S20- Low Dimensional Correlated Magnetic Materials I

Room: Colorado D
Session Chair: Sara Mills, US Naval Research Laboratory

10:00 AM

(EMA-S20-001-2025) Spin Entanglement in 2D Dimer Magnets (Invited)

H. Cao*[1]

1. Oak Ridge National Lab, Neutron Scattering Division, USA

Magnetic frustration disrupts conventional magnetic ordering, leading to exotic magnetic states such as quantum spin liquid, spin ice, spin glass, and intricate magnetic orders with incommensurate, noncollinear, or noncoplanar spin arrangements. Polarized neutron diffraction is a powerful tool for probing local spin properties, including single-ion and exchange magnetic anisotropy, in small crystal samples. Utilizing this method, we have uncovered several intriguing quantum and topological states and are progressing towards more challenging inelastic neutron scattering measurements to further establish these magnetic ground states. In this presentation, I will discuss spin entanglement in spin dimer systems as studied through neutron scattering technique. *The research was supported by the U.S. Department of Energy (DOE), Early Career Research Program Award KC0402020 and used resources at the HFIR and SNS, DOE Office of Science User Facilities operated by ORNL.

10:30 AM

(EMA-S20-002-2025) Complex Magnetism and Its Coupling with Transport in Layered $Mn_{2-x}Zn_xSb$ (Invited)

M. Rafique Un Nabi[1]; R. Basnet[1]; G. Acharya[1]; D. Upreti[1]; S. Karki Chhetri[1]; J. Hu*[2]

1. University of Arkansas, USA
2. University of Arkansas, Physics, USA

The rapid development of two-dimensional (2D) magnetic materials has fueled the exploration of novel magnetic properties and their potential applications. So far, most 2D magnets are based on hexagonal or near-hexagonal magnetic lattices. Identifying new 2D magnetic materials, especially those with different lattice symmetries, could significantly enhance our understanding of 2D magnetism. $Mn_{2-x}Zn_xSb$ is a prime example. Derived from the Cu2Sb-type tetragonal layered compound Mn2Sb, Zn substitution induces a range of magnetic behaviors in $Mn_{2-x}Zn_xSb$, including various ferrimagnetic, antiferromagnetic, and room-temperature ferromagnetic states. These rich magnetic phases are accompanied by unusual electronic transport properties, with magnetism-driven transport anomalies and even metal-to-insulator-like transitions. Furthermore, $Mn_{2-x}Zn_xSb$ stabilizes non-trivial spin textures, such as magnetic skyrmions, at high temperatures, along with a pronounced topological Hall effect across a wide compositional range. These characteristics, combined with the ability to obtain thin flakes via mechanical exfoliation, present promising opportunities for spin-based device applications. We acknowledge the MonArk NSF Quantum Foundry DMR-1906383, NSF Career Award DMR-2238254, and DOE Career Award DE-SC0019467. Ref: Adv Phys Res, 2300145 (2024); Acta Mater 259, 119251 (2023); PRB 104, 174419 (2021).

11:00 AM

(EMA-S20-003-2025) Growth and Properties of Layered Magnetic Materials (Invited)

A. May*[1]

1. Oak Ridge National Laboratory, USA

The development of new technologies that harness quantum materials will rely on an ability to predict and control complex electronic and magnetic phenomena. Single crystal growth and characterization play a vital role in the foundational studies necessary for developing the theoretical understanding and practical knowledge required for these lofty goals. In this talk, we will discuss the coupling of magnetism, structure and transport properties in emerging layered materials.

11:30 AM

(EMA-S20-004-2025) Spectrum Insight in Magnetism with A Twist (Invited)

X. Wang*[1]

1. Washington University in St Louis, Physics, USA

Moiré superlattices of two-dimensional (2D) materials are an emerging platform for studying new physical phenomena with high tunability. Strong excitonic responses in 2D semiconductors allow optical access to the wealth of physics. In this talk, I will present our results about interactions between excitons and charge carriers trapped in moiré potentials. We have discovered novel exciton many-body ground states composed of moiré excitons and correlated electron lattices, resulting from new interaction between exciton and charges enabled by unusual quantum confinement in 2D moiré superlattices. The interaction further enriches the magnetic phases in such moiré superlattices. We have observed that the spin-spin interactions between moiré trapped holes can be drastically tuned by optical excitation power. The mechanism points to the unique excitons-mediated long-range exchange interaction between moiré trapped carriers. This discovery adds a new and dynamic tuning knob to the rich many-body Hamiltonian of moiré quantum matter. Our work provides the framework for understanding and engineering electronic and excitonic states in moiré quantum matters.

12:00 PM

(EMA-S20-022-2025) Highly Tunable Superconductivity at the $KTaO_3$ Interfaces (Invited)

K. Ahadi*[1]

1. The Ohio State University, USA

2D superconductivity is a fertile landscape for exotic quantum phenomena. Rashba and Gor'kov suggested that the interfaces with broken inversion symmetry could be an ideal platform for unconventional 2D superconductivity, including finite momentum and triplet pairing, with enhanced critical field beyond Pauli limit. The nature of superconductivity and its interplay with strong spin–orbit coupling at the $KTaO_3(111)$ interfaces remain a subject of debate. This talk will focus on our recent experiments of epitaxial growth and superconductivity of $KTaO_3$ heterostructures. Superconductivity at $KTaO_3$ interfaces is robust against the in-plane magnetic field, with the critical field of superconductivity reaching ~25 T in optimally doped heterostructures. The superconducting order parameter is highly sensitive to the carrier density and orientation of the magnetic field. The strong violation of Pauli limit for the upper critical field of the $KTaO_3$ interfaces is due to spin–orbit coupling which motivates the formation of anomalous quasiparticles with vanishing magnetic moment. These results offer design opportunities for superconductors with extreme resilience against the applied magnetic fields.

*Denotes Presenter

12:30 PM

(EMA-S20-006-2025) Exploiting the angular dependency of the magnetic anisotropy for sub-THz devices utilizing hexaferrites

D. Hedlund*[1]; P. Kulik[1]

1. University of Central Florida, Department of Electrical and Computer Engineering, USA

An approach to exploiting the angular dependency of the magnetic anisotropy of a hexaferrite for sub-THz devices will be described, along with spin-wave evolution due to rotation along the crystallographic axes. High-frequency devices, like those in 6G telecommunications (30 to 3000 GHz), cannot use traditional materials due to physical limitations. Dielectric relaxation typically occurs below 10 GHz, and other materials have issues like skin effects, thermal management and size. Hexaferrites are materials suitable for high frequency applications, are made from abundant elements and can be designed to fit many needs. We studied the dynamical magnetic properties of a macroscopic single crystal hexagonal ferrite, grown with a flux-melt technique. The measurements were performed using a quasi-optical resonance technique with a maximum frequency of 120 GHz. Measurements were performed in field-swept mode, with a maximum applied field of 5 T. Angular-dependent measurements along both crystallographic axes captured the crystal's symmetry, allowing analysis of spin-wave evolution across frequency, field, and rotation. Using these measurements, we studied spin-wave evolution over frequency, field and rotation. We analyzed the results using well-known dispersion relationships and show how frequency tunable devices can be engineered exploiting the angular dependency of the anisotropy.

S22 Advanced Electronic Materials- Processing structures and applications

S22- Advanced electronic materials, including ferroelectric, piezoelectric, dielectric, electrostrictive, and pyroelectric materials

Room: Colorado F

Session Chairs: Hana Uršič, Jozef Stefan Institute; Keisuke Yazawa, Colorado School of Mines

10:00 AM

(EMA-S22-019-2025) $BiFeO_3$-$BaTiO_3$ for High-Temperature Piezoelectric Applications: Synthesis, Defect Studies and Nonlinear Harmonic Analysis (Invited)

A. Iacomini*[1]; J. Roknić[1]; H. Uršič[2]; T. Rojac[2]

1. Institut Jozef Stefan, Electronic Ceramics Department K5, Slovenia
2. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia

$BiFeO_3$-$BaTiO_3$ (BFO-BT) emerges as a promising lead-free ferroelectric system for high-temperature piezoelectric applications. This study focuses on synthesizing and investigating BFO-BT ceramics, addressing current challenges related to heterogeneous composition and low DC electrical resistivity. Mechanochemical activation (MA) proves efficient in producing high-quality BFO-BT ceramics with high densities (>93% of theoretical) and minimal core-shell structures and secondary phases. Point defect studies were conducted by evaluating electrical conductivity and Seebeck coefficient under various temperatures (25–700°C) and O_2 partial pressures (10^{-6}–1 atm) to address in situ redox processes, oxygen non-stoichiometry, and defect states. Temperature- and field-dependent piezoelectric harmonic analysis on Mn-doped morphotropic composition (~0.67 mol BFO) revealed a nonlinear response resembling that of lead-based relaxor ferroelectrics, like $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT), suggesting the key role of BFO-BT's relaxor nature in its piezoelectric response. The study highlights BFO-BT potential as a prime candidate for high-temperature piezoelectric applications, offering a viable alternative to lead-based systems by addressing composition heterogeneity and electrical resistivity challenges through defect engineering and systematic point defect investigation.

10:30 AM

(EMA-S22-020-2025) PZ-based antiferroelectric ceramics for dielectric cooling

B. Rozic*[2]; B. Asbani[4]; H. Uršič[3]; M. El Marssi[4]; R. Pirc[1]; M. Morgan[2]; Z. Kutnjak[2]

1. Jozef Stefan Institute, Slovenia
2. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia
3. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia
4. Université de Picardie Jules Verne, LPMC, France

The electrocaloric (EC) effect has attracted great interest in developing new cooling devices that have the potential to reach better efficiency than the existing cooling technologies. This contribution will present our direct measurements of the large EC effect in antiferroelectric PbZrO3 (PZ) based ceramics. In addition, the EC effect in antiferroelectric n/95/5 PLZT ceramics will be investigated by direct experiments, including the compositions with coexisting ferroelectric and antiferroelectric order such as 6/40/60 PLZT ceramics. The annealing effect on EC response will be discussed. It will be shown that under certain conditions, both inverse and positive EC responses can be arbitrarily invoked in antiferroelectric materials by adequately controlling the electric field and temperature, which significantly enhances the electrocaloric cooling power.

10:45 AM

(EMA-S22-021-2025) Stress- and temperature-dependent tailoring of functional properties in antiferroelectric $AgNbO_3$

N. H. Khansur*[1]

1. Case Western Reserve University, Materials Science and Engineering, USA

Although there have been a number of energy storage solutions presented, including fuel cells, electrochemical batteries, and supercapacitors,[4] solid-state dielectric ceramic capacitors remain important for energy storage applications due to the exceptional power densities (~10^4 - 10^5 W/kg) that can be orders of magnitude higher than other technologies, resulting from their fast charge-discharge times (~ns-μs). This, in addition to low cost, high thermal (>150 °C) and mechanical stability, and low fatigue (>10^6 cycles), has made solid-state capacitors an indispensable technology for pulse power applications in, for example, DC/DC converters for electromobility, medical defibrillators, high-power lasers, electromagnetic devices, electric propulsion systems, and commercial pulse forming networks. Antiferroelectric $AgNbO_3$ is one of the most interesting compositions for high-energy storage responses. However, the influence of external perturbations on the functional properties and structural phase transitions is not well established. This presentation will discuss the influence of temperature and compressive stress on the structure-property relationships in $AgNbO_3$. A suite of in situ structure-microstructure-property characterization methods was utilized to provide a comprehensive understanding and highlight the possible ways to engineer the functional properties.

11:00 AM

(EMA-S22-022-2025) Enhancing Vertical Ferroelectric Properties in Aurivillius Phase Thin Films (Invited)

D. Dutta[1]; T. Simonian[2]; M. Schmidt[3]; S. Hussain[1]; V. Nicolosi[2]; L. Keeney*[1]

1. Tyndall National Institute, University College Cork, Advanced Materials and Surfaces Group, Ireland
2. Trinity College Dublin, School of Chemistry, Ireland
3. Tyndall National Institute, Speciality Products and Services, Ireland

Aurivillius phase materials are valuable ferroelectrics in technology, renowned for their fatigue resistance, enabling their commercial application in ferroelectric random access memory. Despite their

promising attributes, incorporating Aurivillius phases into miniaturized devices presents significant challenges, primarily because their polarization is largely confined to the in-plane direction. This creates a challenge for industries that rely on out-of-plane (OOP) polarization for compatibility with conventional vertical devices. To address this, industrially relevant Direct Liquid Injection Chemical Vapor Deposition processes were developed to enhance OOP polarization in odd-layered films. By controlling supersaturation and oxygen partial pressure, the growth mechanism is directed to proceed through either 2D nucleation/growth or dislocation-mediated spiral growth. Piezoresponse force and atomic resolution electron microscopy studies reveal that samples exhibiting growth-spiral morphology and associated dislocations show enhanced OOP ferroelectric properties. Notably, the minimum vertical switching voltage is reduced from ±20V to ±5V. The improvement is attributed to disruptions in elastic strain, electrostatic energy and local symmetry-lowering distortions within the lattice. These findings provide valuable insights into the tailored growth of Aurivillius phases for targeted device applications.

11:30 AM

(EMA-S22-023-2025) Reversible dynamics of ferroelectric domain walls

N. Domingo Marimon*[1]; S. Raghuraman[1]; K. Kelley[1]; R. K. Vasudevan[1]; M. Zahn[2]; S. Neumayer[1]; J. Schultheiss[2]; D. Meier[2]; S. Jesse[1]

1. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
2. Norges teknisk-naturvitenskapelige universitet Fakultet for naturvitenskap, Department of Materials Science and Engineering, Norway

The dynamics of ferroelectric domain walls which determine the dynamics of ferroelectric switching are known to depend on several factors such as bulk structure and boundary conditions, being very sensitive to defects, chemical and structural pinning sites. However, domain walls also show a sub-coercive field dynamics as a reversible motion, with vibrational states that strongly coupled to local structure and composition of the domain wall. In this presentation, I will talk about the imaging and study of domain wall dynamics in both, an out of field quasi-static and an on-field dynamic approach. I will show the singular E field-driven motion of domain walls in improper ferroelectrics and also discuss Scanning Oscillator PFM, a novel microscopy mode based on a multifrequency approach which allows us to quantify domain wall oscillations under sub-coercive electric fields, distinguishing piezoelectric from electrostatic signals that introduce severe distortions on the net piezoelectric response around domain walls. This technique allows quick visualization of domain wall displacement, their velocities and dependence on pre-existing domain configurations and defects. This work was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

11:45 AM

(EMA-S22-024-2025) Improving multiline thru-reflect-line calibrations for high-frequency materials characterization

N. Jungwirth*[1]; F. Bergmann[1]; R. Jones[1]; B. Bosworth[1]; J. Cheron[1]; L. Enright[1]; A. Osella[1]; C. Long[1]; N. Orloff[1]

1. National Institute of Standards and Technology, USA

On-wafer methods are a broadband approach for characterizing the complex permittivity of materials from dc to terahertz frequencies. At low frequencies, interdigitated capacitors are useful because the net capacitance scales linearly with both the device length and with the real part of the permittivity. At higher frequencies, where the electrical length exceeds the device length, the multiline thru-reflect-line (TRL) calibration algorithm is the preferred method. In this regime, a collection of on-wafer measurements is used to extract the propagation constant, which is then combined with finite element simulations to infer the frequency dependent permittivity. In this work, we demonstrate that by combining two co-fabricated multiline TRL kits, one may significantly decrease the uncertainty in the extracted permittivity. We measure the propagation constant of two coplanar waveguide kits: one fabricated on fused silica, and an identical kit with a superstrate of SU-8, a common photo-definable polymer. Our method uses the ratio of the propagation constants to quantify the complex permittivity to 220 GHz. We compare the results of our approach to traditional techniques. Our results validate our approach for measuring permittivity of photo-definable polymers, and to 220 GHz and beyond.

12:00 PM

(EMA-S22-025-2025) Complex permittivity measurements of substrates and thin films at millimeter-wave

L. Enright*[1]; B. Jamroz[1]; N. Orloff[1]

1. National Institute of Standards & Technology, Communications Technology Laboratory, USA

Complex permittivity describes a material's behavior under an applied electric field. Complex permittivity is therefore a key parameter for the design and modeling of electronic devices. Researchers' understanding of the complex permittivity of a given material is fundamentally limited by their ability to measure it, especially at higher frequencies (e.g., millimeter-wave: 30 – 300 GHz) where materials, devices, and measurement tools are still maturing. Here, we show advances in the standardization of millimeter-wave complex permittivity measurements of substrates (e.g., fused silica) using split-cylinder resonators, and we extend the use of these resonators to measure dielectric thin films (e.g., AlN, SU-8). We describe the electromagnetic theory behind these measurements and the limitations of these measurements. This work enables split-cylinder resonator measurements of isotropic substrates and thin films for low-loss applications in telecommunications, electronics, and quantum computing.

12:15 PM

(EMA-S22-026-2025) Improving equivalent circuit models of interdigitated capacitors

N. Jungwirth*[1]; B. Bosworth[1]; F. Bergmann[1]; E. Marksz[1]; L. Enright[1]; A. Osella[1]; J. Cheron[1]; A. Hagerstrom[1]; I. Takeuchi[2]; C. Long[1]; N. Orloff[1]

1. National Institute of Standards and Technology, USA
2. University of Maryland, USA

Interdigitated capacitors are nearly ubiquitous circuits found in everything from telecommunications components to superconducting quantum computers. When the electrical wavelength becomes comparable to the length of the capacitor, lumped-element models fail to describe how the admittance changes as a function of frequency. This failure limits the frequency range where one can accurately predict the performance of interdigitated capacitors and extract material properties. Here, we imnplement a multi-mode, distributed theory for interdigitated capacitors and quantify the trade-offs between a lumped-element and distributed approach. To test our model, we measured interdigitated capacitors fabricated on $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ substrate and interdigitated capacitors with same geometry fabricated on a $BaSrTiO_3$ thin film.

S1 Ceramics for the Hydrogen Economy

S1- Ceramic processing and manufacturing techniques for hydrogen applications

Room: Colorado J
Session Chairs: Ming Li, University of Nottingham; Till Frömling

2:00 PM

(EMA-S1-001-2025) Promises and challenges of protonic ceramic electrolysis cells (Invited)

S. Ricote*[1]; R. J. Kee[1]

1. Colorado School of Mines, Mechanical Engineering, USA

Over the past forty years, protonic ceramics have garnered increasing attention, with a notable rise in interest in recent years. This trend can be explained by an improved understanding of their properties and advancements in scalable and reproducible manufacturing techniques. This presentation will start with a detailed overview of protonic ceramics, highlighting their conductivity and hydration characteristics. It will then focus on protonic ceramic electrolysis cells (PCECs). After some examples of the latest advancements, the major challenges and their potential solutions will be addressed: (1) Faradaic efficiency: the discrepancies in the Faradaic efficiency trends will be discussed and strategies to achieve high faradaic efficiencies will be offered. (2) Steam electrodes (positrode): their mechanisms are more complex compared to those in solid oxide cells. Efforts are ongoing to develop high-performance and stable materials for intermediate temperatures.

2:30 PM

(EMA-S1-002-2025) Proton-conducting cells for membrane reactors and electrochemical cells – An overview (Invited)

W. Deibert*[1]; N. H. Menzler[1]; S. Baumann[1]; O. Guillon[1]; W. A. Meulenberg[1]

1. Forschungszentrum Julich GmbH, IMD-2, Germany

The Institute of Energy Materials and Devices, Materials Synthesis and Processing (IMD-2) is specialised on the development of planar electrochemical cells for broad range of hydrogen-related activities. This talk will give an overview of different concepts, materials and fabrication methods applied at IMD-2. Starting with protonic ceramic fuel cells and protonic ceramic electrolysis cells with comparably low operation temperatures (typically 400 °C - 600 °C). Another research field is the multi-fuel approach as different energy carriers can be used to generate electricity or to provide high purity hydrogen. Proton conducting ceramic materials offer the possibility to build membrane reactors, where the ceramic membrane either provides pure hydrogen to or extracts hydrogen from a chemical reaction. In one example ethane is converted to ethylene and hydrogen on one side of the membrane. Hydrogen is extracted via the membrane, leading to two valuable products. A mixed proton and electron conducting membrane can be applied as well as an electrically driven cell. In all of these concepts, layered ceramic structures are fabricated by scalable and industrial relevant methods. Tape-casting, screen-printing or wet powder spraying are available at IMD-2. For endothermal reactions electrical heating has to be implemented. In this case solar radiation shows a sustainable alternative for the heat input.

3:00 PM

(EMA-S1-003-2025) Operation-Specific Electronic Leakage in Protonic Ceramic Electrolytes for Solid Oxide Cells (Invited)

B. Guan[3]; H. Tian[3]; Y. Picard[2]; J. Liu[2]; T. Kalapos[2]; H. Abernathy[2]; L. Zhou[1]; X. Li[3]; W. Li[3]; X. Liu*[1]

1. West Virginia University, Mechanical & Aerospace Engineering, USA
2. National Energy Technology Laboratory, USA
3. West Virginia University Benjamin M Statler College of Engineering and Mineral Resources, USA

In this study, we explore the electron and ion mixed transport properties of four common protonic ceramics. BZCYYb1711 exhibits the highest ionic conductivity, but 2-3 times higher electronic leakage when exposed to oxygen-containing environments than the others. BZY82 exhibits ~2 times higher electronic leakage in hydrogen-containing environment. BZCY721 demonstrates excellent ion transport numbers across these four operating conditions. The most challenging operating environment for all candidates is the air side of fuel cell mode, which leads to a high initial electronic leakage, followed by a significant increase with polarization. The probable cause for this behavior is a H_2-free, polarization-induced reduction that leads to the formation of $Vo^{\cdot}$. The electron small polaron associated with $Vo^{\cdot}$ is released by the electrical field due to the Poole-Frenkel effect. ZnO and NiO sintering aids are found to be detrimental to the ionic conductivity of the electrolytes. In particular, NiO substantially lowers the ion transport number.

4:00 PM

(EMA-S1-004-2025) Chemical Modulation of Grain Boundaries and Electrochemical Interfaces - New Opportunities for Improved Energy Conversion Devices (Invited)

H. L. Tuller*[1]; M. Yasutake[2]; H. Seo[3]; J. Matsuda[2]; K. Sasaki[2]; T. Defferriere[1]; C. Gilgenbach[1]; Z. Sha[1]; J. LeBeau[1]

1. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
2. Kyushu University, Department of Mechanical Engineering, Japan
3. Dankook University, Department of Materials Science and Engineering, Republic of Korea

Functional ceramics play an increasingly more critical role in energy conversion devices given unique electrical, electrochemical, and mechanical properties with ability to operate in harsh chemical and thermal environments at relatively low cost. Key challenges commonly include optimized initial performance and minimized degradation rates. Both objectives are often tied to how both internal (e.g. grain boundaries, phase boundaries) and external interfaces function during device operation. I begin by reviewing recent advances in our laboratory demonstrating extraordinary ability to control and manipulate catalytic activity at the rate controlling solid oxide fuel/electrolysis cell electrodes, allowing for both enhanced initial performance and markedly decreased degradation rates. I then go on to describe our ability to modulate ionic transport at grain boundaries in polycrystalline solid electrolytes with promise for reduced ohmic losses and reduced degradation resulting from current induced delamination and porosity.

4:30 PM

(EMA-S1-005-2025) Enhancing Nanocatalyst Design: Unraveling the Role of Surfaces on Nanoparticle Exsolution by Advanced Characterization (Invited)

J. Hidalgo*[1]; R. Li[2]; I. Waluyo[2]; A. Hunt[2]; B. Yildiz[1]

1. Massachusetts Institute of Technology, USA
2. Brookhaven National Laboratory, NSLS II, USA

Nanocatalysts are key in advancing energy conversion systems, with one recent breakthrough being exsolution – the in-situ growth of metal nanoparticles anchored to a parent oxide, such as perovskites. However, the influence of surface chemistry and microstructure on exsolution mechanisms remains not fully understood. Using synchrotron-based surface-sensitive characterization techniques, we unravel the effect of near-surface microstructure and surface chemistry on the formation of nickel nanoparticles from the exsolution of perovskite polycrystalline thin films. By grazing-incidence wide-angle X-ray scattering, we analyze and observe that crystallinity and plane orientation at the near-surface impact nucleation and growth. Additionally, in-situ near-ambient-pressure X-ray photoelectron spectroscopy reveals that chemical surface modifications influence nickel reduction behavior, altering the formation kinetics and increasing the nanoparticle's surface area, potentially enhancing nanocatalyst performance. Establishing correlations between surface chemistry, structure, and nanoparticle characteristics is essential for designing exsolution surfaces tailored to specific electrochemical reactions, such as water splitting for hydrogen production.

5:00 PM

(EMA-S1-006-2025) Blacklight sintering of $BaZrO_3$-based proton conductors

J. N. Ebert*[1]; D. Jennings[2]; O. Guillon[2]; W. Rheinheimer[1]

1. Universitat Stuttgart, IFKB, Germany
2. Forschungszentrum Julich GmbH, IMD-2, Germany

For millennia, ceramics have been densified via sintering in a furnace, a time-consuming and energy-intensive process. The need to minimize environmental impact calls for new physical concepts beyond large kilns relying on thermal radiation and insulation. Especially acceptor-doped $BaZrO_3$, a ceramic proton conductor, has to be sintered at high temperature (> 1600 °C) for long times (~ 24 h). At these sintering conditions BaO is prone to evaporate, increasing the difficulty to produce stoichiometric, dense, and large grained ceramics. Here, we realize ultra-rapid heating by blacklight sintering with intense blue laser light to sinter bulk $BaZr_{0.8}Y_{0.2}O_{3-\delta}$ (BZY20) and $BaZr_{0.8}Y_{0.1}Sc_{0.1}O_{3-\delta}$ (BZY10Sc10) in under four minutes. While the problem of extensive BaO evaporation was mitigated by blacklight sintering as XRD revealed single phase materials, a remaining challenge is the heterogenous microstructure. During blacklight sintering a grain size and porosity gradient developed from the laser irradiated surface (top) to the surface in contact with the carbon substrate (bottom) with larger grains and low porosity at the top. Still the proton conductivity of the blacklight sintered samples was only slightly worse (BZY20) or even comparable (BZY10Sc10) to conventionally sintered samples. As such blacklight sintering is a promising technology to rapidly densify proton conductors based on $BaZrO_3$.

5:15 PM

(EMA-S1-007-2025) Application of advanced ceramic materials for fuel cell and green hydrogen production at Ceres: achievements and future opportunities

R. T. Leah*[1]; S. Mukerjee[1]; C. Hargrove[1]

1. Ceres Power Holdings plc, United Kingdom

Ceres is one of the world's leading developers of SOC technology, based in Horsham in the UK. Ceres has developed a unique low-temperature metal-supported SOC technology applicable to both power generation and green hydrogen production. Ceres has developed IP around cell and stack design and manufacture, system and control system design, which has been licenced to a number of global OEMs to manufacture and deploy in their products. Well-known licensees include Bosch in Germany, Doosan in South Korea, Weichai Power in China, Delta Electronics in Taiwan and Denso in Japan. Ceres unique cell architecture has numerous advantages over more conventional SOC designs, particularly around robustness and cost, but does present some unique challenges in both the functional performance of the ceramic materials used in the electrolyte and electrodes and cell manufacture. This presentation will discuss both the challenges which have been overcome and areas where advancements in materials design and characterization can be used to further improve future generations of the technology, including state-of-the-art techniques developed in collaboration with academic partners to further scientific understanding of the performance and degradation of the cell materials.

S2 Electronic and Ionic Materials for Energy Storage and Conversion Systems

S2- Computational and experimental advances in mixed electronic and ionic conductors for energy storage and conversion systems

Room: Colorado I

Session Chairs: Fudong Han, Rensselaer Polytechnic Institute; Nicola Perry, University of Illinois at Urbana-Champaign

2:00 PM

(EMA-S2-008-2025) Molecular Simulations and Machine Learning for Computational Design of Materials with Fast Oxygen Kinetics (Invited)

D. Morgan*[1]; R. Jacobs[1]; J. Meng[1]; M. Sheikh[1]; J. Liu[2]; M. Polak[1]

1. University of Wisconsin-Madison, Materials Science and Engineering, USA
2. NETL, USA

In this talk I will describe some of our recent work demonstrating that molecular simulation and machine learning based screening can discover new materials with outstanding oxygen kinetics. First, I will describe our work using ab-initio calculations of p-bands and correlations with surface exchange, as well as calculations of band gap and stability, to predict that $BaFe_{0.125}Co_{0.125}Zr_{0.75}O_{3-d}$ (BFCZ) could be a promising solid oxide cell electrode material. We then showed experimentally that trends in measured performance and stability are consistent with the modeling predictions, including a significant reduction in Area Specific Resistance for a $(La,Sr)(Co,Fe)O_3$ (LSCF)/BFCZ composite vs. LSCF alone. I will then share our work on machine learning methods for predicting oxygen kinetics, with a focus on Area Specific Resistance (ASR) in solid oxide fuel cell electrodes. We demonstrate that machine learning predictions based on simple elemental properties are quite good (MAE 0.2 log units) and can be used for effective materials discovery. Finally, I will share how emerging data extraction methods based on large language models may greatly reduce the time needed to develop databases for constructing these types of machine learning materials property models.

2:30 PM

(EMA-S2-009-2025) Fundamental thermodynamics and kinetics of cathode and anode materials of Li-ion and Na-ion batteries (Invited)

A. Van der Ven*[1]

1. University of California Santa Barbara, Materials, USA

The electrodes of Li-ion and Na-ion batteries have unique electronic properties and complex crystal structures that play a decisive role in determining their electrochemical properties. Computational approaches based on first-principles statistical mechanics are capable of elucidating how properties at the electronic and atomic scale ultimately determine measurable thermodynamic and kinetic properties at the macroscopic scale. In this talk I will focus on electrode materials used in Li-ion and Na-ion batteries and survey the rich variety of redox mechanisms and diffusion mechanisms that enable high capacity and high-rate cycling. Layered intercalation compounds used as cathodes exhibit a wide variety of atomic hop mechanisms that make them sensitive to guest ion concentration and variations in lattice parameters. The hop mechanisms in layered compounds are sensitive to the stacking sequence of the host, with Li diffusion mediated by vacancy clusters and Na transport mediated by the motion of extended defects such as anti-phase boundaries. New redox mechanisms are increasingly being harnessed to enable higher capacities. Anion redox mechanisms have the potential to increase the capacity of cathode materials, while extended molecular orbital-like redox mechanisms show promise in anodes such as Wadsley-Roth phases.

3:00 PM

(EMA-S2-010-2025) Probing Reaction Heterogeneity in Thick Battery Electrodes: Effects of Electrode Thermodynamic Properties and Electronic Conductivity *WITHDRAWN*

M. Tang*[1]

1. Rice University, Materials Science & NanoEngineering, USA

Making battery electrodes thick is a practical way to increase the battery energy density, but this approach is impeded by the inferior rate and cycle performance of thick electrodes due to nonuniform reaction distribution. Reaction heterogeneity is often attributed to limited charge transport kinetics. However, here we present experimental results that it is also impacted by the thermodynamic properties of the electrode active material. We charterized the reaction distributions in $LiFePO_4$ (LFP) and $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC) thick electrodes with XANES imaging and ToF-SIMS measurement. Despite having similar porosity, tortuosity and thickness, the LFP electrodes possess a more pronounced reaction gradient than NMC discharged at the same rates. The disparate reaction gradients in LFP and NMC electrodes are attributed to their distinct SOC dependence of the open circuit potentials. The relatively higher reaction uniformity in NMC electrodes leads to better active material utilization and reduced capacity fade, which highlights the intrinsic properties of the active materials as an important factor in thick electrode design.

3:15 PM

(EMA-S2-011-2025) Extended oxygen defects modulate the ethylene selectivity in the electrochemical oxidative coupling of methane

F. Grajkowski*[1]; B. Liu[1]; S. Koohfar[1]; S. Chandra[1]; B. Yildiz[1]

1. Massachusetts Institute of Technology, USA

The electrochemical oxidative coupling of methane (EOCM) to ethylene (C_2H_4) is a promising way to decarbonize global C_2H_4 production, which today is the 2nd-biggest contributor to industrial CO_2 emissions (>300Mt/yr). However, a key challenge with EOCM is understanding how to form active oxygen species at the anode surface which can selectively activate CH_4 to C_2H_4. In this presentation, we discuss how these oxygen species can be formed at the surface of $La_{0.3}Sr_{0.7}TiO_{3+\delta}$ (LST) and the key materials properties that enable selective CH_4 activation. In particular, we discuss how nucleating extended shear defects in LST using the oxygen overstoichiometry δ can promote oxygen evolution (OER) to occur at the anode surface. By then coupling the EOCM reactions to OER and utilizing the intermediates of OER to activate CH_4, we demonstrate a >3x enhancement in the C_2 (C_2H_6 and C_2H_4) selectivity of EOCM relative to the baseline performance. We then provide mechanistic insights into the surface reactions and how the identity of the active oxygen species influences the reactions. Our results demonstrate that by utilizing structural transformations at/near the electrode surface, we can significantly modify the surface chemistry and greatly enhance the selectivity of the EOCM reactions by specifically forming the active oxygen species which are most selective for C_2 formation.

4:00 PM

(EMA-S2-012-2025) Advanced oxides for solid oxide cells (Invited)

J. Sirvent[2]; F. Baiutti[2]; F. Chiabrera[2]; K. Kreka[2]; F. Buzi[2]; A. Morata[2]; A. Maria[2]; L. Bernadet[2]; A. Tarancon*[1]

1. ICREA/IREC, Spain
2. Institut de Recerca en Energia de Catalunya, Spain

Solid Oxide Cells (SOCs) for power generation and electrolysis represent a mature technology for energy conversion, rapidly approaching commercialization. However, several challenges remain unresolved, including the excessive use of critical raw materials, high manufacturing costs, and limited performance and durability. These practical issues are closely linked to gaps in our understanding of the processing and mass transport properties of the relevant materials, especially at the interface level. In this talk, I will discuss our group's recent advances in addressing these problems, such as the use of high entropy oxides, thin film technologies, ultrafast sintering of ceramics, and high-throughput and operando characterization techniques.

4:30 PM

(EMA-S2-013-2025) Complex mixed electronic and ionic conduction in protonic ceramics (Invited)

S. Ricote*[1]

1. Colorado School of Mines, Mechanical Engineering, USA

$Ba(Ce,Zr,Y)O_{3-d}$, referred to as BCZY, is a widely studied protonic ceramic with complex conductivity characteristics. In oxidizing atmospheres, O-site polarons are created by the dissociation of oxygen into oxide vacancies. Their contribution increases with the oxygen partial pressure. At oxygen partial pressures below 10^{-5} bar, BCZY is an ionic conductor, with pure proton conduction below 600 C and mixed oxide-ion and proton conduction above 600 C. High cerium content compositions can display n-type conductivity at elevated temperatures and very reducing conditions. Following a detailed overview of protonic ceramic conductivity, we will explore various applications, including protonic ceramic fuel cells (PCFCs), protonic ceramic electrolysis cells (PCECs), and membrane reactors. Additionally, it is important to note that the electrodes in these protonic ceramic cells are also made from mixed ionic and electronic conductive ceramics. Examples will be provided in the case of PCFCs and PCECs.

5:00 PM

(EMA-S2-014-2025) In-situ and Ex-situ Impedance Spectroscopy Analysis of Li_2OHCl Antiperovskite Solid Electrolyte Grown by Pulsed Laser Deposition

K. Lan*[1]; E. Cho[1]; Y. Lee[1]; X. Ji[1]; P. V. Braun[1]; D. G. Cahill[1]; A. Schleife[1]; N. H. Perry[1]

1. University of Illinois at Urbana-Champaign, Material Science and Engineering, USA

Solid-state lithium-ion batteries (ASSLIBs) have garnered significant interest due to their enhanced safety compared to flammable organic liquid electrolytes and their potential for higher energy density through efficient packaging. Li_2OHCl, an antiperovskite material, is a promising lithium-ion conductor as a solid electrolyte for ASSLIBs. However, the fundamental relationship between processing conditions, microstructure, and conductivity remains unclear due to the hygroscopic nature of these materials. Plus, there are knowledge gaps in the lithium ionic transport properties of Li_2OHCl thin film compared to their bulk form. In this study, in-situ in-plane AC-impedance spectroscopy (AC-IS) was conducted during the growth of Li_2OHCl thin films to better understand how PLD processing parameters affect the ionic conductivity of solid electrolytes as thin films develop. This technique effectively prevents moisture adsorption, which can dominate in-plane impedance. A kinetic model was established to quantitatively analyze the in-situ PLD data, providing insights into the nucleation and growth of antiperovskite thin films during deposition and their impact on ionic transport within the films. Ex-situ in-plane AC-IS was also performed. Our findings can guide the design of solid electrolytes with lower processing temperatures for future ASSLIB applications.

S3 Nano4Neuro-Mechanisms and Materials for Next Generation Computing

S3- Phase transitions for information

Room: Colorado C
Session Chair: Yiyang Li, University of Michigan

2:00 PM

(EMA-S3-007-2025) Low-Power and High-Temperature Computing with III-Nitride ferroelectrics (Invited)

D. Jariwala*[1]
1. University of Pennsylvania, USA

In this talk I will discuss memory devices from 2D materials integrated with emerging wurtzite structure ferroelectric nitride materials namely aluminium scandium nitride (AlScN). First, I will present on Ferroelectric Field Effect Transistors (FE-FETs) made from 2D materials when integrated with AlScN and make the case for 2D semiconductors in this application. Next I will introduce our work on Ferroelectric Diode (FeD) devices also based on thin AlScN. In addition, I will also present how FeDs provide a unique advantage in compute-in-memory (CIM) architectures for efficient storage, search as well as hardware implementation of neural networks. Finally, I will present ongoing work and opportunities to extend the application of AlScN memory devices into extreme environments.

2:30 PM

(EMA-S3-008-2025) Measurements of electron and phonon transport and scattering in ferroelectric thin films using ultrafast and infrared spectroscopy

S. Makarem*[1]; S. Zare[2]; C. Skidmore[3]; I. Mercer[3]; J. Maria[3]; P. Hopkins[2]
1. University of Virginia, Materials Science and Engineering, USA
2. University of Virginia, USA
3. Pennsylvania State University, Materials Science and Engineering, USA

Ferroelectric materials possess a spontaneous electrical polarization that can be switched between stable states by an external electric field, making them uniquely functional among piezoelectrics. As the demand for miniaturized sensors and actuators in microelectromechanical systems (MEMS) grows, and with the integration of ferroelectric properties into integrated circuits (ICs), there is increasing interest in ferroelectric thin films. However, many oxide perovskite ferroelectrics face challenges such as low transition temperatures and poor compatibility with CMOS and III-nitride technologies, limiting their adoption in microtechnology. This study focuses on ferroelectric wurtzite nitrides, which offer dynamic tunability over light, charge, spin, and heat. We characterize the phonon transport, sound speed, and phonon lifetimes of $Al_{1-x}B_xN$ ferroelectric thin films using ultrafast spectroscopy. Combined with infrared variable angle spectroscopy ellipsometry (IR-VASE), these methods enable precise monitoring of scattering rates. Temperature-dependent measurements further illuminate changes in optical phonon energies, enhancing our understanding of phonon dynamics and paving the way for improved ferroelectric materials in next-generation microtechnology.

2:45 PM

(EMA-S3-009-2025) Theoretical Switching Mechanism of Wurtzite Aluminum Nitride

D. Behrendt*[1]; A. Samanta[1]; A. M. Rappe[1]
1. University of Pennsylvania, Chemistry, USA

The advent of wurtzite ferroelectrics is enabling a new generation of ferroelectric devices for computer memory that has the potential to bypass the von Neumann bottleneck, due to their robust polarization and silicon compatibility. However, the microscopic switching mechanism of wurtzites is still undetermined due to the limitations of density functional theory simulation size and experimental temporal and spatial resolution. Thus, physics-informed materials engineering to reduce coercive field and breakdown in these devices has been limited. Here, the atomistic mechanism of domain wall migration and domain growth in wurtzites is uncovered using molecular dynamics built on a machine learned force field and dynamics-informed Monte Carlo simulations of aluminum nitride. We further show how the unique shape of the domain wall breaks assumptions in the KAI model and leads to the anomalously fast switching in wurtzite structured ferroelectrics.

3:00 PM

(EMA-S3-010-2025) Crystalline Phase Evolution, Dimensional Scaling and Reliability of Hafnia-Zirconia Ferroelectric Thin Films (Invited)

P. McIntyre*[1]
1. Stanford University, Materials Science and Engineering, USA

Ferroelectric (FE) $Hf_{0.5}Zr_{0.5}O_2$ (HZO) based devices such as random-access memory and field-effect transistors have emerged as promising candidates for non-volatile memory applications due to their robust FE properties at nanoscale dimensions. Many research efforts in the field have focused on reducing the programming voltage, improving reliability and achieving compatibility with back-end-of-line process temperatures. To fully realize their potential, it is essential to understand the switching dynamics and the structural changes that dictate the reliability of HZO FE thin films. This presentation describes the influence of growth conditions, electrode material and post-growth annealing on phase evolution in HZO films synthesized by plasma-enhanced atomic layer deposition. It is possible to tune the properties of the resultant films by controlling the crystalline phase exhibited by HZO in as-fabricated devices. In addition, the scaling of FE properties to ultra-small film thickness and lateral dimensions, and their heterogeneity, are investigated. Field-induced transformations among different non-polar and polar phases are probed as a function of time and temperature to understand their influence on the switching reliability in HZO memory capacitors by utilizing correlated, temperature-dependent electrical measurements and grazing incidence X-ray diffraction (GIXRD).

4:00 PM

(EMA-S3-011-2025) Ferroelectric Hafnia for Neuromorphic Computing: Overcoming Obstacles Imposed by Metastability (Invited)

J. Ihlefeld*[1]
1. University of Virginia, Department of Materials Science and Engineering, USA

Ferroelectricity in hafnium oxide reenergized the thin film ferroelectric community owing to its unprecedented compatibility with CMOS and back end of line processes. In addition to conventional memory devices, such as FeRAM, the switchable polarization in hafnia holds promise for neuromorphic computing, particularly in Ferroelectric Tunnel Junctions (FTJs). This presentation will highlight some of the promising attributes of hafnia and how improved processing and understanding of the ferroelectric-phase-stabilizing-mechanisms have resulted in advances in material properties. It will be shown that selection of electrode materials is important for stabilizing the ferroelectric phase and that they directly impact the defect concentration and retention performance. Results will be shown that suggest that electronic barriers to charge transport differ with electrodes and that with use, some of these barriers are modified, presumably due to motion of charged defects. Some final obstacles facing hafnia in scaled environments will be discussed to inspire future research to make ferroelectric hafnia-based devices a reality in the near future.

4:30 PM

(EMA-S3-012-2025) Opening the Neuromorphic Design Space: Engineering Spin Crossover Devices with Compositional Complexity (Invited)

E. J. Fuller*[1]

1. Sandia National Laboratories California, Materials Physics, USA

We have recently demonstrated the utility of spin crossover oxides, such as $LaCoO_3$, in various computational paradigms including axon-like signal transmission[1] and true random number generation[2]. However, the design space for electrothermally induced spin crossover devices is limited by conventional material constraints. Here, we explore expanding material candidates with oxides that can be engineered beyond traditional design limits through a focus on compositionally complex oxides. These materials, often called high entropy oxides, have lattice sites that share more than four cations, forming single-phase solid solutions with unique properties. Here, we demonstrate compositional complexity as a tunable parameter in the spin-transition oxide semiconductor $La_{1-x}(Nd,Sm,Gd,Y)_{x/4}CoO_3$, by varying the population x of rare earth cations over $0.00 \leq x \leq 0.80$. Across the series, increasing complexity is revealed to systematically improve crystallinity, increase the amount of electron versus hole carriers, and tune the spin transition temperature and on-off ratio[3]. Some unconventional properties that emerge and the potential to engineer them into next generation computing devices will be discussed. [1] T.D. Brown et. al. Nature, 2024 [2] K.S. Woo et. al. Nature Communications, 2024 [3] A. Zhang et. al. Advanced Materials, 2024.

5:00 PM

(EMA-S3-013-2025) Exploring electro-thermal localizations and metal-insulator transitions in micron to sub-micron thin film VO_2 devices

Y. Yu*[1]; A. Bradicich[1]; T. D. Brown[3]; F. Jardali[1]; S. Kumar[3]; R. S. Williams[2]; P. Shamberger[1]

1. Texas A&M University System, Materials Science and Engineering, USA
2. Texas A&M University, Electrical and Computer Engineering, USA
3. Sandia National Laboratories California, USA

In select transition metal oxides, non-linear electronic transport can lead to negative differential resistance (NDR), resulting in spiking neuronal behavior. However, several mechanisms contribute to this non-linear behavior, including 1) intrinsic temperature-dependent electrical transport, 2) localization of current density within high current-density 'hot' channels, and 3) spatially heterogeneous metal-insulator transitions (MIT). In complex systems like VO_2, which exhibit multiple of these behaviors, the interaction between these mechanisms remains unclear, especially as device dimensions decrease. In this study, we explore the relationship between phase-homogeneous electro-thermal localizations and MIT through 3D-multiphysics simulations of the two-terminal VO_2 devices. Our results reveal that MIT is spatially heterogeneous, triggered by dramatic increases in local current density and temperature due to system instabilities. Furthermore, we show that spatial heterogeneity formation is strongly dependent on device size, with a critical device width of approximately 0.7 μm, below which the localizations and MIT cease to occur heterogeneously. Our findings offer a clearer understanding of how current-induced coupled electrothermal localizations lead to heterogeneous phase transformations, showing that NDR is not always directly tied to one specific mechanism.

5:15 PM

(EMA-S3-014-2025) Measuring Dynamic Data

P. Maksymovych*[1]; N. Bauer[6]; O. Popova[2]; M. Lavrentovich[4]; M. A. Susner[3]; A. V. Levlev[5]; S. Neumayer[2]

1. Clemson University, Materials Science and Engineering, USA
2. Oak Ridge National Laboratory, USA
3. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
4. Worcester State University, Earth, Environment and Physics, USA
5. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
6. The University of Tennessee Knoxville Tickle College of Engineering, Physics, USA

The challenge of connecting device function and fundamental physical processes is particularly pronounced in neuromorphic materials, where resistive, ferroelectric and other kinds of switching dynamics are inherently non-equilibrium. Scanning probe microscopy (SPM) is a promising technique to bridge the nanoscale gap between idealized atomic models and the functional scale of information devices. However, SPM data often lacks calibration due to reduced sampling volume, while the exact values of applied forces are difficult to determine and correlate to larger scales. Here I will focus on a systematic approach to quantify "dynamic data" in SPM – such as hysteresis loops or oscillatory response, which reflect the underlying multiplicity of accessible material states. Through methods of dynamic mode decomposition and topological data analysis we can systematically distinguish hysteresis loops of ferroelectric and spurious processes, identify the signatures of multiwell ferroelectric potential in model $Sn_2P_2S_6$, and point to the specific dynamics leading to the rare memcapacitive behavior, prohibited in ideal double-well ferroelectrics. I will also demonstrate this approach for resistive switching in binary oxides. Research supported by DOE Office of Science Microelectronics Codesign Program through the Abisko Project. Experiments carried out at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, a DOE User facility.

S4 Oxide Quantum Materials: Synthesis, Properties and Application

S4- Advanced Characterization

Room: Colorado B
Session Chairs: Grace Pan, University of California Berkeley;
Seung Sae Hong, University of California, Davis

2:00 PM

(EMA-S4-019-2025) Electron-Beam Writing of Atomic-Scale Reconstructions at Oxide Interfaces (Invited)

G. Segantini*[1]; C. Hsu[1]; C. W. Rischau[1]; P. Blah[2]; M. Matthiesen[2]; S. Gariglio[1]; J. Triscone[1]; D. Alexander[3]; A. Cavglia[1]

1. Universite de Geneve, Switzerland
2. Technische Universiteit Delft, Netherlands
3. Ecole Polytechnique Federale de Lausanne, Switzerland

Transition metal oxides exhibit a variety of functionalities and epitaxial growth enables the synthesis of high-quality films. However, it confines the choice of substrates to those meeting symmetry and lattice parameter constraints. A way to overcome these constraints is releasing epitaxial oxides from their growth substrate, by means of sacrificial layers, thus obtaining oxide membranes. Here, we report on the controlled formation of interfacial ionic bonds between a 30 nm-thick SrTiO3 membrane and a niobium-doped SrTiO3(001) carrier substrate. Scanning transmission electron microscopy in electron energy-loss spectroscopy mode (STEM-EELS) was used to investigate electronic/bonding state of Ti and O going across the interface from the substrate to the membrane as a function of annealing temperature. For a certain annealing temperature, and for a certain flux of STEM electron-beam, rastering it across the interface between the membrane and the substrate induces a perfect interface reconstruction with formation of ionic bonds between the membrane and the substrate. STEM-EELS analysis confirmed a change of Ti valence from Ti 2+ to Ti 4+, and restoration of oxygen octahedral coordination in the interface region. This study presents a method to selectively create ionic bonds between perovskite oxides, enabling the local manipulation of physical properties at their interface.

2:30 PM

(EMA-S4-020-2025) Revealing the Intricacies of Vibrations in Complex Oxides using Polarization Selective Electron Energy-loss Spectroscopy (Invited)

E. R. Hoglund*[1]; H. A. Walker[2]; S. T. Pantelides[3]; J. A. Hachtel[1]

1. Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, USA
2. Vanderbilt University, Interdisciplinary Materials Science Program, USA
3. Vanderbilt University, Dept. of Physics and Astronomy, USA

Vibrational electron energy-loss spectroscopy (EELS) in a monochromated scanning transmission electron microscope is a useful tool to understand how local heterogeneity impacts atomic vibrations.[1–3] Such vibrations are typically measured with optical spectroscopies that have superior spectral resolution with lower spatial resolution. Effort has been put into decreasing the energy resolution gap between optical spectroscopies and monochromated EELS in an to enable vibrational spectroscopy with high-spatial resolution.[4] However, optical spectroscopies can also utilize polarized light, which provides details about vibration eigenvectors. While polarization selectivity has been examined in aloof EELS[5] it has been overlooked in off-axis EELS. Recent efforts have demonstrated that the direction of the off-axis deflection in reciprocal space enables sensitivity to anisotropies in the eigenvectors enabling analysis of incipient transformations in oxides or anisotropic behavior in other ceramics.[6,7] Here we demonstrate high-spatial resolution polarization selectivity in vibrational EELS and its application anisotropic vibrations at nitride interfaces and complex oxides heterostructures. By operating at nanometer-scale resolution, we gain mixed-space insights into the behavior of unique vibrations.[8]

3:00 PM

(EMA-S4-021-2025) Terahertz switching of ferroelectric polarization in Hafnia films (Invited)

H. Park*[1]

1. Ulsan National Institute of Science and Technology, Department of Physics, Republic of Korea

Silicon-compatible HfO_2 has been attracting significant attentions for ferroelectric applications. HfO_2 orthorhombic phase exhibits robust ferroelectricity even within half-units of cell width, which distinguishes it from perovskites. This unique property has been demonstrated theoretically to be the result of polar domains with extremely localized phonon bands. The light-induced polarization dynamics of HfO_2 have not been fully understood despite its exceptional properties, primarily because of its high coercive field, which exceeds 1-2 MV/cm, and the orthogonal relationship between terahertz electric field and ferroelectric polarization in typical planar configurations. In this work, we employed a time-resolved THz pump-THz probe spectroscopy technique to observe ferroelectric polarization switching within sub-1 picoseconds (ps) in $Hf_{0.5}Z_{0.5}O_2$ (HZO). This was achieved by combining vertically-oriented HZO films with THz nanoresonators, allowing THz waves to be squeezed to tens of MV/cm. In order to achieve ultrafast dynamics in HZO, its improper nature and non-interacting polar domains have been attributed to its resistance to depolarization fields during the ultrafast process. In addition, we observed for the first time S-shaped hysteresis curves during light-induced polarization switching, revealing the intrinsic negative capacitance within the switching pathway of their double well energy landscape.

S4- Theory and Calculations

Room: Colorado B

Session Chairs: Elizabeth Nowadnick, University of California, Merced; Ho Nyung Lee, Oak Ridge National Lab

4:00 PM

(EMA-S4-022-2025) Coupling Between Magnetic Multipoles and Crystal Structure in Altermagnets (Invited)

T. Birol*[1]; L. Buiarelli[1]; R. M. Fernandes[2]

1. University of Minnesota Twin Cities, USA
2. University of Illinois Urbana-Champaign, USA

Altermagnetism has a short but contentious history. In this talk, we will argue that it is possible to define altermagnetism as a new and distinct phase of matter that hosts certain higher order magnetic multipoles. By using a combination of first principles methods (DFT) and group representation theory we will show that the common structural distortions present in oxides can couple with these multipoles and have a strong impact on the electronic structure of altermagnets, as well as lead to novel macroscopic responses such as piezomagnetism.

4:30 PM

(EMA-S4-023-2025) Electron-Crystal Structure Symmetry Breaking in Quantum Correlated Electron Materials (Invited)

A. Georgescu*[1]

1. Indiana University Bloomington, Chemistry, USA

Abstract: In this talk, I will focus on theoretical insights into coupling between crystal structure and electronic properties, in correlated electron materials. Correlated electron materials can be understood as having properties arising from local, quantized degrees of freedom (spin, charge order, orbital polarization) which give rise to emergent phenomena such as superconductivity, magnetism, metal-insulator transitions. I will describe - based on computational and theoretical tools - how the interaction between local crystal structure motifs and electronic symmetry determines the resulting quantum states, as well as their propagation at different length scales. Finally, I will show how machine learning can be used to assist at all steps of discovery of quantum materials, from their identification to proposed synthesis pathways. Acknowledgement: This work is partially supported by the Lilly Endowment, Inc., through its support for the Indiana University Pervasive Technology Institute, which allowed DFT computations to be performed at Indiana University on the BigRed200 and Quartz high-performance computing clusters.

5:00 PM

(EMA-S4-024-2025) Piezoelectricity in Ruddlesden-Popper and Dion-Jacobson ferroelectrics from first principles

K. Hasin*[2]; N. Pokhrel[1]; E. Nowadnick[2]

1. Oak Ridge National Laboratory, Division of Materials Science and Technology, USA
2. University of California Merced, Department of Chemical and Materials Engineering, USA

Layered perovskites, such as the Ruddlesden-Popper and Dion-Jacobson oxides, are of significant interest due to their novel properties, including hybrid improper ferroelectricity and complex domain structures. We use first-principles calculations to determine piezoelectric tensors for n = 2 Ruddlesden-Popper ($Ca_3Ti_2O_7$, $Sr_3Zr_2O_7$, $Sr_3Sn_2O_7$, $Li_2SrNb_2O_7$) and Dion-Jacobson ($CsBiNb_2O_7$, $CsNdNb_2O_7$, $CsSmNb_2O_7$, $RbBiNb_2O_7$) ferroelectrics. Conventional piezoelectrics typically show positive longitudinal coefficients with two negative transverse coefficients. In contrast, we identify an unconventional form of transverse piezoelectricity in $Ca_3Ti_2O_7$ and $Li_2SrNb_2O_7$, where one transverse piezoelectric coefficient is negative and the other is positive. In addition, we discover a distinct behavior in Dion-Jacobson perovskites, where all the transverse piezoelectric coefficients exhibit the same sign as of the longitudinal one, indicating potential for designing materials with large hydrostatic piezoelectric responses. Furthermore, we demonstrate that octahedral rotation distortions, which are coupled to the polarization in these families of layered ferroelectrics, can tune the amplitudes of the piezoelectric coefficients. These findings provide new insights into the piezoelectric behavior of layered perovskites and suggest avenues for tuning these properties in functional materials.

5:15 PM

(EMA-S4-025-2025) Metal-Insulator Transitions in Multicomponent Oxide: Ruthenate Pyrochlores *WITHDRAWN*

S. Akhbarifar*[1]

1. The Catholic University of America, Physics, USA

The interplay between charge, spin, orbital, and lattice in strongly correlated oxide materials, like multicomponent ruthenate, provides opportunities to explore quantum phenomena that could significantly impact electronic and thermoelectric applications. In this study, we investigate the metal-insulator transition (MIT) in these oxides, focusing on lead substitution with yttrium between 293 and 575 K. All compounds were isometric, with no miscibility gap, and the unit cell contracted linearly with increasing Y concentration. The parent material shows strong electron correlation, while the fully substituted system exhibits Mott insulating behavior. A critical MIT occurs at ~0.2 moles of yttrium, independent of temperature. Our results show that the MIT is governed by the Mott-Hubbard mechanism, where electron localization occurs via bandgap opening at critical yttrium concentrations. Additionally, we model the impact of these transitions on thermoelectric properties, utilizing quantum modeling to analyze changes in carrier concentration, scattering mechanisms, and conductivity across the transition.

S6 Two-Dimensional Quantum Materials-Synthesis, theories, properties and applications

S6 – Two dimensional quantum materials: Synthesis, theories, properties & applications

Room: Colorado G

Session Chair: Cheng Gong, University of Maryland

2:00 PM

(EMA-S6-012-2025) Hyperbolic phonon-polariton electroluminescence in graphene-hBN van der Waals heterostructures (Invited)

Q. Guo*[1]

1. CUNY Advanced Science Research Center, Photonics Inititative, USA

Phonon-polaritons are electromagnetic waves resulting from the coherent coupling of photons with optical phonons in polar dielectrics. They are uniquely poised to enable a suite of applications beyond the reach of conventional photonics, such as sub-diffraction imaging and near-field energy transfer. The conventional approach to exciting phonon-polaritons through optical methods, however, necessitates costly mid-infrared and terahertz coherent light sources along with near-field scanning probes. Here, we demonstrate that under proper conditions, phonon-polaritons can be excited all-electrically by flowing charge carriers. Specifically, in hexagonal boron nitride (hBN)/graphene heterostructures, by electrically driving charge carriers in ultra-high-mobility graphene out of equilibrium, we observe bright electroluminescence of hBN's hyperbolic phonon-polaritons (HPhPs) at mid-IR frequencies. The HPhP electroluminescence shows a temperature and carrier density dependence distinct from black-body thermal emission. Moreover, the carrier density dependence of HPhP electroluminescence spectra reveals that HPhP electroluminescence can arise from both inter-band transition and intra-band Cherenkov radiation of charge carriers in graphene. The HPhP electroluminescence offers fundamentally new avenues for realizing electrically-pumped, tunable mid-IR and THz phonon-polariton light sources.

2:30 PM

(EMA-S6-013-2025) Interlayer, intralayer, and defect-bound excitons in transition metal dichalcogenide moiré heterostructures (Invited)

A. Kunin*[1]; Z. Withers[2]; Z. Li[3]; J. Ding[2]; A. Adler[2]; J. Guo[4]; S. Chernov[2]; W. Zhou[3]; S. Cheng[3]; V. Chang Lee[4]; B. Hou[4]; G. Schonhense[5]; X. Du[2]; D. Qiu[4]; R. Kawakami[3]; T. Allison[2]

1. Princeton University, USA
2. Stony Brook University, USA
3. The Ohio State University, USA
4. Yale University, USA
5. Johannes Gutenberg Universitat Mainz, Germany

Monolayer transition metal dichalcogenides (TMDs) are of major interest for their strongly bound, long-lived excitons. Twisted vertical heterostructures of TMDs yield spatially separated, interlayer excitons and the emergence of new, tunable excitonic properties due to the moiré superlattice that is formed. The moiré superlattice also gives rise to exciton localization, which has stimulated interest in a variety of quantum applications. Defect sites in TMDs also act as localizing traps, and both moiré and defect engineering of TMD systems are promising avenues for control of exciton localization but require a clear understanding of the momentum-space exciton wave function. Here, we use time-resolved momentum microscopy to visualize excitons in pristine and defective twisted $MoSe_2/WS_2$ heterobilayers. $MoSe_2/WS_2$ presents a distinct case among TMD heterobilayers as the conduction band alignment is believed to be nearly degenerate, which has been proposed to lead to intralayer and interlayer exciton hybridization. With momentum microscopy, the electron sharing between the two layers can be directly visualized. In defective samples, we observe unique, diffuse momentum-space spectral signatures that reveal the extent of the exciton wave function localization in these systems.

3:00 PM

(EMA-S6-014-2025) Tunable magnons in van der Waals antiferromagnet (Invited)

B. Kim*[2]; S. Xu[1]; X. Lu[3]; Z. Wang[2]; J. Jin[2]; C. Qian[2]; L. He[2]; D. Chica[4]; X. Roy[4]; B. Zhen[2]

1. Southern University of Science and Technology, Electrical and Electronic Engineering, China
2. University of Pennsylvania, Physics and Astronmy, USA
3. University of Pennsylvania, Electrical and Systems Engineering, USA
4. Columbia University, Chemistry, USA

Spin wave precessions, known as magnons, offer a promising avenue for ultrafast information transmission and reading without the associated Joule heating. However, their practical device applications are limited by the lack of an efficient and facile switching mechanism. In this study, we discuss a switching effect of magnons in CrSBr, a van der Waals antiferromagnet. Specifically, the switching effect can be enabled by controlling magnon-magnon coupling through external magnetic and electric fields. Our ultraclean CrSBr with long magnon lifetimes (> 1ns) enables us to probe magnon eigenfrequencies and their transport properties by ultrafast spectroscopy. Our findings suggest a new approach to control magnon transport in an atomically thin antiferromagnet, promising next-generation information applications in ultrafast computing and hybrid quantum information systems.

4:00 PM

(EMA-S6-015-2025) Excitonic band structure of monolayer hexagonal boron nitride (hBN) (Invited)

L. Liu[1]; S. Woo[2]; J. Wu[3]; B. Hou[3]; C. Su*[3]; D. Qiu[3]

1. Yale University, Applied Physics, USA
2. Oak Ridge National Laboratory, USA
3. Yale University, USA

Despite the simple crystal structure of monolayer hBN, there is still an ongoing debate about whether it is a direct or indirect bandgap insulator. In this talk, I'm going to introduce our recent progress on measuring the band structure of hBN using momentum-resolved electron energy loss spectroscopy. We have identified a direct optical band gap which is larger than the previously measured value, and a photon-like excitonic band in the lowest excitonic state.

4:30 PM

(EMA-S6-016-2025) Strong Light-Matter Coupling in Excitonic 2D semiconductors (Invited)

D. Jariwala*[1]

1. University of Pennsylvania, USA

In this talk, I will first focus on the subject of strong light-matter coupling in excitonic 2D semiconductors, namely chalcogenides of Mo and W. Visible spectrum band-gaps with strong excitonic absorption makes transition metal dichalcogenides (TMDCs) of molybdenum and tungsten as attractive candidates for investigating strong light-matter interaction formation of hybrid states. We will present our recent work on the fundamental physics of light trapping in multi-layer TMDCs when coupled to plasmonic substrates. Next, we will show the extension of these results to halide perovskites, metal organic chalcogenates and superlattices of excitonic chalcogenides. These hybrid multilayers offer a unique opportunity to tailor the light-dispersion in the strong-coupling regime. We will discuss the physics of strong light-matter coupling and applications of these structures. If time permits, I will also present our recent work on scalable, localized quantum emitters from strained 2D semiconductors and control of light in magnetic semiconductors. Our results highlight the vast opportunities available to tailor light-matter interactions and building practical devices with 2D semiconductors. I will conclude with a broad vision and prospects for 2D materials in the future of semiconductor opto-electronics and photonics.

S7 Additive manufacturing for power sources in electronics

S7 - AM for Lithium Batteries II

Room: Colorado E
Session Chair: Bin Li, Oak Ridge National Lab

2:00 PM

(EMA-S7-005-2025) Advanced Manufacturing of Multiscale Controlled Electrodes for Lithium-Ion Batteries (Invited)

J. Park*[1]

1. Missouri University of Science and Technology, Mechanical and Aerospace Engineering, USA

This work presents a multiscale approach to electrode fabrication for lithium-ion batteries (LIBs), focusing on both microstructure and macrostructure control to address key performance challenges. At the microstructural level, an electric field is applied during fabrication to align particles more effectively, optimizing ion pathways and improving overall ion transport within the electrode. Simultaneously, at the macrostructural level, microcasting and femtosecond laser processing are used to enhance the structural integrity and scalability of hyper-thick electrodes. By combining these multiscale techniques, the resulting electrodes exhibit significantly improved ion diffusion, low tortuosity, and mechanical stability. The process enables the production of hyper-thick electrodes (~700 µm) that maintain high areal capacities (~8 mAh/cm2) and long cycle life, even under high C-rate cycling. Furthermore, the microstructure alignment via the electric field and the macrostructure control through laser processing ensure the electrodes retain their structural integrity after 1000 cycles at 2C, addressing the common challenges of poor ion transport and degradation in thick electrodes. This multiscale-controlled electrode design represents a significant advancement in battery manufacturing, providing a scalable solution for high-performance, high-capacity lithium-ion batteries.

3:00 PM

(EMA-S7-006-2025) Architected Carbon Electrodes for Supercapacitors (Invited)

Y. Li*[1]

1. University of California Santa Cruz, Chemistry and Biochemistry, USA

Carbon materials have long been valued for their electrical conductivity, affordability, and versatility, making them popular for energy storage devices like batteries and supercapacitors. However, the capacitance of carbon-based supercapacitors has remained between 100 and 200 F/g for decades. Recently, a breakthrough in hierarchical porous carbons has pushed capacitance beyond 300 F/g, renewing interest in carbon materials for supercapacitors. In this talk, I will discuss how combining traditional material synthesis with 3D printing can develop architected carbon electrodes. We have created hierarchical porous carbon aerogels using methods like freeze-drying, templating, and chemical etching, along with 3D printing. These materials feature interconnected pores that provide a large, accessible surface area, enabling ultrafast charging and discharging, even at -70°C. Additionally, they can act as 3D conductive scaffolds for pseudo-capacitive materials with ultrahigh mass loadings. This approach demonstrates how a deterministic structure can overcome key challenges in improving supercapacitor rate capability, capacitance at high current densities and high mass loadings, and performance at low temperatures.

4:00 PM

(EMA-S7-007-2025) Printed Graphtie Electrodes for Fast Charging Lithium-Ion Batteries (Invited)

Q. Wu*[1]

1. Western Michigan University College of Engineering and Applied Sciences, Chemical and Paper Engineering, USA

Fast charging capability has become one of the key features of lithium-ion batteries (LIBs) to facilitate the rapid growth of the electric vehicle (EV) market. However, charging thick electrodes in conventional EV batteries at high current densities always leads to adverse battery performance and safety issues. To address these challenges, thick graphite electrodes with patterned porous architecture were developed through a screen printing process at room temperature. The porous structure including pore diameter and pore-to-pore distance was controlled via adjusting the designed patterns on the screens. The presence of porous structure was confirmed through microscopic images. Used as anodes in LIBs (half and full cells), the printed graphite electrodes exhibited superior electrochemical behaviors over traditional electrodes in terms of rate capability and cycle life. The post-mortem analysis of cycled cells reveals that the printed electrodes have the capability to suppress the Li plating related to fast charging rates. Combining with the advantages of low cost and high throughput, the printed electrode with patterned pores, thus, has the potential of replacing conventional electrodes in commercial LIBs to realize the fast-charging application.

4:30 PM

(EMA-S7-008-2025) 3D Printed Anodes for Next-Generation Batteries (Invited)

M. Wood*[1]; M. C. Freyman[1]; Y. Xiao[1]; B. Wang[1]; N. R. Cross[2]; T. Lin[2]; G. Bucci[2]; C. Zhu[2]; S. Li[2]

1. Lawrence Livermore National Laboratory Physical and Life Sciences Directorate, Materials Science Division, USA
2. Lawrence Livermore National Laboratory, USA

As the demand for energy continues to rise, there is a greater need for high energy density batteries that can operate well under a variety of extreme conditions. These conditions include fast charging and low-temperature environments, where mass transport limitations significantly hinder battery performance. Architected electrodes have the potential to help solve these challenges by improving mass transport throughout the electrode material, and 3D printing enables precise control over the electrode architecture. However, the relationship between architecture and performance is not well understood. We explored how anode architecture impacts performance to better understand the cycling behavior of graphite and Li anodes. Electrodes with well-controlled geometries were fabricated by 3D printing and characterized by SEM and XPS before cycling to evaluate their performance. Modeling was used to predict how anode microstructure affects intercalation behavior and Li nucleation probability, and these results were used to help guide anode design. This work provides valuable insight that will facilitate the development of versatile high-energy-density batteries in the future. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

5:00 PM

(EMA-S7-009-2025) Advancing 3D-Printable Battery Systems: AI-Guided Coatings and Composite Conductors for Enhanced Performance and Scalability (Invited)

S. Thummalapalli[1]; M. T. Sobczak[1]; A. Ramanathan[1]; K. Song*[1]

1. University of Georgia, Mechanical Engineering, USA

This work explores the development of advanced 3D-printable battery systems, focusing on innovative coatings and composite conductors designed to enhance battery performance and manufacturability. By integrating AI-guided additive manufacturing techniques, we achieve precise deposition of multifunctional materials, including polymer/nanoparticle composites, to create intricate electrode structures and conductive pathways. These systems incorporate advanced coatings that improve ionic and electronic conductivity, enhance mechanical stability, and provide superior thermal management. The use of composite conductors, such as silver-infused polymers, significantly reduces internal resistance and boosts energy density, while maintaining a low defect rate. This approach not only enables the production of customized, high-performance battery components but also addresses key challenges in scalability and sustainability, positioning 3D-printed batteries as a transformative solution in energy storage technology.

S11 Complex oxide thin films and heterostructures- from synthesis to strain/interface-engineered emergent properties

S11- Emergent phenomena in complex oxide thin films II

Room: Colorado A

2:00 PM

(EMA-S11-016-2025) Heterogeneous Doping via Nanoscale Coating Impacts Mechanics of Li Intrusion in Brittle Solid Electrolytes (Invited)

X. Xu*[1]

1. Arizona State University, USA

Lithium metal electroplating and short-circuiting limit fast charging in solid-state batteries, yet the mechanisms and methods to regulate lithium intrusions are not well-understood. In this work, we discover that nanoscale heterogeneous Ag^+ doping dramatically affects lithium intrusion in $Li_{6.6}La_3Zr_{1.6}Ta_{0.4}O_{12}$ (LLZO), a brittle solid electrolyte. We generate nanoscale Ag^+ doping by thermally annealing a 3-nm-thick metallic film. The metallic Ag undergoes Ag-Li ion exchange and diffuses into LLZO bulk and grain boundaries to a depth of 20-50 nm. Density functional theory calculations predict this Ag-Li ion exchange exhibits negligible impact on electronic properties. Mechanically, nanoindentation experiments (n = 69) show a fivefold increase in the force required to fracture Ag^+ surface-doped LLZO (Ag^+-LLZO), providing direct evidence that surface modification due to Ag^+ incorporation prevents crack opening. Conducting 121 plating experiments via operando microprobe scanning electron microscopy, we further confirm that the Ag^+-LLZO surface exhibits improved lithium plating even under a large local indentation stress of 3 GPa, demonstrating its role in enhancing the defect tolerance of LLZO. Our study reveals a chemo-mechanical mechanism via surface heterogeneous doping, complementing the present bulk design rules to prevent mechanical failures in solid-state batteries.

2:30 PM

(EMA-S11-017-2025) VO_2 nanocomposite thin films integrated on glass substrates for tunable properties

C. Mihalko*[1]; J. Lu[1]; Z. He[2]; N. Bhatt[1]; Y. Zhang[1]; H. Dou[1]; J. P. Barnard[1]; H. Wang[1]

1. Purdue University, Materials Engineering, USA
2. Purdue University, Electrical and Computer Engineering, USA

Successful tuning of the metal-to-insulator transition (MIT) near room-temperature for VO_2 thin films have been previously reported via a variety of methods, from strain and defect engineering to energy band restructuring. In this study, a nanocomposite VO2 design has been integrated on glass substrates resulting in tuning of the transition, morphology, and optical and electrical properties. Specifically, VO_2-Au nanocomposite and VO_2 thin films have been grown using pulsed laser deposition (PLD) on glass with a ZnO buffer layer. The variations in film composition result in unique morphology, transition characteristics, and optical properties. Notably, the introduction of the ZnO buffer layer results in a redshift of the surface plasmon resonance (SPR) wavelength and unique hyperbolic characteristic for most films. Overall, this work discusses the effect on the tuning of the MIT and optical properties through a novel multifaceted approach using both defect engineering and energy band restructuring. These films integrated on glass show promise for applications in sensing, thermochromics, and optical switching.

2:45 PM

(EMA-S11-018-2025) Low-loss Ruddlesden-Popper ferroelectrics varactors ***WITHDRAWN***

N. Orloff*[1]; F. Bergmann[1]; S. J. Freed[2]; M. R. Barone[3]; D. Schlom[3]
1. NIST, Communications Technology Laboratory, USA
2. University of Maryland, Materials Science & Engineering, USA
3. Cornell University, Department of Materials Science and Engineering, USA

Frequency agile electronics require tunable circuit elements. Tunable capacitors or varactors are a common tunable element. Many varactor applications use semiconductor materials that are lossy above 10 GHz, limiting the potential applications in commercial applications. Ruddlesden-Popper ferroelectrics from $SrTiO_3$ could offer a solution to low loss tunable varactors, but the best demonstrations to date only showed in-plane tunability. Here, we designed an experiment to test if targeted chemical pressure with barium atoms could generate out-of-plane tunability in $SrTiO_3$ Ruddlesden-Popper ferroelectrics. We tested 8 different samples that were 200 nm thick films. The samples had periodicities with different concentrations (15 % and 45 %) of barium to achieve different chemical pressures. These variations help illuminate the limits of defect mitigation in our system how periodicity and targeted chemical pressure can help optimize the tradeoff between tunability and microwave loss.

3:00 PM

(EMA-S11-019-2025) Emergent phenomena in complex oxides via extreme electron doping (Invited)

S. Ramanathan*[1]
1. Rutgers University, ECE, USA

Many classes of complex oxide semiconductors host hidden electronic phases that emerge at certain carrier concentrations. The question is how to sufficiently introduce dopants without destroying the parent lattice or atleast in a reversible manner such that the properties can be toggled with external stimuli. I will present a novel approach to use hydrogen as a dopant that enables discovery of simply stunning physical properties in nominally semiconducting or metallic perovskite nickel oxides. From ten orders of magnitude non-thermal resistance tuning range to onset of ferroelectric behavior in parent metal compounds, hydrogen is among the most powerful electron dopants to explore emergent phenomena in complex oxides. The doping techniques are readily transferable to various solid-state systems beyond oxides. The doping density exceeds electrostatic gating charge by orders of magnitude which is essential for phase emergence. I will also compare hydrogen against lithium in this context as well as solid versus liquid electrolytic gating dynamics. Not only are these properties of interest to advancing condensed matter theory, the large and dynamic tunability opens new application frontiers. I will describe examples in ocean sensing, haptic interfaces and neural probes from our collaborative studies.

4:00 PM

(EMA-S11-020-2025) Unconventional Polar Phenomena in Epitaxial Magnetic Heterostructures (Invited)

L. M. Caretta*[1]
1. Brown University, USA

Crystal symmetry in condensed-matter materials largely dictates their micro- and macroscopic properties and, in turn, their functionalities. A key challenge in quantum materials is to stabilize and control symmetry breaking in polar materials. To this end, the intimate coupling between spin, charge, and lattice degrees of freedom in complex oxides provides a platform to manifest correlations between broken inversion symmetry and materials properties. Polar materials, such as ferroelectrics, are a particularly pervasive example of broken inversion symmetry. Here, we show pathways by which symmetry in unconventional phenomena in polar materials can be engineered via epitaxial constraints. First, by engineering octahedral tilt distortions in epitaxial multiferroic superlattices, we demonstrate that electric (polar) fields can be used to both erase and introduce centrosymmetry, effectively erasing and writing ferroelectric order, and resulting in orders-of-magnitude changes in the nonlinear optical response, resistivity, and piezoresponse. Second, we show that epitaxial strain and heterostructure boundary conditions in non-centrosymmetric oxide metals can be used to establish multiferroic order and topological defects in ultrathin films.

4:30 PM

(EMA-S11-021-2025) Continuous Lattice Symmetry Control of Oxide Films (Invited)

T. Z. Ward*[1]
1. Oak Ridge National Laboratory, USA

Strain engineering is generally imposed by heteroepitaxial film growth on non-lattice-matched substrates. This method involves perturbation in all three unit cell dimensions since the in-plane strain induced into a film's lattice is accommodated by an elastic reaction along the out-of-plane lattice direction driven by the Poisson effect. This talk will give an overview of our group's recent work in developing low energy, low dose He ion implantation as a means to strain dope thin film materials. Unlike conventional epitaxy-based strain tuning methods, strain doping a lattice by implanting noble helium atoms into epitaxial films is an effective means of continuously controlling lattice expansion along the out-of-plane axis while leaving the in-plane axes locked to the substrate. We will focus on our recent works related to magnetic oxides, where induced uniaxial lattice expansion is shown as an effective route to manipulating orbital populations, magnetic anisotropy, and spin coupling. We will also demonstrate how local functionalization may be applied for direct-write device applications.

S14 A1 in Materials research: from data analysis, autonomous experimentation, to human AI cooperation

S14- AI for smart lab and microscopy

Room: Matchless
Session Chairs: Yongtao Liu, Oak Ridge National Lab; Yan Zeng, Florida State University

2:30 PM

(EMA-S14-005-2025) Creating Smart Labs of the Future (Invited)

R. Moore*[1]
1. Oak Ridge National Laboratory, USA

The Interconnected Science Ecosystem (INTERSECT) Initiative at Oak Ridge National Laboratory aims to create smart labs of the future—self-driving, AI and machine learning-driven laboratories where interconnected instruments and compute resources work in harmony to help researchers tackle significant scientific challenges. While this vision is ambitious and transformative, it also remains somewhat abstract. In this talk, I will outline the steps being taken to turn this vision into reality. The INTERSECT science domain test cases encompass a broad range of activities from fundamental sciences like materials, microscopy, and quantum computing to applied fields such as advanced manufacturing and the electrical grid. This wide-ranging scope is designed to cultivate an INTERSECT ecosystem that is both robust and adaptable. I will outline the architecture and software developments that form the foundation of this ecosystem and then focus on the autonomous materials workflows that are advancing interactions between humans and AI assistants. Additionally, I will explore the design's flexibility and its potential impact on addressing the scientific challenges of today and the future.

3:00 PM

(EMA-S14-006-2025) Autonomous Scanning Electron Microscope Powered by Vision Language Models (Invited)

Z. Ren*[1]; J. Li[1] ***WITHDRAWN***

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA

We developed a prototype of an autonomous Scanning Electron Microscope (SEM), designed to reduce the complexity of SEM operation for researchers. Traditional SEMs require significant expertise, but this system leverages AI to automate the entire imaging process. Researchers can verbally simply describe the SEM image they need in natural language, and the AI autonomously handles the workflow, from image capture to optimization, without further human intervention. This autonomous SEM represents a significant leap in AI-assisted research, simplifying the use of complex scientific instruments and enabling more efficient, precise results with minimal human effort.

S14- Automated synthesis and characterization of 2D materials

Room: Matchless

Session Chairs: Yongtao Liu, Oak Ridge National Lab;
Esther Tsai, Brookhaven National Laboratory

4:00 PM

(EMA-S14-007-2025) Automated 2D materials fabrication and characterization (Invited)

S. Park*[1]; H. Jang[1]; K. Yager[1]; G. Doerk[1]; A. Stein[1]; J. Sadoski[1]; C. Black[1]

1. Brookhaven National Laboratory, center for functional nanomaterials, USA

Two-dimensional (2D) materials are highly versatile building blocks for creating novel heterostructures, as individual layers can be stacked without the limitations of epitaxy. Since the pivotal discovery of mono- and few-layered graphene through mechanical exfoliation in 2004, research in 2D materials has made remarkable progress. However, the widespread application of 2D materials has been limited by the labor-intensive fabrication process, which requires significant expertise. In this talk, I will present ongoing work on a robotic 2D material fabrication platform called the Quantum Material Press (QPress). This cluster tool integrates three specialized machines: a robotic exfoliator, a machine vision-based cataloger for flake detection, and a robotic stacker for assembling 2D homo- and heterostructures, all operating within an inert gas glovebox. QPress aims to provide a more reliable fabrication method by optimizing conditions to improve yield and reproducibility.

4:30 PM

(EMA-S14-008-2025) Approaches for AI-driven pulsed laser deposition using in situ diagnostics (Invited)

S. Harris*[1]; A. Biswas[3]; R. Fajardo[2]; F. Bao[2]; C. Rouleau[1]; A. Puretzky[1]; K. Xiao[1]; R. K. Vasudevan[1]

1. Oak Ridge National Laboratory, Cener for Nanophase Materials Sciences, USA
2. Florida State University, USA
3. University of Tennessee Knoxville, USA

The promise of using AI to accelerate synthesis with physical vapor deposition methods relies on exploiting various in situ diagnostics that encode key correlations between the growth environment and film properties. In this talk, I will show how we combined in situ and real-time diagnostics to enable both data-driven and model-driven synthesis approaches with pulsed laser deposition (PLD). First, I will discuss a data-driven method using in situ Raman spectroscopy as a material quality metric to drive an autonomous PLD system to optimize WSe_2 films in a 4D space. Next, I will show that the complex characteristics of the PLD environment can be used to predict thin film growth kinetics by applying deep learning to intensified CCD image sequences of the PLD plume. Using the predictive capabilities of plume dynamics on film properties provides a means for rapid pre-screening of growth conditions prior to deposition. Finally, I will discuss an on-line state estimation method towards real-time model-based control of synthesis trajectories. We developed a film growth model based on fractional area coverage of discrete layers and show that the model parameters can be rapidly estimated in real-time during synthesis of 1T'-$MoTe_2$. This work was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

S19 Frontiers in ferroic ceramics-synthesis, properties and applications

S19- Frontiers in Ferroic Ceramics: Synthesis, properties and applications

Room: Colorado H

Session Chair: Jayakanth Ravichandran, University of Southern California

2:00 PM

(EMA-S19-001-2025) Controlling spin current transport in multiferroic oxides (Invited)

D. Yi*[1]

1. Tsinghua University, Material Science and Engineering, China

Spin-orbitronics, which use pure spin currents to deliver spin angular momentum without net charge flow, holds great promises to revolutionize next-generation information technologies by significantly reducing Joule heating. A key challenge is to control the propagation of pure spin currents, ideally by using electric-field. Multiferroic oxides, with a coexistence of ferroelectric and magnetic ordering, provide a promising material platform to address this challenge. In this talk, I will present our recent studies on the spin current transport in perovskite complex oxides, as exemplified by the multiferroic $BiFeO_3$. We show that the insulating perovskite oxides can efficiently deliver the spin current, which is closely correlated to the antiferromagnetic ordering. Moreover, we demonstrate that the spin current transport behaviors in the multiferroics can be manipulated by using electric-field due to the coupling of ferroelectric polarization and antiferromagnetic order. This progress could pave pathway for developing energy-efficient magnon-based logic and memory devices.

2:30 PM

(EMA-S19-002-2025) In situ cryogenic TEM study of electric field control of magnetic skyrmions (Invited)

M. Han*[1]

1. Brookhaven National Laboratory, USA

Topologically nontrivial spin structures in chiral magnets and two-dimensional (2D) van der Waals (vdW) materials have garnered significant interest due to their implications for fundamental spin physics in low dimensions and potential applications in spintronics and quantum computing. Controlling skyrmionic spin structures and dynamics via electric means is essential for realizing these novel applications. Utilizing in situ electrical and magnetic biasing in a transmission electron microscope (TEM) at liquid helium temperatures, we investigate deterministic control of skyrmions in two insulating magnets by directly imaging magnetic spin structures and their responses to external electric fields. In the skyrmion-hosting chiral magnet Cu_2OSeO_3, we demonstrate that an external electric field can stabilize or destabilize skyrmion lattices, depending on the field direction relative to the crystallographic orientation. Additionally, we show that the skyrmion chirality in the insulating centrosymmetric 2D vdW magnet $Cr_2Ge_2Te_6$ can be controlled by the direction of the external electric field applied during the magnetic field cooling process. Our results demonstrate that electric fields can effectively control the stability and chirality of magnetic skyrmions in insulating systems, providing a crucial foundation for designing skyrmion-based spintronic and quantum computing devices.

3:00 PM

(EMA-S19-003-2025) Interfacial Effects and the Magnetism of Epitaxial Perovskite Thin Films (Invited)

P. Woodward*[1]

1. Ohio State University, Chemistry and Biochemistry, USA

In this talk I will discuss the surprising ways in which the magnetism of epitaxial thin films of three oxide perovskites—$LaFeO_3$, $LaCoO_3$, Sr_2FeMoO_6—is altered by interactions with the underlying substrate. (1) In bulk samples, $LaFeO_3$ is a G-type antiferromagnet with a robust Neel temperature of 740 K. Epitaxial films of $LaFeO_3$ grown on $SrTiO_3$ substrates exhibit an unexpected spin-state disproportionation at the interface that stabilizes a thin ferromagnetic insulating layer. (2) In the bulk, the Co^{3+} ions in $LaCoO_3$ adopt a diamagnetic low-spin state at low temperature that prevents development of cooperative magnetic order. In contrast, there are numerous reports of ferromagnetism arising in thin film samples of $LaCoO_3$. We have studied the effects of epitaxial strain on the magnetism of $LaCoO_3$ films grown by off-axis RF sputtering on substrates with varying degrees of lattice mismatch. The results reveal a complex interplay of strain and defects on the spin states and cooperative magnetism of these films. (3) The double perovskite Sr_2FeMoO_6 is a half-metallic ferrimagnet, where the minority spin electrons become itinerant. While the bulk T_C is ~420 K, this value is reduced to nearly room temperature in thin film samples. However, when Sr_2FeMoO_6 are grown on antiferromagnetic $LaFeO_3$ films, Fe–O–Fe superexchange interactions at the interface increase the ferrimagnetic Curie temperature substantially.

4:00 PM

(EMA-S19-004-2025) Unlocking Atomically Precise Oxide Membrane Growth with Molecular Beam Epitaxy (Invited)

B. Jalan*[1]

1. University of Minnesota, USA

Advances in thin-film exfoliation techniques have enabled the creation of oxide membranes, unlocking new possibilities for assembling heterostructures from materials that are structurally and chemically incompatible. The sacrificial layer method facilitates the integration of these membranes with dissimilar materials. However, the complexity of conventional sacrificial layers limits their utility. In contrast, binary alkaline earth metal oxides with a simple rock salt crystal structure — such as (Mg, Ca, Sr, Ba)O — offer a more accessible alternative. These oxides, covering a broader range of lattice parameters, are easier to grow and can be dissolved in deionized water, making them ideal sacrificial layers. In this presentation, I will present epitaxial single-crystalline growth of perovskite $SrTiO_3$ (STO) on the sacrificial layer of crystalline SrO and BaO films. By dissolving the sacrificial layer in the DI water, we exfoliate millimeter-sized STO membranes. Using high-resolution x-ray diffraction, atomic-force microscopy, scanning transmission electron microscopy, impedance spectroscopy, and scattering-type near-field optical microscopy (SNOM), we demonstrate epitaxial STO membranes with bulk-like intrinsic dielectric properties. The talk will conclude with an exploration of the potential applications of 3D nanomembranes in materials physics and device engineering.

4:30 PM

(EMA-S19-005-2025) Moiré induced polar topologies in twisted oxide membranes (Invited)

J. Santamaria*[1]

1. Universidad Complutense, Materials Physics, Spain

The recent realization of freestanding membranes of perovskite oxides, has enabled their deterministic mechanical assembly into twisted homo bilayers. Twisted oxide membranes surpass the limitations of epitaxial growth, which lock the direction of the crystalline axes of the growing layer, and open the way to a completely new generation of interfaces. In this talk I will show that twisted interfaces of transition metal oxides feature a non homogeneous pattern of shear strains determined by the atomic registry though the strong ionic bonding of this family of compounds. Twisted ferroelectric membranes unlock a "chirality" degree of freedom opening an unprecedented opportunity to tailor topological polar landscapes in a way determined by the lateral strain modulation driven by twisting. We find that the peculiar pattern of polarization vortices driven by strain gradients through flexoelectric coupling of strain gradients to polarization are an indirect measure of the interlayer interaction which can be modulated by inserting graphene layers in between of the twisted layers. This finding opens exciting opportunities to manipulate the remote moiré interaction between the layers allowing for the exploration of novel physical effects and functionalities.

5:00 PM

(EMA-S19-006-2025) Two-step phase transition enabled superelasticity in quasi-two-dimensional freestanding perovskite ferroelectric films (Invited)

X. Pan*[1]

1. University of California Irvine, Materials Science and Engineering; Physics and Astronomy, USA

The weak elasticity and high brittleness of most perovskite ferroelectrics make it challenging to utilize their unique properties for applications in the next-generation flexible electronic devices. Herein, we demonstrate the possibility to overcome this challenge by showing superelasticity of a freestanding $BiFeO_3$ film, a prototype of multiferroics, using in situ transmission electron microscopy and in situ scanning transmission electron microscopy. The film exhibits a tremendous lattice strain of up to 34.4%, which is two orders of magnitude higher than its bulk counterpart and even comparable to that of ductile metals. First-principles calculations and in situ experimental results indicate that such superelasticity is enabled by a reversible 2-step phase transition that includes a conventional rhombohedral-to-tetragonal step and a tetragonal-to-super-tetragonal step which has not been reported before. This work reveals the largest strain tolerance ever reported for $BiFeO_3$ films and provides new insights into perovskite strain engineering, opening new avenues for the development of advanced flexible electronic devices.

S20 Magnetic and superconducting materials-from basic science to applications

S20- Novel applications of magnetic materials

Room: Colorado D
Session Chair: Timothy Haugan, U.S. Air Force Research Laboratory

2:00 PM

(EMA-S20-007-2025) Symmetry and Chemical Stability of 2D M_3X_8 (M = Nb, X= Cl, Br, I) and Related Ionic Kagome Materials

V. Kumari*[1]; J. Bauer[2]; A. Georgescu[1]

1. Indiana University, Chemistry, USA
2. Yale University, USA

Correlated electron materials display a wide array of applications due to their interplay between charge, spin, orbital, and crystal structure leading to a wide variety of emergent states including magnetism and superconductivity. The 2D van der Waals transition metal Kagome halides M_3X_8, are a class of correlated materials showing potential multiferroic properties and spin liquid behavior which have recently been used in field-free Josephson diodes[1] for quantum computing applications. However, a limited number of these materials, only M = Nb and X = Cl, Br, I compounds are reported in the literature - as opposed to the wider variety of 2D dihalides and trihalides (MX_2 and MX_3). Using density functional theory, we show that these materials' chemical stability is driven by the symmetry of the trimer orbital formation across M_3 ions which stabilizes a breathing distortion. Using Crystal Orbital Hamiltonian Populations (COHP) and symmetry analysis we find that the materials that have been successfully synthesized have an optimal trimer orbital bonding/antibonding filling ratio. Our theoretical analysis easily extends to insulating Kagome oxides as well, including $Li_xScMo_3O_8$,[2] $Li_2InMo_3O_8$, and $LiZn_2Mo_3O_8$,[2] which all follow the same symmetry criterion. Finally, we use our analysis to propose new potential materials for potential synthesis.

2:15 PM

(EMA-S20-008-2025) Frontiers in AM3X4 and AM6X6 kagome compounds; development of new kagome metals (Invited)

B. R. Ortiz*[1]; W. Meier[6]; G. Pokharel[5]; D. Parker[1]; H. Miao[1]; J. Chamorro[3]; F. Ye[1]; S. Sarker[4]; G. D. Samolyuk[1]; K. Gornicka[1]; F. Yang[1]; S. Mozaffari[6]; A. Thaler[6]; A. May[1]; S. Wilson[2]; B. Sales[1]; D. Mandrus[6]; M. McGuire[1]

1. Oak Ridge National Laboratory, USA
2. University of California Santa Barbara, USA
3. Carnegie Mellon University, USA
4. Cornell University, USA
5. University of West Georgia, USA
6. The University of Tennessee Knoxville Tickle College of Engineering, USA

Continued efforts into understanding complex electronic and magnetic states in kagome metals has served as a great impetus for the discovery of new kagome metals. This is particularly the case for low-dimensional crystal structures (e.g. our prior discovery of the AV3Sb5 kagome superconductors and recent discoveries in the AM3X4 kagome magnets, both of which are exfoliable). In this chemistry-focused talk, we present our experimental methodology for discovering new kagome metals alongside a discussion of several new families of compounds. Examples include; our ability to tune magnetism in a new series of AM3X4 layered magnets, a new density-wave transition in a nonmagnetic kagome metal, a new kagome prototype built from the AM3X5 structural motif, and new frontiers in the larger AM6X6 kagome family. Our results provide the community with new single-crystal platforms for the exploration of magnetic, structural, and electronic instabilities in kagome metals.

2:45 PM

(EMA-S20-009-2025) Magnetization dynamics of $LnMn_6Sn_6$ (Ln = Tb, Dy) ferimagnetic kagome metals (Invited)

K. Collins*[1]; J. Flores[1]; M. A. Susner[2]; M. Newburger[3]

1. Air Force Research Laboratory/Azimuth Corp, Materials and Manufacturing Directorate, USA
2. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
3. Air Force Research Lab, USA

The $LnMn_6Sn_6$ family of materials, where Ln is a generic lanthanide trivalent cation, have attracted much interest due to their complex electronic and magnetic structures. This complexity arises from the coupling of highly anisotropic lanthanide ions spins with large spin-orbit couplings to the spins of the Mn atoms, which are arrayed in a kagome lattice, a lattice topology known to give rise to exotic topological phenomena. This interplay of magnetic anisotropy and electronic topology motivates investigation into the magnetic excitations of these materials, which unlike the ground state magnetic structures of this family have not been extensively studied. Herein, we use Brillouin light scattering to measure the magnon spectra of $TbMn_6Sn_6$ and $DyMn_6Sn_6$, measuring the magnon frequency, lifetime, and intensity as a function of applied magnetic field and sample temperature. We find that despite a difference in their magnetic ground states between a canted easy-axis (Tb) and easy-cone (Dy) spin orientation, these two structural isomers host markedly similar magnon dispersions, both with respect to magnetic field and temperature.

3:15 PM

(EMA-S20-010-2025) Evolution of Magnetism and Transport Properties through Electrochemical Intercalation for a 2D Magnetic Semiconductor

Z. Zhai*[1]; W. Liu[1]; X. Guo[3]; N. Agarwal[4]; A. Stangel[4]; D. Schulze[2]; T. Kuo[2]; L. Deng[2]; N. Jalali[5]; K. Brenner[5]; L. Zhao[3]; R. Hovden[4]; C. Chu[2]; B. Lv[1]

1. The University of Texas at Dallas, Physics, USA
2. University of Houston, Physics, USA
3. University of Michigan, Physics, USA
4. University of Michigan, MSE, USA
5. The University of Texas at Dallas, MSE, USA

Van der Waals(vdW) magnets currently receive increasing research interest for both fundamental 2D materials research and their potential in future spintronic and information applications. The superior crystalline quality with minimum defects for these vdW magnet bulk crystals is extremely important for many aspects of 2D magnet studies. CrSBr is an air-stable vdW layered orthorhombic antiferromagnet which shows high Néel temperature of 132 K with A type magnetic ordering structure, where each atomic layer CrSBr shows in-plane ferromagnetic ordering along the b axis, and the adjacent layers stack antiferromagnetically along the c axis. Interesting properties such as structural phase transformations, magneto-optical and magneto-transport, the coupling of excitons and magnons, and surface magnetism have been reported. Here we carry out electrochemical intercalation studies to probe the magnetic and transport properties of high quality bulk CrSBr crystals we have synthesized. The detailed results and their implications will be presented and discussed. In addition, we will discuss and report our efforts on bulk crystal growth on large series of orthorhombic magnetic oxyhalide phases, their crystal quality and related physical properties will be properly discussed.

4:00 PM

(EMA-S20-011-2025) Opportunities for Advanced Magnetism in Hybrid Organic-Inorganic Materials (Invited)

E. Mozur*[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA

Hybrid Organic-Inorganic Materials inhabit a diverse phase space, encompassing metal-organic frameworks, hybrid halide perovskites, and many traditional oxide structure types. This structural versatility is coupled to varied mechanisms of organic-inorganic coupling that modify the local structure and bonding around the magnetic inorganic ion. Hybrid materials, therefore, have the potential to have varied, tunable magnetism. Here, we discuss available knowledge, limitations, and open questions in the design of the magnetic structure of hybrid organic-inorganic mateirals.

4:30 PM

(EMA-S20-012-2025) Engineering Electromagnetic Properties of Yttrium Iron Garnet Thin-Films Through Ion Implantation (Invited)

P. Kulik*[1]

1. University of Central Florida, ECE, USA

Epitaxially grown high quality Yttrium Iron Garnet (YIG) on Gadolinium Gallium Garnet (GGG) substrates have recently gathered attention for tunable filter and optical devices. Yet, the prohibitive manufacturing cost and limited electromagnetic property tunability has prevented their wide adoption. In this talk, we will discuss our recent efforts in understanding the effects of aluminum (Al) and holmium (Ho) ion implantation on thin film YIG/GGG substrates utilizing low and high ion fluencies. Our study focuses on both the static and dynamic magnetic properties of the implanted films which reveal that higher ion fluency leads to a more significant reduction in magnetic saturation, resulting in a shift of ferromagnetic resonance. Additionally, the static magnetic properties suggest a localized shift in magnetic anisotropy. These modifications in material properties indicate the potential for post-growth alterations similar to semiconductor doping, paving the way for the development of innovative devices on high quality thin-film YIG.

5:00 PM

(EMA-S20-013-2025) Aerosol deposition of yttrium iron garnet/iron magnetic composites

S. C. Mills*[1]; E. Patterson[1]

1. US Naval Research Laboratory, Material Science and Technology, USA

Aerosol deposition (AD) was used to produce dense and polycrystalline films of yttrium iron garnet (YIG, $Y_3Fe_5O_{12}$) and iron (Fe) and their composites. Magnetic composites, particularly 0-3 composites, composed of 'hard' (Fe) and 'soft' (YIG) magnetic materials can become exchange coupled via nanoscale interactions, enhancing various magnetic properties such as remnant magnetization, coercivity, and magnetic energy product $(BH)_{max}$. The bonding and densification of a film produced by AD is facilitated by high pressure, impact and fracture of the particles, resulting in a nanocrystalline film that has the potential to exhibit exchange coupling between materials, such as with Fe_2O_3 (soft) and FeCo (hard) nanocomposites. Deposition was carried out onto alumina substrates with a range of YIG:Fe compositions. Various powder pre-treatment methods and AD parameters were first optimized to produce dense and adherent films. After deposition, the properties of the films were characterized via X-ray diffraction, ferromagnetic resonance (FMR), and vibrating sample magnetometry (VSM) to determine the effect of composition on YIG/Fe AD films. The ability to deposit magnetic composites into microns thick, dense, and polycrystalline films at room temperature via AD has promise for a variety of applications that require the integration of high-melting point materials in CMOS-compatible manufacturing processes.

5:15 PM

(EMA-S20-014-2025) "Easy peel" 1T-$CrTe_2$: Studying the Chemistry Change from $ACrTe_2$ (A=K, Rb) to 1T-$CrTe_2$ (Invited)

J. Wang*[1]; K. Prasad[1]

1. Wichita State University, Chemistry and Biochemistry, USA

Among several ferromagnetic materials with transition temperatures above room temperature, 1T-$CrTe_2$ has garnered increasing attention due to its combination of ferromagnetic properties and its two-dimensional (2D) crystal structure. 1T-$CrTe_2$ is classified as a 2D ferromagnet, making it an excellent candidate for exploring magnetism in low-dimensional systems. Typically, 1T-$CrTe_2$ is synthesized indirectly by extracting potassium (K) from $KCrTe_2$. However, the presence of residual potassium complicates the exfoliation of 1T-$CrTe_2$ crystals. In this study, we investigate the chemical changes that occur when transitioning from pristine $ACrTe_2$ (where A = K or Rb) to 1T-$CrTe_2$, focusing on changes in the oxidation state of chromium (Cr) and the physical properties of $ACrTe_2$. We present the crystal structure and physical properties of $ACrTe_2$ and examine the oxidation states of Cr in the transition from $ACrTe_2$ to $CrTe_2$ using X-ray photoelectron spectroscopy (XPS). Additionally, we developed a straightforward method to remove residual potassium from 1T-$CrTe_2$, which significantly makes exfoliation easier, making it "easy to peel."

5:45 PM

(EMA-S20-015-2025) Atomistic Magnetoelastic Simulations Using Molecular Dynamics

M. McIntosh*[1]; G. Carman[1]

1. University of California Los Angeles, Mechanical Engineering, USA

Understanding magnetism and its role in magnetomechanical forces at the atomic level has traditionally been limited by Density Functional Theory (DFT), which can only characterize electron orbits in periodic structures at zero temperature. This limitation excludes the impact of thermal fluctuations and long-range order on magnetic energies. In this work, we extend the Atomic Spin Dynamics (ASD) and Molecular Dynamics (MD) framework by incorporating magnetoelastic energy to capture both magnetic and lattice responses to external stimuli, such as applied pressure or magnetic fields. Unlike DFT, this model relies on empirical data, enabling it to be applied to small, discrete structures—only a few nanometers in size—and to more complex geometries. Our results demonstrate consistency with real-world experiments of both the Villari effect (inverse magnetostriction) and magnetostriction, while maintaining atomic-level accuracy down to the angstrom scale. Furthermore, we explore the influence of defects, such as voids and interstitials, on these small-scale systems. This approach advances our understanding of dynamic magnetic responses in exchange-coupled structures near complex boundaries.

Friday, February 28, 2025

S1 Ceramics for the Hydrogen Economy

S1- Ceramic components for solid oxide cells, including electrolytes, electrodes, and sealants

Room: Colorado J
Session Chairs: Vaibhav Vibhu, Forschungszentrum Julich GmbH; Till Frömling, Technische Universität Darmstadt

8:30 AM

(EMA-S1-008-2025) Probing protonic transport in ceramic electrolytes for solid oxide cell applications (Invited)

S. Skinner*[1]; K. Huang[1]; C. Liao[1]; Y. Han[1]; M. Gonzalez[2]

1. Imperial College London, United Kingdom
2. Institut Laue-Langevin, France

As there is increasing interest in the development of all ceramic electrolysers it is apparent that a new generation of materials are required with exceptional perfomance over a wide oxygen partial pressure regime, with a drive to develop devices operating at intermediate temperatures of 500-700°C. To address this need there is signifciant focus on protonic ceramic electrochemical cells (PCEC).

Leading materials contenders in this space include the $BaZrO_3$ based electrolytes, with cation substitution, but increasingly there is a need for new materials comnbined with detailed understanding of the protonic transport mechanism. Here we embrace two parallel strategies focusing on the identification of proton tranport mechanisms in oxides, with attention on the BZCYYb ($BaZr_{1-x-y-z}Ce_xY_yYb_zO_{3-d}$) and $LaNbO_4$ based systems. Our work indicates that the BZCYYb phases contain signifcant immobile proton content even in nominally dry conditions, whilst the $LaNbO_4$ based phases exhibit enhanced proton mobility under reducing conditions. These data provide new insights that will underpin the development of PCEC technologies.

9:00 AM

(EMA-S1-009-2025) New Hexagonal Perovskite Derivatives for Hydrogen Applications (Invited)

S. Fop*[1]; A. Mclaughlin[1]

1. University of Aberdeen, Chemistry, United Kingdom

Proton and oxide ion ceramic conductors are important materials with electrolyte applications in hydrogen-based technologies. Several ceramic ionic conductors crystallize with the perovskite ABO_3 structure, which is composed by a three-dimensional network of corner-sharing BO_6 octahedra, with the larger A cations occupying the interstitial voids. In these materials, extrinsic defects necessary for ionic transport are typically introduced by acceptor doping. In our quest to find new conductors with enhanced performances, we have explored the hexagonal perovskites family. Hexagonal perovskites form from mixed stacking sequences of hexagonal (h) and cubic (c) close-packing of $[AO_3]$ layers, which result in the formation of face-sharing and corner-sharing BO_6 octahedra. By controlling the composition and crystal chemistry, it is possible to introduce intrinsic cation and anion vacancies, with the formation of inherently defective layers of general composition $[AO_{2\pm\delta}]$. The intrinsic oxygen disorder within these functional layers can result in oxide ion conduction, as well as enable water absorption and migration of protonic defects. Here, I will report a few examples of hexagonal perovskite derivatives exhibiting high oxide ion and proton conductivity. Overall, our results highlight the importance of exploring alternative crystal structure systems for the design of innovative ionically conducting ceramic materials.

9:30 AM

(EMA-S1-010-2025) High electrical conductivity of 0.01 - 0.001 S/cm at room temperature in yttria-stabilised zirconia

L. Thompson*[1]; L. Paulsson-Habegger[1]; M. Li[2]

1. University of Nottingham, Engineering, United Kingdom
2. University of Nottingham, Department of Mechanical, Materials and Manufacturing Engineering, United Kingdom

Yttria-stabilised zirconia (YSZ), developed by Walther Nernst in the 1890s, find important technical applications due to its excellent chemical, thermal and mechanical properties. YSZ has been known to exhibit 'pure' oxide ion conductivity but negligible electronic conductivity at high temperatures. Its oxide ion conductivity reaches 0.01 S/cm at 700-750 °C and is stable in both oxidising and reducing atmospheres, enabling it to be used as a solid electrolyte in solid oxide fuel cells. We have developed a way to enhance the electrical conductivity of YSZ by more than 10 orders of magnitudes to the range of 0.001 - 0.01 S/cm at room temperature. The high electrical conductivity is presumably related to electronic conduction. Thermogravimetric analysis (TGA) reveals an oxygen loss of approximately 1-2% by mass in the reduced YSZ, which maintains its typical cubic structure as determined by X-ray diffraction (XRD). The potential roles of the reduced YSZ in the hydrogen economy will be discussed.

9:45 AM

(EMA-S1-011-2025) Low Chemical Strains in Orthorhombic Ferrite Perovskites: Relating Bond Angles, Hybridization, and Redox Coefficients of Chemical Expansion

L. O. Anderson[1]; D. Nordlund[2]; N. H. Perry*[1]

1. University of Illinois Urbana-Champaign, USA
2. Stanford Linear Accelerator Center, USA

Chemical strains are associated with mechanical degradation in multilayer ceramic energy devices. For oxide mixed ionic/electronic conductors operating at high temperatures, a relevant metric is the redox coefficient of chemical expansion (CCE), which normalizes the isothermal chemical strain to the change in oxygen stoichiometry. The location of electrons that form during oxygen release is significant in the magnitude of the CCE: redox on cations can create large strains, while redox on anions can yield near-zero strains; however, such charge localization may hinder electronic transport. In this study we investigated the role of charge distribution in the B-O bonds of ABO_3 perovskites, expecting greater covalency to lower redox CCEs. We synthesized and characterized $(La,Ca)FeO_{3-x}$ (LCF) and $(Y,Ca)FeO_{3-x}$ (YCF) with synchrotron XRD and XAS, and in-situ dilatometry and TGA. Despite expecting lower Fe-O hybridization in YCF owing to smaller Fe-O-Fe angles, the reverse was observed and attributed to the role of the more polarizable A-site cation in LCF. While both compositions exhibited low redox CCEs compared to most perovskites, the lower CCE of YCF coincided with both greater distortions and greater hybridization. However LCF exhibited higher electronic conductivity. Implications for design of near-zero-strain materials will be discussed.

10:30 AM

(EMA-S1-012-2025) All-ceramic solid oxide fuel cells utilizing phase-inversion derived scaffolds and impregnated nanoparticles as cathodes (Invited)

C. Chen*[1]; C. Huang[1]

1. University of Science and Technology of China, Materials Science and Engineering, China

Solid oxide fuel cells (SOFCs) supported on ceramic cathodes exhibit better redox stability and allow for a broader selection of anode materials compared to those supported on the Ni-yttria stabilized zirconia (YSZ) cermet anodes. In the present study, a cathode-supported all-ceramic SOFC was proposed and investigated. The cathode consisted of a phase-inversion derived porous yttria-stabilized zirconia (YSZ) scaffold in which $LaCoO_3$ (LCO) nanoparticles were impregnated. Through testing with symmetric cells, the optimal LCO loading was determined to be 15 wt%, resulting in a polarization resistance (R_P) of 0.05 Ω cm^2 at 800 °C. The anode was composed of a thin porous YSZ scaffold impregnated with $Sr_{1.9}Fe_{1.4}Ni_{0.1}Mo_{0.5}O_{6-\delta}$ (SFMN) nanoparticles. The optimal loading of SFMN was found to be 40 wt%, corresponding to an R_P of 0.16 Ω cm^2 at 800 °C. An SOFC featuring a 400 μm thick LCO@YSZ cathode, a 10 μm thick YSZ electrolyte, and a 30 μm thick SFMN@YSZ anode achieved a peak power density of 1084 mW cm^{-2} at 800 °C with wet H_2. By utilizing composite of LCO and $Gd_{0.1}Ce_{0.9}O_{2-\delta}$ (GDC) in a 7:3 ratio as the cathode, the cell's stability, as indicated by the change in power density over time, showed a notable improvement. Further investigation of the cathode-supported all-ceramic SOFC is warranted to enhance stability and reduce operating temperatures.

11:00 AM

(EMA-S1-013-2025) $SrCo_{0.9}Ta_{0.1}O_{3-d}$ vs. $BaCo_{0.9}Ta_{0.1}O_{3-d}$: Which Is a Better Oxygen Electrocatalyst? (Invited)

K. Huang*[1]

1. University of South Carolina, Mechanical Engineering, USA

Oxygen deficient perovskites are highly active catalysts toward oxygen catalysis needed for high-performance solid oxide cells (fuel cells and electrolyzers), metal-air batteries, and air-oxygen separation membranes. In this presentation, we compare physiochemical properties of $BaCo_{0.9}Ta_{0.1}O_{3-d}$ (BCT) with $SrCo_{0.9}Ta_{0.1}O_{3-d}$ (SCT) of primitive cubic structure. The comparison reveals that BCT exhibits a thermal expansion coefficient (TEC) close to the commonly used electrolytes (10-12 ppm/K), whereas SCT exhibiting nearly doubled TEC. Electrically, SCT is a much better conductor than BCT, showing nearly two orders of magnitudes of electronic conductivity. Thermally, SCT gives off more oxygen at higher temperatures than BCT, resulting in higher oxygen nonstoichiometry. Electrochemically, SCT shows lower and more stable area-specific polarization resistance than BCT. Crystallographically, SCT10 contains larger Co-O octahedra than BCT10, even though the latter has a larger unit cell. This implies that the oxygen catalytic activity is controlled by the size of Co-O octahedron, not the size of unit cell of the perovskite.

11:30 AM

(EMA-S1-014-2025) Development of high-performing and durable fuel electrodes for Solid Oxide Electrolysis Cells (Invited)

V. Vibhu*[1]; R. Kumar[1]; S. E. Wolf[1]; J. Uecker[1]; I. Unachukwu[1]; L. de Haart[1]; R. Eichel[1]

1. Forschungszentrum Julich GmbH, Institute of Energy Technologies (IET-1), Fundamental Electrochemistry, Germany

The conventional Ni-yttria stabilized zirconia (YSZ) fuel electrode shows strong degradation in SOEC operation under steam-containing fuels due to Ni migration and agglomeration. As an alternative, Ni-gadolinium doped ceria (GDC) electrode exhibit higher performance than Ni-YSZ owing to the mixed ionic and electronic conductivity of GDC under reducing conditions, however it couldn't prevent Ni-migration. To overcome these issues, we have considered perovskites-based fuel electrodes, e.g. $Sr_2Fe_{2-x}Mo_{x-y}M_yO_{6-\delta}$ (x=0.5, 1.0 and M = Ni), as they exhibit mixed ionic and electronic conducting properties and good redox stability under reducing atmospheres. SFM based fuel electrode materials also show higher electrochemical performances than Ni-YSZ electrode. Moreover, we have also investigated Ni-free fuel electrode materials and considered single-phase ceria-based materials e.g. $Ce_{0.8}Gd_{0.2}O_{1.9}$ and $Ce_{1-x}Pr_xO_{2-\delta}$ ($0.0 \le x \le 0.3$). These ceria-based materials are mixed ionic and electronic conductors and exhibit high catalytic activity under reducing atmospheres. For instance, the single cell with the GDC fuel electrode has similar performance as that of the Ni-YSZ electrode but shows significantly lower degradation rates under SOEC operation. The structural, physicochemical, and electrochemical properties of newly developed fuel electrodes including long-term degradation tests will be presented.

12:00 PM

(EMA-S1-015-2025) Toward the rational design of high entropy perovskite oxide for Solid Oxide Cells with the machine learning approach

Y. Kim*[1]; P. Rand[1]; C. Miesel[2]; J. Yang[1]; N. Sullivan[2]; R. O'Hayre[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA
2. Colorado School of Mines Department of Mechanical Engineering, USA

Solid oxide cells (SOCs) are promising candidates for renewable energy-conversion devices. Due to their reversible capabilities, they can operate both in fuel cell mode (producing electric power) or in electrolysis mode (producing hydrogen). SOC performance is often constrained by rate-limiting processes found at the air electrode, which must activate the oxygen reduction reaction. Conventional air electrodes in SOCs are typically based on single perovskite oxides such as $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$. However, these materials face challenges in terms of stability under harsh gas environment conditions, including CO_2 and high humidity. High entropy oxides (HEO) have emerged due to their high configurational entropy with high catalytic activity and stability. HEOs necessarily entail high compositional complexity, and thus their design can be aided by machine learning. Here, symbolic regression (SR) offers benefits, as it enables the development of interpretable models based on physical mathematical formulas. In this work, we designed novel high-entropy double-perovskite ($AA'BB'O_6$) oxides for SOC air-steam electrode materials. We then identify chemical descriptors for HEO performance based on our experimental results and use these descriptors to further optimize our HEO composition. Finally, we deploy our optimized HEO composition as a reversible SOC air/steam electrode.

12:15 PM

(EMA-S1-016-2025) Oxygen Non-Stoichiometry and Thermochemical Hydrogen Production in Novel Machine Learned Oxides

T. C. Douglas*[1]; K. King[1]; M. Witman[1]; P. A. Salinas[1]; A. McDaniel[1]; E. Coker[1]; S. Bishop[1]

1. Sandia National Laboratories, USA

Thermochemical hydrogen production (TCH) is a promising approach to convert water into hydrogen by harnessing thermal energy. In this two-step process, a material undergoes thermal reduction at high temperatures (~ 1300 – 1500 °C) under low oxygen partial pressures of $\sim 10^{-3} - 10^{-5}$ atm, resulting in the formation of oxygen vacancies. Then, the temperature of the system is reduced to ~800 – 1000 °C in the presence of steam, enabling water splitting through oxidation of the material. Commercial feasibility of TCH is reliant on identifying a material with an optimal reduction enthalpy that supports both the thermal reduction of redox-active cations and its subsequent re-oxidation, while also maintaining high cycle stability. Our team has developed a machine learning algorithm to discover materials suitable for TCH. From the thousands of compounds predicted by the model, we have selected candidates based on criteria for oxygen vacancy formation energy and stability and focused on compounds with redox-active cations beyond the commonly studied first-row transition metals such as, Fe, Co, and Mn. We will present the oxygen vacancy concentrations of selected compounds derived from thermogravimetric measurements, analysis of point defect equilibria, and hydrogen production data obtained from flow reactor experiments. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

S2 Electronic and Ionic Materials for Energy Storage and Conversion Systems

S2- Next generation electrodes and electrolytes

Room: Colorado I
Session Chairs: Hui Xiong, Boise State University

8:30 AM

(EMA-S2-015-2025) Materials Design and Structural Understanding of Cation-Disordered Oxides For Battery Applications (Invited)

D. Chen*[1]

1. University of New Mexico College of Arts and Sciences, Chemistry, USA

Cation disordering, a fascinating phenomenon that represents random cation distribution in a long range, has drawn significant attention among solid-state chemists and functional materials scientists. Due to the younger age of cation-disordered materials, exploration of chemical and structural space of cation disordered materials is still at a preliminary stage. In this presentation, we will demonstrate our effort in developing all-new cation-disordered battery electrode materials and investigating their electrochemical properties for battery applications. Moreover, we will present our approach in characterizing the unique structural features and working mechanisms of these novel electrode materials via a comprehensive array of spectroscopic techniques, ranging from X-ray absorption, solid-state UV-Vis absorption, vibrational spectroscopy, etc. The materials developed and the knowledge obtained in the study not only contribute to the advancement of fundamental solid-state chemistry but also generate transformative insights for various subfields of energy storage materials with disordered structures.

9:00 AM

(EMA-S2-016-2025) Mn_3O_4 as an Anion-Hosting Cathode for Aqueous Batteries (Invited)

S. Sandstrom[1]; Q. Li[2]; Y. Sui[1]; D. Jiang[2]; X. Ji*[1]

1. Oregon State University, Chemistry, USA
2. Vanderbilt University, USA

In this talk, I will address the unconventional utility of MnO_x as a cathode material for storing anions, where we paid close attention to Mn_3O_4. Our initial studies reveal that through structural amorphization, Mn_3O_4 can host NO_3^- ions reversibly upon anodic charging by exhibiting a capacity of nearly 120 mAh/g. This finding is the first example of the reversible hosting of anions by a dense ceramic structure. Later, we explored the anion-hosting of Mn_3O_4 in concentrated $ZnCl_2$-based electrolytes, where Mn_3O_4 exhibits intriguing electrochemical behaviors. If Mn_3O_4 is discharged first, it shows a modest capacity of 50 mAh/g at low potentials around 0.3 V vs. Zn^{2+}/Zn. However, upon subsequent charging, this compound delivers a large capacity of nearly 200 mAh/g at high potentials above 1.5 V vs. Zn^{2+}/Zn. The much greater capacity from a substantially higher potential suggests that the first discharge process is irreversible, where the inserted Zn^{2+} ions are trapped in the structure. We found that the irreversible Zn^{2+} trapping confers an environment that enhances the subsequent reversible anion hosting, where this mechanism is referred to as counter-ion insertion (CCI). The question is, what ion insertion constitutes the observed large capacity for the charging? Our integrated characterization and simulation suggest that the storage of polychloride is responsible for the capacity.

9:30 AM

(EMA-S2-017-2025) Designing Fast and Stable Li-Ion Batteries through Inter- and Intra-Polyhedral Connectivity

M. M. Butala*[1]

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

Early transition metal oxides, e.g., α–V2O5 and Wadsley-Roth materials, are promising future Li-ion battery electrodes. A range of inter- and intra-polyhedral connectivities between V_2O_5 and Wadsley-Roth structures highlight the roles of composition, atomic structure, and battery cycling behavior. We describe the use of chemical modification and soft-chemical synthesis routes to access metastable materials related to these widely studied Li-ion battery materials. These include a metastable polymorph of Nb_2O_5 and a compositional series of Mo-substituted V_2O_5. Synchrotron X-ray and neutron diffraction and battery cycling studies show how differences in inter- and intra-polyhedral connectivity affect reaction pathways during Li intercalation and de-intercalation. Through this work, we identify strategies for mitigating structural evolution during cycling toward enhanced battery performance. To further understand the relationship between structural connectivity and battery performance, we employed data science and machine learning techniques. By assembling encoded atomic structure information and cycling data for select Wadsley-Roth and related materials, we investigate more general correlations between inter- and intra-polyhedral connectivity and electrochemical energy storage. These insights can guide the design of future synthetic targets and the development of advanced battery materials.

9:45 AM

(EMA-S2-018-2025) Local and Global Structural Effects of Doping on Ionic Conductivity in Na3SbS4 Solid Electrolyte

C. Lee*[1]; M. Maegawa[2]; H. Akamatsu[2]; K. Hayashi[2]; S. Ohno[3]; P. Gorai[4]

1. Colorado School of Mines, USA
2. Kyushu Daigaku, Japan
3. Tohoku Daigaku, Japan
4. Rensselaer Polytechnic Institute, USA

Solid electrolytes (SEs) used in solid-state batteries suffer from low ionic conductivity and limited (electro)chemical stability that have impeded their commercialization. Na-ion battery technology offers tremendous potential for grid-scale energy storage. Among Na-ion SEs, Na_3SbS_4 has an ionic conductivity of 10^{-3} S/cm, which is increased to 10^{-2} S/cm with W doping. It has been suggested that aliovalent W doping increases the Na vacancy concentration, which increases ion conductivity. However, doping also affects the mobility of Na ions by modifying their migration barrier, but such effects are not fully understood for doped-Na_3SbS_4. We use first-principles defect calculations to quantitatively demonstrate the increase/decrease in Na vacancy concentration due to aliovalent doping of Na_3SbS_4. In conjunction with experiments, we reveal local and global structural effects of doping on the migration barrier. These effects and their interplay manifest even in the case of isovalent doping where doping does not change the mobile ion concentration.

10:30 AM

(EMA-S2-019-2025) Iron (Fe) redox chemistry in concentrated aqueous electrolytes: from unexpected discovery to thermodynamic modeling (Invited)

T. Gao*[1]

1. The University of Utah, USA

Addressing the climate change challenge requires widespread deployment of renewable energy and the decarbonization of emission-intensive industries. Although the redox chemistry of iron (Fe) in aqueous electrolytes has been studied for decades, recent advancement in electrolyte science has revealed unprecedented phenomenon in the concentrated regime, which opens new opportunities to design rechargeable batteries for renewable energy deployment. In this talk, I will first introduce Fe metal battery and how concentrated electrolytes address some key barriers of Fe metal batteries, then discuss some unexpected fundamental discovery during this journey and share how thermodynamic modeling can explain these discoveries.

11:00 AM

(EMA-S2-020-2025) Single-particle electrochemistry of cathode particles using microelectrode arrays (Invited)

Y. Li*[1]

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

Porous battery electrodes are comprised of an ensemble of many redox-active battery particles, binders, and conductive additives infilitrated with liquid electrolytes. This heterogeneity makes it difficult to uncover the intrinsic redox behavior of individual battery particles. We overcame this challenge by using the microelectrode array to isolate individual micron-sized cathode particles and conduct electrochemistry on individual particles. Our key findings are that the electrolyte penetrates into polycrystalline NMC particles due to cracking, and that this electrolyte penetration enables fast charge and discharge. Single-crystal NMC particles do not benefit from this electrolyte penetration and therefore have substantially worse rate capability than polycrystalline ones, making them challenging for use in commercial batteries. We further discuss other opportunities for microelectrode arrays to uncover the intrinsic electrochemistry of cathode particles.

11:30 AM

(EMA-S2-021-2025) Uncover Transport, Mechanics and Failure in Electroceramics through Atomic and Dynamic Visualization (Invited)

X. Xu*[1]

1. Arizona State University, USA

Electroceramics with superior ionic conductivity, fast interfacial kinetics, and high mechanical strength are promising for renewable energy storage and conversion systems. However, fundamental mechanisms of charge transport and the related electro-chemo-mechanics are not well understood. In this talk, I will highlight my recent work on two types of electroceramics: an oxygen-ion conductor CeO_2 for fuel cells, and a Li-ion conductor $Li_7La_3Zr_2O_{12}$ for solid-state batteries. First, I will present a unique approach to study the charge transport at grain boundaries in polycrystalline CeO_2: a combination of electron holography and atom probe tomography. The atomic visualization of electric fields and chemical species reveals the chemical origins of resistive grain boundaries. These insights suggest chemical tunability of grain boundary transport properties which can potentially benefit the design of low temperature solid-oxide fuel cells and electrolytic cells. Second, I will discuss the Li intrusion phenomena in $Li_7La_3Zr_2O_{12}$, a failure mechanism in solid-state batteries involving both electrochemistry and mechanics. Using operando electron microscopy, statistical analysis and nanoscale characterization, I will discuss the mechanical origins of Li intrusion and highlight the mechanical tunability of electrochemical plating reactions in brittle electroceramics.

12:00 PM

(EMA-S2-022-2025) Understanding Calendaring Decay of Bulk-Type Solid-State Batteries

F. Han*[1]

1. Rensselaer Polytechnic Institute, USA

Solid-state batteries based on the LiPON thin film solid electrolyte have been demonstrated to exhibit a long calendar life of more than 10 years. Such a long calendar life is also assumed to be transferable to bulk-type solid-state batteries with superionic sulfide-based solid electrolytes. However, quantitative studies of calendaring decay of bulk-type solid-state batteries have been rarely reported. In this presentation, we will introduce our preliminary study on understanding the mechanisms of capacity decay in a sulfide-based solid-state battery. Through voltage decay measurement of solid-state cells with variable thicknesses of solid electrolyte and cathode, we highlight the important role of electronic conductivity in calendaring decay of solid-state batteries.

S3 Nano4Neuro-Mechanisms and Materials for Next Generation Computing

S3- Neuroinformatics and architectures

Room: Colorado C

Session Chairs: Sangmin Yoo, Oregon State University; Anton Ievlev

8:30 AM

(EMA-S3-015-2025) Axon-like Active Signal Transmission at the Edge of Chaos (Invited) *WITHDRAWN*

S. Kumar*[1]

1. N/A, USA

Neuromorphic computing has made impressive advances, but has ignored the issue of moving signals efficiently like the brain. Any electrical signal propagating in a metallic conductor loses amplitude due to the metal's natural resistance. Compensating for such losses presently requires repeatedly breaking the conductor and interposing amplifiers that consume and regenerate the signal. This century-old primitive severely constrains the design and performance of today's interconnect-dense chips. Here we present a fundamentally different primitive based on semi-stable Edge of Chaos (EoC), a long-theorized but experimentally elusive regime underlying active (self-amplifying) transmission in biological axons. By electrically accessing the spin crossover in $LaCoO_3$, we isolate semi-stable EoC, characterized by small-signal negative resistance and amplification of perturbations. In a metallic line atop a medium biased at EoC, a signal input at one end exits the other end amplified, without passing through a separate amplifying component. Operando thermal mapping reveals the mechanism of amplification – the EoC medium's bias energy, instead of fully dissipating as heat, is partly used to amplify signals in the metallic line, thus enabling spatially continuous active transmission, which could transform the design and performance of complex electronic chips. Main Reference: Brown et al., Nature (2024) DOI: 10.1038/s41586-024-07921-z.

9:00 AM

(EMA-S3-016-2025) Emergent oxide thin films and heterostructures based memristive devices for neuromorphic computing (Invited)

S. Kunwar*[1]; A. Chen[1]

1. Los Alamos National Laboratory, Center for Integrated Nanotechnologies, USA

Emergent metal-oxide thin films and heterostructures hold great promise for applications in next-generation non-volatile memory and neuromorphic systems, as they can exhibit dynamic resistive switching (RS) properties. These RS properties can be tuned by controlling the interface, crystal structures/phases, and ion densities (including oxygen vacancies) to achieve energy efficient and reliable performance. In this talk, I will discuss our recent efforts on exploiting RS characteristics in phase-change materials and interface-type metal/metal oxide heterostructures. Our recent study on the vanadium dioxide (VO_2) based memristive devices have suggested that a reconfigurable RS i.e., both volatile (as neurons) and non-volatile (as synapse) can be achieved for energy and area efficient artificial neural networks. Meanwhile, the interface-controlled system is explored for emulating synaptic functions such as long-term and short-term plasticity based on its multi-level non-volatile resistance states that can be controlled by the modulation of metal/oxide Schottky interface.

9:30 AM

(EMA-S3-017-2025) Co-design of power-efficient intelligent systems (Invited)

S. Yoo*[1]

1. Oregon State University, Electrical Engineering and Computer Science, USA

Hardware advances for better AI have been mainly accomplished by minimizing data movement and accelerating multiply-and-accumulate (MAC) operations in systems such as GPUs and dedicated accelerators. Emerging memory technologies, such as memristors, have shown promise in analog programmability and 3D integration, potentially leading to faster MAC operation and smaller chip areas. In the meantime, another main component of AI, non-linear functions, has been less investigated. The non-linearity inspired by neurons and synapses makes AI models "neuromorphic", while the complications of a higher order than linear calculations offered by digital computers cause high power and long latency. As a solution, electronic devices whose native internal physics can be analogous to the mathematical description of the non-linearities have been investigated. In particular, volatile memristors demonstrate non-linear decay in conductance, which has implemented memristor-based reservoir computing systems. Despite its great performance and efficiency at a certain time scale, the lack of systematic control of the device dynamics hinders its wide adoption to various time scales.

Here, our study to obtain the controllability by entropy-stabilized oxides and its systematic efficacy will be discussed. An algorithmic framework of hierarchical RC systems based on controllability and a neuromorphic vision sensor and potential research topics will be followed.

10:30 AM

(EMA-S3-018-2025) Characterization and Assessment of Oxide-Based Resistive and Electrochemical Memories for Energy Efficient Space-Based Analog In-Memory Computing (Invited)

M. Marinella*[1]

1. Arizona State University, Electric, Computer and Energy Engineering, USA

Analog in-memory computing (AIMC) offers orders of magnitude energy efficiency improvements over traditional architectures. Dot product operations at the heart of neural networks are computed by representing weights as conductances and using analog circuits for multiplication and summation. Excellent energy efficiency makes AIMC particularly appealing for space computing. However, achieving high accuracy on neural network inference using AIMC is challenging even for terrestrial systems – a challenge intensified in space due to radiation effects. Although charge-based memories are sensitive to ionizing radiation, oxide-based resistive memory (ReRAM) and electrochemical memory (ECRAM) offer potential solutions. Both devices modulate oxygen vacancy concentration in switching regions to control the conductance states – a process that is relatively insensitive to ionizing radiation. However, ReRAM must address drift and read noise which degrade AIMC accuracy. Oxide-based ECRAM can maintain precise, high resistance analog states with years-long retention. Initial ECRAM radiation testing is promising, although care must be exercised at the highest resistance states. This talk will discuss the characterization of device noise, variability, radiation effects, and modeling of these devices in energy efficient, space-based AIMC systems.

11:00 AM

(EMA-S3-019-2025) Filament-free Resistive Memory with Long Retention Time

S. Lee*[1]; Y. Li[1]

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

ReRAM memory holds promising prospects in the area of memory technologies. Among these, interfacial-type memory has attracted significant research attention due to its excellent device-to-device and chip-to-chip uniformity and capability for analog operations. However, it suffers from drawbacks such as shorter retention time and longer writing time compared to filamentary-type memristors. In this work, we investigated multi-level and filament-free memory using tantalum oxide (Ta_2O_5). Like other types of interfacial memristors, it demonstrates area-dependent currents and gradual switching. However, unlike other devices, we achieved over 24 hours of retention at 190°C, which is comparable to filamentary ReRAM and can achieve over 10 years at 85°C. Through complementary materials and device characterizations, we propose this retention occurs from the composition phase separation between metal-rich and oxygen-rich phases of amorphous tantalum oxide. This study provides a comprehensive understanding of the underlying mechanisms and offers insights into potential improvements for future ReRAM devices.

11:15 AM

(EMA-S3-020-2025) Boosting lifetime and resistive switching in TaOx memristors

O. Popova*[1]; W. S. Wahby[2]; R. Jacobs-Gedrim[2]; C. Bennett[2]; P. S. Finnegan[2]; A. V. Levlev[1]; A. A. Talin[2]; M. Marinella[3]; P. Maksymovych[1]

1. Oak Ridge National Laboratory, CNMS, USA
2. Sandia National Laboratories, USA
3. Arizona State University, USA

In this study, we successfully pieced together the puzzle of controlling resistive switching in TaOx thin-film memristive devices. The characterization of memristive switching behaviors is crucial for the development of next-generation memory and neuromorphic computing devices. These devices exhibit complex and asymmetric hysteresis loops, which present significant challenges in understanding the underlying switching mechanisms. To address these challenges, we used advanced techniques including cAFM, I-Vmeasurements and ToF-SIMS. Our analysis revealed critical insights into the processes of filament formation, localized conduction, and the impact of electrical dissipation on device performance. By carefully controlling the lifetime and resistive switching, we uncovered dynamics that conventional methods often overlook, providing a deeper understanding of how resistive switching can be fine-tuned. These experimental observations not only deepen our understanding of TaOx memristive devices but also offer a practical framework for improving device efficiency. This includes reducing power consumption and optimizing switching reliability, paving the way for more sustainable thin-film memristive devices. Our findings contribute to the broader field of memristive technology, moving it closer to real-world integration into advanced computing systems.

11:30 AM

(EMA-S3-021-2025) Linearly programmable halide perovskite memristors for neurocomputing (Invited)

S. Kim*[1]; J. Yang[1]

1. University of Southern California, Electrical and Computer Engineering, USA

Exotic properties of three-dimensional halide perovskites, such as mixed ionic-electronic conductivity and feasible ion migration, have been challenging traditional memristive materials. However, the poor moisture stability and difficulty in controlling ion transport due to their polycrystalline nature have hindered their use as a neuromorphic hardware. Recently, two-dimensional (2D) halide perovskites have emerged as promising artificial synapses due to their phase versatility, microstructural anisotropy, and excellent moisture resistance. However, their asymmetrical and nonlinear conductance changes still limit the efficiency of training and accuracy of inference. Here, we achieve highly linear and symmetrical conductance changes in Dion-Jacobson 2D perovskites, previously unachievable in 2D perovskites. We further build a 7×7 crossbar array based on analog perovskite synapses, achieving a high device yield, low variation, multilevel analog states, and moisture stability over 7 months. We explore the potential of such devices in large-scale image inference via simulations and show an accuracy within 0.08% of the theoretical limit. The remarkable device performances are attributed to the elimination of gaps between perovskite layers, allowing the halide vacancies to migrate homogenously regardless of grain boundaries. This was confirmed by first-principles calculations and experimental analysis.

12:00 PM

(EMA-S3-022-2025) Oxide-Oxide Vertically Aligned Nanocomposite Memristor as High-Performance Electronic Synapses via Interface Engineering *WITHDRAWN*

Z. Hu*[1]; H. Dou[2]; J. Lu[2]; A. Choudhury[2]; K. N. Evancho[2]; J. Huang[2]; H. Wang[2]

1. Purdue University, School of Electrical and Computer Engineering, USA
2. Purdue University, School of Materials Engineering, USA

Oxide-based memristors have attracted significant research interest due to their resistive switching properties and compatibility with existing CMOS technologies, making them promising candidates for neuromorphic microchips in artificial intelligence (AI) and machine learning (ML) applications. However, challenges remain in implementing and scaling memristor-based neuromorphic microchips due to limitations including poor device reliability, severe device-to-device variation, and relatively high set/reset voltage. Recent advances in oxide-oxide vertically aligned nanocomposite (VAN) memristors offer a solution by using vertical interfaces to facilitate oxygen vacancy ($V_o^{\cdot\cdot}$) migration. In this study, a novel $SrTiO_3$-CeO_2 (S-C) VAN-based memristor was successfully demonstrated. The effect of interface density on device performance was systematically examined. Results show that devices with higher interface densities exhibit improved power efficiency (~50% reduction in set/reset voltage), enhanced device reliability (up to 10^8 cycles in endurance and 10^4 seconds in retention), reduced device-to-device variation, and improved device plasticity. Additionally, the spiking neural network (SNN) built on the S-C memristor achieved a high recognition rate (~94%) after training, highlighting its potential for large-scale neuromorphic microchips.

12:15 PM

(EMA-S3-023-2025) Understanding the Non-Volatility of Hafnium Oxide Resistive Memory through Oxygen Tracer Diffusion

D. Shin*[1]; A. V. Levlev[2]; K. Beckmann[3]; J. Li[1]; P. Ren[1]; N. Cady[4]; Y. Li[1]

1. University of Michigan, Materials Science and Engineering, USA
2. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
3. NY CREATES, USA
4. University at Albany, College of Nanotechnology, USA

This work investigates oxygen tracer diffusion in amorphous hafnium oxide (HfO_2) thin films, a material widely used in resistive memory devices. The discrepancy between experimentally measured data retention times and oxygen diffusion rates in HfO_2 has posed a challenge for device performance predictions. Using isotope tracer diffusion techniques, we measured oxygen transport in amorphous HfO_2 thin films deposited by atomic layer deposition (ALD) and sputtering. Our results show significantly lower oxygen diffusion rates in amorphous HfO_2 compared to previous studies on monoclinic HfO_2, with a diffusion activation energy of ~1.5 eV. Furthermore, we observed that ALD-deposited films exhibit lower oxygen diffusion rates than sputtered films, suggesting a strong correlation between film density and diffusion behavior. This study reconciles the long data retention times observed in HfO_2-based resistive memories and provides insights into controlling oxygen diffusion through processing conditions, paving the way for optimized device performance in memory and neuromorphic computing applications.

S6 Two-Dimensional Quantum Materials-Synthesis, theories, properties and applications

S6 – Two dimensional quantum materials: Synthesis, theories, properties & applications

Room: Colorado G
Session Chairs: Haozhe Wang, Duke University; Cheng Gong, University of Maryland

8:30 AM

(EMA-S6-017-2025) Designer 2D materials with new phononic and photonic properties (Invited)

S. Huang*[1]

1. Rice University, USA

2D materials offer enormous opportunities to build designer structures with widely tunable properties. The precise atomic engineering and quick characterization approach are critical to advance the application of designer 2D materials. This talk will introduce new optical features of designer 2D materials, including dipole-induced mechanical behavior, phonon interference, and single photon emission.

9:00 AM

(EMA-S6-019-2025) New Theoretical Insights into Moiré Solids and 2D Magnets from Machine Learning Assisted First-Principles Calculations (Invited)

T. Cao*[1]

1. University of Washington, USA

This talk will show our recent theoretical and computational investigations into moiré superlattices and 2D magnets. We start by demonstrating that a deep neural network guided by first-principles data can be used to examine moiré structural reconstruction in various homobilayers and heterobilayers of transition metal dichalcogenides. Going beyond the capacity of direct DFT calculations, our machine-learning enabled workflow discovers salient structural features and key topological characters controlled by twist angles, layer composition, and other tuning knobs. This knowledge can be used to inform accurate continuum model, and to predict new forms of moiré potential and moiré topology. In the second part, we show that the magnetism in 2D magnets like CrSBr is highly tunable by strain, pressure, chemical doping, and interfacing with other vdW materials like graphene. This allows for multi-dimensional control of magnetic orders and noncollinear magnetism. We demonstrate the strong light-matter interactions and unique excitonic structures in CrSBr provide possibility to control material transparency by ultrafast means. Finally, we connect our theoretical discoveries to experimental results and explore potential applications.

S7 Additive manufacturing for power sources in electronics

S7 - AM for Lithium Batteries and Beyond

Room: Colorado E
Session Chair: Kun Fu, University of Delaware

8:30 AM

(EMA-S7-010-2025) Direct Ink Writing of 3D Batteries with High Energy and Power Density (Invited)

B. Dunn*[1]; Y. Wang[1]; M. Choi[1]; C. Wang[3]; M. Worsley[2]; M. Wood[2]; E. P. Ramos Guzman[2]

1. University of California Los Angeles, Materials Science and Engineering, USA
2. Lawrence Livermore National Laboratory, USA
3. University of California Los Angeles, USA

Additive manufacturing, particularly direct ink writing (DIW), has emerged as a promising technology for the next generation of battery production, offering significant advantages for 3D-structured batteries. Three-dimensional battery architectures have the potential to overcome the traditional trade-off between energy density and power density inherent in conventional planar designs. By constructing electrodes in the vertical (z) direction, 3D batteries enable higher mass loading, which significantly improves areal energy density. Simultaneously, the 3D configuration shortens ion diffusion pathways, maintaining high power density. In this study, we successfully employed DIW to fabricate lithium iron phosphate (LFP) and niobium pentoxide (Nb_2O_5) electrodes, serving as the cathode and anode, respectively. Lattice-structured electrodes with varying pitch lengths up to five layers were printed. The highest areal capacities achieved were 2.75 mAh/cm^2 for LFP and 1.85 mAh/cm^2 for Nb_2O_5, with mass loadings of 20 mg/cm^2 and 12.3 mg/cm^2, respectively. The printed electrodes exhibited excellent capacity retention, maintaining 96% of their theoretical capacity after 25 cycles. The present work demonstrates the feasibility of DIW for fabricating high-performance 3D-structured electrodes and underscores its potential as a scalable approach for the commercialization of 3D battery architectures.

9:00 AM

(EMA-S7-011-2025) Shape matters: Understanding the effect of electrode geometry and microstructure (Invited)

G. Bucci*[1]; T. Lin[1]; N. W. Brady[1]; N. R. Cross[1]; V. M. Ehlinger[1]; H. Li[1]; S. P. Mish[1]; T. Roy[1]; S. T. Sarnecki[1]; D. A. Tortorelli[1]; M. Wood[1]; J. Ye[1]; C. Orme[1]; M. Worsley[1]

1. Lawrence Livermore National Laboratory, USA

Electrodes with a three-dimensional (3D) shape allow batteries to overcome some of the capacity and rate performance trade-offs. For instance, they enable higher active-material loading, while keeping the transport pathways fixed, or they allow for better material utilization. Our models and experiments show that the benefit of 3D shapes is more apparent in extreme conditions, such as low temperature and high charge/discharge rate. Specifically, when ion transport in the electrolyte is limiting, electrode shape contributes to lowering the cell electrical resistance and enables for a more uniform current distribution. We show how dimensional analysis can be used as a tool to understand when shape matters, i.e., when it acts on the limiting kinetic and transport processes. We also investigate porous scaffolds for Li-metal anode, by leveraging a meshing tool that simulates large topological changes associated with Li plating/stripping in 3D. We analyze in what conditions porous anode architectures are effective in expanding the surface area of the charge-transfer interface, and in self-regulating current density and dendrite growth. This work was supported by Lawrence Livermore National Laboratory (LLNL) LDRD SI 23-SI-002, and was performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344.

9:30 AM

(EMA-S7-012-2025) Automated High Throughput Screening of Solid Polymer Electrolytes (Invited) *WITHDRAWN*

J. J. Schwartz*[1]

1. Lawrence Livermore National Laboratory, Materials Science Division, USA

Advancement of increased ionic conductivity polymer electrolyte materials for Li-ion battery applications has traditionally required formulations to be hand-mixed by researchers, limiting progress and adding potential batch-to-batch variability. Through our Studying-Polymers-On a-Chip (SPOC) platform, we seek to solve the challenge of developing safe, stable, and cost effective batteries. We do so by accelerating screening of polymer electrolyte materials through integration of additive manufacturing, impedance characterization, and machine learning experimental planning systems. Various monomers, salts, and nanoparticle fillers were screened to modify the amorphous character in semicrystalline polyethylene glycol-based polymer electrolytes. Ultimately, long-term cycling, aging, and stability measurements need to be made for identified polymer electrolytes to be useful for battery applications. The end of the talk will discuss some of our ongoing SPOC platform developments to create and couple high-throughput aging and degradation assessments into our screening platform.

10:30 AM

(EMA-S7-013-2025) Direct Deposition of Separator Materials for the Additive Manufacturing of Lithium Ion Batteries (Invited)

A. Fassler*[1]; R. Kohlmeyer[2]; S. Rajput[2]; G. Horrocks[1]; J. Deneault[1]; R. Green-Warren[3]; N. McAllister[3]; M. Arkhipov[3]; M. Grzenda[3]; A. Juhl[1]; J. Singer[3]; M. Durstock[1]

1. Air Force Research Laboratory Materials & Manufacturing Directorate, USA
2. Xerion Advanced Battery Corp, USA
3. Rutgers The State University of New Jersey, USA

In order to achieve fully additively manufacturable batteries, materials and processes must be developed to yield components with suitable composition, microstructure, and functionality. Furthermore, each step and material used in the process must be compatible to not degrade the properties of the final device. Our research is focused on the challenge of additively fabricating multilayer structures of lithium ion cell materials, with particular attention given to the separator membrane. Direct deposition of the separator onto an electrode presents the first step for fully additive cells and can simplify mass manufacturing. The separator itself demands non-trivial properties, requiring a porous network for electrolyte penetration and ion transport while being physically robust to prevent shorting and dendrite growth. We have developed a solution processable PVDF and Al_2O_3 separator utilizing an evaporation induced phase separation technique. This process generates porosity within the material upon drying, making it compatible with a variety of casting and printing approaches. The separator was deposited onto printed graphite anodes using aerosol jet printing, and assembled to create functional lithium ion cells in both coins and non-planar configurations. We examined the microstructures and interfaces produced in this and other methods, and how they can impact performance.

11:00 AM

(EMA-S7-014-2025) Exploiting advanced scan strategies in Laser Powder Bed Fusion towards the manufacturing of rechargeable Zn-based batteries (Invited)

L. Caprio*[1]; E. Emanuele[2]; C. Baldi[1]; A. G. Demir[1]; B. Bozzini[2]; B. Previtali[1]

1. Politecnico di Milano, Mechanical Engineering, Italy
2. Politecnico di Milano, Energy, Italy

Additive Manufacturing (AM) technologies are appealing production routes for the on-demand deposition of batteries with freeform geometries. Amongst the various AM techniques, Laser Powder Bed Fusion (LPBF) enables the deposition of metallic structures with

tailored shapes and complex surfaces. These features are particularly attractive for the development of secondary Zn-based batteries, as they can help mitigate typical morphochemical issues that arise during cycling, such as dendrite growth, surface passivation, and hydrogen evolution reactions. Nonetheless, there are several challenges associated with the laser processing of pure Zn and its alloys due to strong fume formation caused by the vicinity of its melting and evaporation points. To overcome such issues a reconfigurable LPBF platform was exploited to flexibly manipulate the trajectory and the spatial and temporal profile of the laser beam during the deposition process. This approach allowed to deposit pure Zn thin walled with different geometries and characteristics to investigate their applicability as anodes in secondary batteries with an aqueous electrolyte. Samples where characterized in terms of their morphology and electro-chemical tests were conducted to assess their cycling behaviour.

11:30 AM

(EMA-S7-015-2025) Laser Additive Manufacturing of Battery Cathode Films (Invited)

J. Ye*[1]; Y. Xiao[1]; E. P. Ramos Guzman[1]; R. Kim[2]; M. Wood[1]; E. Brown[2]; H. Du[2]

1. Lawrence Livermore National Laboratory, USA
2. Ampcera, USA

There is urgent need to develop low-cost high-performance battery manufacturing technologies for the electrical vehicle, energy storage and consumer electronics markets in the United States. Transition from wet processing of battery electrodes to dry processing is anticipated to reduce the capital investment, energy consumption, and environmental impact. Here, we report a laser additive manufacturing approach to fabricate cathode films. This approach reduces energy consumption and material waste and can achieve comparable production rate as conventional slurry casting approach. The resulted electrodes show comparable battery cycling performance as the slurry-casting approach. In this talk, I will discuss powder mixing, spray coating, and laser processing parameters and how they affect the uniformity of the film, the adhesion to the current collector, the composition change, and finally the battery performance. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The project is funded by Advanced Materials and Manufacturing Technologies Office.

12:00 PM

(EMA-S7-016-2025) 3D electrodes for long duration and seasonal energy storage (Invited)

B. S. Jayathilake*[1]

1. Lawrence Livermore National Laboratory, Materials Science Division, USA

With the urgent need for emissions-free economies and to achieve grid-scale energy security we need to rapidly advance and deploy low-cost, scalable, and durable energy conversion and storage technologies. Electrochemically driven such technologies allow clean energy utilization through renewable energy harvesting coupled with power supply. For advancing performance in electrochemical systems, electrode design and architecture play a key role. Engineering structural features of 3D electrodes enable efficient and fast electrochemical reactions at the electrode surface. In this work, we explored two types of key technologies namely: redox flow batteries and power to gas systems for advancing performance through improving the understanding of electrode structural-property relationships. These technologies help solving long duration and seasonal storage challenges. Using the hydrogen evolution reaction and metal plating process as model systems, we identified several high surface area structures that improve the fluid distribution within the reactor. Triply periodic minimal surface structures, like gyroids, enable higher volumetric productivities of hydrogen compared to conventional planar electrodes while gradient 3D electrode structures enabled even distribution of metal deposition. IM release number: LLNL-ABS-869652.

S9 Data-Driven and Model-supported structure-property relationships in complex electroceramics

S9- Data-driven & Model-supported structure- property relationships in complex electroceramics I

Room: Colorado B
Session Chair: Anna Grünebohm, Ruhr-Universitat Bochum

8:30 AM

(EMA-S9-002-2025) Understanding domain size effect on piezoelectricity in ferroelectric perovskite oxides from thermodynamics and phase-field simulations (Invited)

B. Wang*[1]; L. Chen[2]

1. Lawrence Livermore National Laboratory, USA
2. The Pennsylvania State University, USA

Domain structure plays a pivotal role in determining the piezoelectric properties of electroceramic materials, including ferroelectric single crystals and thin films. Understanding this relationship is key to accelerating the design of advanced electroceramic materials through domain engineering. In this presentation, we will introduce a unified theoretical framework to predict the domain size effect on piezoelectric coefficients of ferroelectric materials, based on thermodynamics and phase-field simulations. We demonstrate the application of this framework in two significant case studies, including rhombohedral relaxor-$PbTiO_3$ crystals, which led to the discovery of transparent crystals with high piezoelectric and optical properties, and monoclinic $K_xNa_{1-x}NbO_3$ epitaxial thin films, which revealed unique superdomain structures and their impact on material properties. We will also outlook opportunities and challenges in furthering this physics-modeling approach by leveraging data-driven methods. These examples showcase the power of the theoretical approach in understanding and predicting the complex relationships between domain size and piezoelectric performance in diverse ferroelectric systems, ultimately contributing to the rational design of advanced electroceramic materials.

9:00 AM

(EMA-S9-003-2025) A quest for new antiferroelectrics (Invited)

H. Aramberri*[1]

1. Luxembourg Institute of Science and Technology, Luxembourg

Antiferroelectrics display antiparallel electric dipoles so that their net polarization vanishes, and they can be taken to a polar state under an electric field. Their characteristic non-linear response makes them ideal for energy storage devices with very large energy densities. However, we still know only a relatively small number of such materials. In this talk I will present several data-driven strategies we followed to find new antiferroelectric materials and to optimize their response using modelling and atomistic simulations based on firts-principles calculations. Our findings indicate that (1) the pyroxene materials family (one of the most abundant mineral families on Earth) may host antiferroelectric compounds, and (2) that paraelectric/ferroelectric heterojunctions can workk as antiferroelectrics, and that they can be strongly optimized for energy storage applications in a wide range of working voltages.

9:30 AM

(EMA-S9-009-2025) Automated Quantification and Quality of 'Big' AFM Data for Electro-Ceramics

K. Del Cid-Ledezma[1]; K. Lizu[1]; F. Wang[1]; J. L. Perez Gordillo[1]; B. Huey*[1]

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

PFM is ubiquitous for studying piezoelectrics. But to precisely determine piezocoefficients—especially for polycrystalline piezoelectrics—advanced manufacturer-modes, custom approaches, or expensive new systems are necessary. Furthermore, no matter the sophistication, uncertainties are superimposed due to tip-sample convolution associated with the local surface topography. Two broadly applicable approaches are presented to address these widespread challenges. First: carefully considering the fundamental mechanics of the AFM cantilever improve measurement precision up to an order of magnitude, especially for polycrystalline ceramics. Second: calculating, recognizing, and weighting pixels according to surface geometry parameters, improves automated assessment of hundreds of images—not just for PFM, but also for any AFM results. Removing suspect pixels obviously substantially improves local and statistical analyses of such 'big [AFM] data.' Both of these advances have important implications not just for microscopists, but also modelling, fabrication, and device design that benefits from more and better analysis of local materials properties.

S9- Data-driven & Model-supported structure- property relationships in complex electroceramics II

Room: Colorado B

Session Chair: Bo Wang, Lawrence Livermore National Laboratory

10:30 AM

(EMA-S9-004-2025) Materials informatics meets ferroelectric domain walls: Scale-bridging insights from ab initio based simulations (Invited)

A. Grünebohm*[1]

1. Ruhr-Universitat Bochum, ICAMS and ZGH, Germany

Functional properties of ferroelectric oxides are closely related to field-induced domain wall motion. While ab initio based simulations can contribute to the fundamental understanding and control of this motion, they are challenged by the scale-bridging and statistical nature of the underlying nucleation and pinning processes. This contribution discusses how the combination of atomistic and coarse-grained simulations with methods from materials informatics can overcome this challenge. First, we will discuss the success and limits of machine learning potentials (atomic cluster expansion) to describe ferroelectric phases, domain wall motion and defects. Second, we will discuss the mechanism of domain wall motion in tetragonal and orthorhombic ferroelectrics.

11:00 AM

(EMA-S9-005-2025) Depth-resolved X-ray photoelectron spectroscopy evidence of intrinsic polar states in hafnia-based ferroelectrics (Invited) *WITHDRAWN*

N. Strkalj*[1]

1. Institut za Fiziku, Croatia

The discovery of ferroelectricity in nanoscale films of binary oxides, particularly hafnia, has reignited interest in understanding the emergence of ferroelectric properties at the nanoscale. The unusual size scaling of polarization led to intense investigation and several hypotheses regarding the nature of the polar state in hafnia-based films. In this talk, I will explore the relationship between the ferroelectric switching and electrochemical reactions in hafnia-based films using depth-resolved X-ray photoelectron spectroscopy. Our findings reveal more pronounced electrochemical changes in films with lower polarization, suggesting a lack of direct linkage between polarization and electrochemical changes. These results thus indicate an intrinsic polar state in hafnia-based ferroelectrics. Our study demonstrates the critical role of advanced characterization methods in uncovering the fundamental mechanisms behind the macroscopic properties of nanoscale ferroelectrics.

11:30 AM

(EMA-S9-006-2025) Waste Heat to Electricity (H2E): From 2D Materials Perspective (Invited)

N. Singh*[1]

1. Khalifa University, Physics, United Arab Emirates

Waste heat is everywhere, and every bit of waste heat recycled into green energy can reduce greenhouse emissions, promote sustainable development, and impact the economy. Thermoelectric generators generate electricity from waste heat and can be used to convert even tiny heat into electricity for sensors. The development of efficient devices, however, requires materials with a robust thermoelectric response. Two-dimensional (2D) materials have unique electronic properties due to the quantum confinement and prevent heat transfer between two layers, making them excellent thermoelectric materials. We design 2D materials and their heterostructure using innovative approaches to optimize thermal transport properties by optimizing the electronic properties and simultaneously reducing the thermal conductivity of 2D materials. In this talk, I will discuss a wide perspective and various design principles of 2D materials and their possible applications in thermoelectric generators.

12:00 PM

(EMA-S9-008-2025) Uncovering the mechanisms of the ultra-high, low-hysteresis electrostrain of lead-free piezoelectric $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (Invited) *WITHDRAWN*

H. Amorín*[1]; J. E. García[2]; D. A. Ochoa[2]; M. Venet[3]; P. Ramos[4]; C. Pascual-Gonzalez[1]; A. Castro[1]; M. Algueró[1]

1. Instituto de Ciencia de Materiales de Madrid, Multifunctional Materials, Spain
2. Universitat Politecnica de Catalunya, Departamento de Física, Spain
3. Universidade Federal de Sao Carlos, Departamento de Física, Brazil
4. Universidad de Alcala, Departamento de Electrónica, Spain

High-sensitivity piezoelectric $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ stands out among lead-free perovskite oxides for its large piezoelectric coefficients. However, transfer to industry is being hindered by processing issues, and preparation of reliable materials with tailored microstructure remains a challenge. Best performances are reported for coarse-grained materials, and attempts to refine microstructure below the 10-μm grain size consistently resulted in significant loss of functionality. Electrostrain behaves differently, and enhanced response has been reported for grain sizes of 5 μm [H. Amorín et al. J. Eur. Ceram. Soc. 42, 4907 (2022); Adv. Electron. Mater. 10, 2300556 (2024)]. We provide insights into the mechanisms of the ultrahigh electrostrain of BCZT, and relate it to size effects. This required the processing of high-quality, dense ceramics with refined microstructure by spark plasma sintering of nanopowders obtained by mechanosynthesis. Results show very good overall performance with grain refinement and electrostrain above 2000 pm V^{-1}, while distinctive relaxor features are found below 1 μm. Synchrotron radiation is used to study the mechanisms behind this response, associated with a reversible transition between metastable intermediate states and the ferroelectric phase. Funded by projects PID2021-122708OB-C33 and TED2021-130871B-C21.

S11 Complex oxide thin films and heterostructures- from synthesis to strain/interface-engineered emergent properties

S11- Functional Properties and Applications of Oxides

Room: Colorado A
Session Chair: Lucas Caretta, Brown University

8:30 AM

(EMA-S11-022-2025) Doping Effects on the Structure and Properties of Complex Oxide Thin Films (Invited)

L. Wang*[1]; M. Choi[1]; K. P. Koirala[1]; M. Bowden[1]; P. Sushko[1]; Y. Du[1]

1. Pacific Northwest National Laboratory, USA

ABO_3-type perovskite oxides are renowned for their diverse electronic, optical, magnetic, and catalytic properties, largely due to their large ability to accommodate oxygen-based defects like oxygen vacancies (V_O) and various cation and/or anion doping. Among these, $SrFeO_{3-\delta}$ (SFO) is a particularly intriguing material system, where δ can be finely tuned from 0 to 1, enabling a wide range of functional properties. However, despite extensive research on SFO, the effects of B-site cation doping, particularly with transition metals (TMs) like Cr, Mn, Co, and Ni, are still not well understood. In this talk, I will focus on three specific doping systems within SFO: $SrFe_{1-x}NiO_{3-\delta}$, $SrFe_{1-x}Cr_xO_{3-\delta}$, and Cr/Ni co-doped $SrFeO_{3-\delta}$. I will discuss how the introduction of different dopants influences the phase stability/transitions, oxygen vacancy ordering, charge distribution/charge states, as well as the optical properties of these systems. Through this, we aim to provide a deeper understanding of how tailored doping strategies can be employed to enhance the performance of SFO-based materials for energy and electronic applications.

9:00 AM

(EMA-S11-023-2025) Analog Computing with High Precision and Programmability Enabled by Memristors (Invited)

W. Song*[1]; Y. Xu[1]; J. Yang[1]

1. University of Southern California, Ming Hsieh Department of Electrical and Computer Engineering, USA

Compared with digital computing, analog computing offers superior energy efficiency and throughput. However, its historical limitations in precision and programmability have restricted its use to specific and low-precision areas like neural networks. The growing challenge of large volumes of analog data requires versatile platforms combining high efficiency with sufficient reconfigurability and precision. Recent advances in analog devices, especially memristors, have opened the door to unprecedented analog computing capabilities. By harnessing the multiple roles of memristors, we introduce memristive field-programmable analog arrays (FPAAs), akin to digital field-programmable gate arrays (FPGAs). To improve precision, we study and mitigate the source of reading noise, achieving remarkable 2048 conductance levels in individual memristors. To meet the demand for high-precision computing at the array level, we developed a circuit architecture and programming protocol that allows analog memories to reach arbitrarily high precision with minimal overhead. Our experimental validation with a memristor System-on-Chip demonstrates significantly enhanced precision and power efficiency compared to traditional digital systems. This co-design approach allows low-precision analog devices to perform high-precision computing on a programmable platform, highlighting the transformative potential of analog computing.

9:30 AM

(EMA-S11-024-2025) Functional Topological Defects: Materials at the Edge of Order (Invited)

J. Seidel*[1]

1. University of New South Wales, Australia

Topological defects occur in ordered media as a discontinuity or place where the order cannot seamlessly transition from one area to another. Examples are domain walls and skyrmions in ferroelectric and magnetic materials. These nanoscale features can be created and manipulated in ferroic materials and are the focus of research efforts to exploit their structure, symmetry, chemistry and unique intrinsic properties. I will discuss our recent work on various ferroelectric and multiferroic material systems using scanning probe microscopy and electron microscopy as the main investigative tools, with a focus on nanoscale functional property measurements of individual topological defects. The discussion will include a newly developed method to investigate crackling noise of domain walls in ferroelectrics with an AFM system.

10:30 AM

(EMA-S11-025-2025) Electrochemical control of oxygen deficiency in $(La,Sr)FeO_{3-\delta}$ thin films for precise modulation of magnetic and electrical properties

P. Nizet[1]; F. Chiabrera*[1]; N. López-Pintó[2]; P. Langner[1]; F. Baiutti[1]; A. Morata[1]; J. Sort[2]; A. Tarancon[3]

1. Institut de Recerca en Energia de Catalunya, Spain
2. Universitat Autonoma de Barcelona, Spain
3. ICREA/IREC, Spain

Oxygen deficiency offers a fundamental tool to tune electronic and magnetic properties of metal oxide thin films. Traditionally, control of oxygen stoichiometry has been achieved by adjusting deposition conditions or by high temperature annealing in various atmospheres. However, these strategies fail in providing a rapid, reversible, and modular adjustment of oxygen content, limiting the understanding of oxygen defects–functionality relationships. Here, we show that the application of a Nernstian voltage through a solid-state oxide-ion electrolyte can be employed to enable accurate control of oxygen concentration of thin films. We investigate mixed ionic-electronic conducting $(La,Sr)FeO_{3-\delta}$ thin films and we show that potentially infinite intermediate states, characterized by different electronic conductivity spanning over 5 orders of magnitude, can be stabilized by changing the oxygen content in a continuous and controlled way. A smart experimental design allowed for the simultaneous characterization of structural, optical, electrical, and magnetic properties of the films, shedding light on the mechanisms that correlate such properties with the oxygen content and temperature. The results demonstrate the applicability of the approach the fundamental investigation of complex oxide systems, as well as for the design of novel information devices.

10:45 AM

(EMA-S11-026-2025) Layer Resolved Cr Oxidation State Modulation in Epitaxial $SrFe_{0.67}Cr_{0.33}O_{3-\delta}$ Thin Films

K. P. Koirala[1]; M. Hossain[1]; L. Wang[1]; Z. Zhuo[4]; W. Yang[4]; M. Bowden[1]; S. R. Spurgeon[2]; C. Wang[1]; P. Sushko[3]; Y. Du*[1]

1. Pacific Northwest National Laboratory, USA
2. National Renewable Energy Laboratory, USA
3. Pacific Northwest National Lab, Physical Sciences Division, USA
4. E O Lawrence Berkeley National Laboratory, USA

Understanding how doping influences physicochemical properties of ABO_3 perovskite oxides is critical for tailoring their functionalities. This study uses $SrFe_{0.67}Cr_{0.33}O_{3-\delta}$ epitaxial thin films as a model system to examine the effects of Fe and Cr competition on structure and B-site cation oxidation states. The films exhibit a perovskite-like structure near the film/substrate interface, while a brownmillerite-like structure with horizontal oxygen vacancy channels predominates near the surface. Electron energy loss spectroscopy shows Fe remains Fe^{3+}, while Cr varies from ~Cr^{3+} (tetrahedral layers) to ~Cr^{4+} (octahedral layers) within brownmillerite phases and becomes ~$Cr^{4.5+}$ in perovskite-like phases. Theoretical simulations indicate that Cr-O bond arrangements and the way oxygen vacancies interact with Cr and Fe drive Cr charge disproportionation. High-valent Cr ions also introduce additional Cr 3d states near the Fermi level, reducing the optical bandgap compared to $SrFeO_{2.5}$. These findings enhance our understanding of B-site cation doping in perovskite oxide framework.

11:00 AM

(EMA-S11-027-2025) Composition-Driven Electrocatalysis: High-Entropy Perovskites for Oxygen Evolution Reaction (Invited)

E. D. Gadea*[1]; V. Molinero[1]

1. The University of Utah, Chemistry, USA

High-entropy perovskite oxides are emerging as promising materials for electrocatalysis, offering exceptional performance in the oxygen evolution reaction (OER) due to the synergistic interplay of multiple cationic species. This "cocktail effect" stems from the complexity of their local active-site environments. Despite progress, the mechanisms behind this efficiency remain unclear, particularly for these diverse oxides. Conventional electronic structure models and active-site availability concepts fail to explain the notably low overpotential observed during OER in these materials. In this study, we develop a model that integrates composition, adsorbate interactions, and surface diffusion kinetics—key factors influencing catalytic performance in high-entropy perovskites. Using a lattice Kinetic Monte Carlo approach, we systematically explore these interactions, revealing how variations in local atomic environments broaden adsorption energy distributions at the most active sites, enhancing catalytic activity. By testing our predictions against electrochemical and spectroscopic measurements, we demonstrate the role of extreme surface heterogeneity in modulating catalytic properties. These insights provide a framework for designing ceramic materials with improved efficiency for OER applications, bridging the gap between material composition and electrochemical performance.

S19 Frontiers in ferroic ceramics-synthesis, properties and applications

S19- Frontiers in Ferroic Ceramics: Synthesis, properties and applications

Room: Colorado H
Session Chair: Ruijuan Xu, North Carolina State University

8:30 AM

(EMA-S19-007-2025) Dynamics of Polar Vortex Crystallization in Ultrathin Ferroelectric Films (Invited)

S. Rijal*[1]; Y. Nahas[1]; S. Prokhorenko[1]; L. Bellaiche[1]

1. University of Arkansas, Physics, USA

Polar vortex crystal (VC) is a periodically repeating vortex structure with alternate vorticity predicted to form in $Pb(Zr,Ti)O_3$ films and observed in $PbTiO_3/SrTiO_3$ superlattices at room temperature. These topological structures spontaneously emerge with a fine balance between electrostatic, elastic and gradient energies. VC are shown to be tunable by several tuning factors and feature interesting properties such as collective "vortexon" excitations, coupling to light and electrons due to which they are promising candidates for technological applications. Although collective motion of the vortices in response to an external stimulus had been demonstrated, a clear understanding of the dynamical origin of polar vortex was still lacking. Here, our investigations employing ab-initio based effective Hamiltonian simulation revealed that vortex crystallizations origins from the softening of a phonon mode and can be described as a Z_2 X SU(1) symmetry breaking transition from a vortex-liquid like state to the vortex state. Further, we predict resonant switching of the vortex crystal orientation driven by a midinfrared laser light employing the idea of collective excitation. Such finding elucidates the dynamical nature of polar vortices and bridges them with other modulated states such as spin spirals in magnetics systems.

9:00 AM

(EMA-S19-008-2025) Optical Creation of Polar Supertextures (Invited)

V. Gopalan*[1]

1. The Pennsylvania State University, Materials Science and Engineering, USA

A strong coupling between electrical polarization and strain in ferroelectrics prevents long range complex polar textures similar to magnetic vortices, spin cycloids, skyrmions and others. One way to create such ferroelectric analogues to magnetic textures is by creating designer heterostructures with competing frustrations, and by pushing on them with external stimuli. In this talk, I will show how an ultrafast laser pulse can create complex polar supertextures with modulation periodicities on tens of nanometers scale. The process of this creation is tracked in time over seven orders of magnitude time scale revealing a subtle balance between photo-induced charges, heat, and strain dynamics between competing phases that gives rise to an incredibly rich phase space of polar supertextures.

9:30 AM

(EMA-S19-009-2025) Polar Textures: Beyond Oxides (Invited)

J. Ravichandran*[1]

1. University of Southern California, Chemical Engineering and Material Science, USA

Topological defects such as vortices, and skyrmions have recently gained significant interest in solid state materials as ferroic materials (ferromagnets and ferroelectrics) have become a test bed to realize and control these nanoscale structures. Although this phenomenon is being investigated as a pathway to energy efficient information storage, broader applications in interaction of electromagnetic waves with such features are emerging. In the case of ferroelectrics, boundary condition engineering is used to achieve vortices, skyrmions, and merons in low dimensional epitaxial oxide heterostructures. In this talk, I will introduce the notion that similar phenomenology but at the atomic scale can be achieved in charge density wave phases, especially nominally semiconducting chalcogenides. I will outline my group and other groups efforts in showing non-trivial toroidal polar topologies at the atomic level in chalcogenides with nominally empty conduction band with d-orbital character such as 1T-$TiSe_2$, Ta_2NiSe_5 and $BaTiS_3$. Specifically, we use X-ray single crystal diffraction as a probe for high quality single crystals of a quasi-1D hexagonal chalcogenide, $BaTiS_3$, to reveal complex polar topologies such as vortices, and anti-vortices. I will also discuss recent experiments and theoretical studies on the stability and dynamics of these features, and the perspective for photonic applications of polarization textures.

10:30 AM

(EMA-S19-010-2025) Origin of enhanced ferroelectricity of hafnia down to 2D limit (Invited)

X. Xu*[1]

1. University of Nebraska-Lincoln, Physics and Astronomy, USA

Although ferroelectric hafnia is known to have enhanced properties in nanoscale, its behavior in the ultrathin limit (< 10 nm) remains under debate. To resolve the debate, we studied the epitaxial growth of 10 mol% La-doped HfO2 (LHO) films under compressive strain by (111)-oriented yttria stabilized zirconia (YSZ). We demonstrate that the high-pressure orthorhombic antipolar (o-AP, space group Pbca) phase can be deposited directly, suggesting thermodynamic stabilization. The o-AP phase can be further converted to the ferroelectric orthorhombic (o-FE, space group Pca21) structure using mechanical poling. We observe enhanced orthorhombic order down to 2D limit (one unit cell thickness) with an unprecedented Curie temperature of 850 °C. We also found no reduction of orthorhombic distortion (clamping) at the LHO/YSZ interface. Hence, the o-AP ground state, more effective strain in thinner films, and absence of interfacial clamping are three key factors for the enhanced order down to the 2D limit. Furthermore, a critical implication is that orthorhombic hafnia is a novel antipolar materials with ferroelectric behavior due to high switching energy barrier. The ferroelectric o-FE structure can be viewed as the o-AP structure in a polarized state. This resolves the stabilization mystery of the o-FE structure which is absent in the pressure-temperature phase diagram of hafnia.

11:00 AM

(EMA-S19-011-2025) Experimental Synthesis, Stability, and Magnetic Properties of Co_3PdN Thin Films

S. Dugu*[1]; S. Mahatara[1]; C. Regier[2]; S. Lany[1]; J. R. Neilson[2]; A. Zakutayev[1]; S. Bauers[1]

1. National Renewable Energy Laboratory, USA
2. Colorado State University, Chemistry, USA

Nitrides of form X_3AN (X is a 3d-metal Fe, Ni, Co) are subset of antiperovskite(AP) materials with exciting properties. Examples of magnetic-APs include: Co_3FeN, which has been reported as half-metallic, Fe_3FeN and its N-vacancy ordered-derivative $Fe_{16}N_2$, which is the strongest known ferromagnet. Recently, several Co-containing APs, including Co_3PdN and Co_3PtN were predicted to be stable, despite no experimental reports. We study the synthesis, stability, and magnetic properties of Co_3PdN thin-films prepared by magnetron-sputtering. We find that the AP-structure persists across a relatively large range of Co:Pd ratios. Synchrotron-XRD from Co_3PdN is fit to a cubic-AP structure with a lattice constant of a=3.806Å. Prior computational-works assumed a ferromagnetic-ground-state, and we confirm these results by comparing total energy of ferromagnetic Co_3PdN to several antiferromagnetic-configurations, which are all at least +88meV/atom higher in energy. Experimentally, we found Co_3PdN is a soft-magnetic-material with a RT H_C=50Oe. We find a $T_C \approx$570K, and a decomposition temperature of ~700K. We also discuss magneto-transport collected from epitaxial films of Co_3PdN grown on STO and MgO. This work represents experimental confirmation of Co_3PdN AP and should motivate further study of this material's magnetoelectric functionality and exploration of similar Co_3AN compounds awaiting experimental realization

11:15 AM

(EMA-S19-012-2025) Emerging Materials, Mechanisms, and Design Principles for Wurtzite Ferroelectrics (Invited)

C. Lee*[1]

1. Colorado School of Mines, USA

Wurtzite ferroelectrics (FEs) have drawn increasing attention due to their promise of better performance and integration than traditional oxide ferroelectrics with semiconductors such as Si, SiC, and III-V compounds. However, wurtzite FEs generally require enormous electric fields, approaching breakdown, to reverse their polarization, preventing scale-up and deployment. In this talk, I will discuss the two complementary approaches we have taken to address the challenge. In the first approach, we computationally explore multinary wurtzite-type compounds for promising FE candidates with low switching barriers (~coercive fields) and high dielectric breakdown fields. In addition, we derive design principles based on metal-anion bond ionicity and lattice softness to lower switching barriers. In parallel, we use first-principles computations to systematically understand the switching behavior of AlN-based alloys at the atomic scale. Our predictions along with experimental verifications suggest that a change in the atomic-scale polarization switching mechanism, from a high-barrier collective to an individual switching process with an overall lower energy barrier, is a strong indicator for experimentally observing polarization reversal near room temperature. Our works offer insights for future engineering and realization of wurtzite FEs and open a door to understand domain structures and motions.

11:45 AM

(EMA-S19-013-2025) Combinatorial Synthesis and Characterization of Quaternary, Wurtzite (Al,Sc,Gd)N

J. Martin*[1]; K. Yazawa[1]; C. Lee[2]; T. Nyugen[1]; R. Smaha[1]; P. Gorai[2]

1. National Renewable Energy Laboratory, USA
2. Colorado School of Mines, USA

Many conventional ferroelectric materials for computing and data storage suffer from oxidative stability, electronic defects, and often require high operating temperatures which limits their performance and scalability. As such, designing and realizing new, stable FE materials is critical for energy-efficient computing. Motivated by the recent demonstration of FE behavior in wurtzite $Al_{1-x}Sc_xN$, our computational efforts herein explore cooperative effects from co-doping with rare earth elements and predict a lower switching barrier from smaller dopant concentrations as compared to the individual barriers for Sc- or Gd-doped AlN. We utilize a computationally-informed approach toward realizing quaternary (Al,Sc,Gd)N that employs combinatorial sputter synthesis to explore these chemical phases experimentally. To probe the interplay between structure and property, we investigate chemical composition and crystal structure via X-ray diffraction and X-ray fluorescence spectroscopy as well as test FE properties. We discuss these results in the context of high-throughput, computationally-guided materials discovery for applications in energy-efficient computing and data storage and piezoelectrics.

12:00 PM

(EMA-S19-014-2025) Ferroelectronics: Reimagining the transistor, the capacitor, and the memristor (Invited)

S. Cheema*[1]

1. Massachusetts Institute of Technology, Research Laboratory of Electronics, USA

This talk will explore engineering ferroelectric order in HfO_2-ZrO_2 on silicon – the dielectric used in today's state-of-the-art logic transistors and memory capacitors – to redesign integrated circuit building blocks. First we will present record-low EOT-leakage performance in HfO_2-ZrO_2 negative capacitance thin films down to two-nanometers and one-nanometer thickness, leveraging our previous work on the atomic limits of fluorite-structure ferroelectricity, leading to breakthrough transistor performance. Due to the seamless transition from high-κ HfO_2 dielectrics to negative-κ HfO_2-ZrO_2 ferroelectrics, these negative capacitance stacks have already been validated and integrated by prototyping foundries and semiconductor foundries. Next wel will discuss our recent work on capacitors demonstrating record-high energy storage and power density for on-chip energy technologies, and memristors demonstrating record-high on-off ratio and rectification for scalable compute-in-memory arrays. This talk will hopefully motivate more researchers in the materials science community to explore ferroic phenomena in simple systems with integration potential.

12:30 PM

(EMA-S19-015-2025) On-demand nanoengineering of in-plane ferroelectric topologies via smart scanning

M. Checa*[1]

1. Oak Ridge National Laboratory, CNMS, USA

Hierarchical assemblies of ferroelectric nanodomains (or superdomains) can exhibit exotic morphologies that lead to distinct behaviors and functionalities. Controlling these superdomains reliably is critical for realizing new states with desired functional properties. Here, using a biased atomic force microscopy tip we reveal a so-called super-switching mechanism of the in-plane superdomains of a model ferroelectric $Pb_{0.6}Sr_{0.4}TiO_3$, demonstrating that the response of this material is dominated by a superdomain nucleation and super-boundary stabilization process. We show that the scanning-probe's trajectory is key in stabilizing complex defect states, enabling on-demand formation of intricate center-divergent/convergent and flux-closure polar structures. Correlative piezoresponse force microscopy and optical spectroscopy confirm the topological nature and significant tunability of these emergent structures. The stability of the generated structures, validated by phase-field modeling, suggests potential for reliable multi-state nanodevice architectures, offering an alternative route for creating tunable topological structures in neuromorphic circuits, forging a new frontier in nanolithography for ferroics.

S20 Magnetic and superconducting materials-from basic science to applications

S20- Superconductivity and Other Correlated Systems

Room: Colorado D
Session Chair: Michael Susner, Air Force Research Laboratory

8:30 AM

(EMA-S20-016-2025) Magnetomechanical Coupling for Artificial Multiferroics (Invited)

M. E. Jamer*[1]

1. United States Naval Academy, Physics, USA

Multiferroics are proposed for a variety of exciting possible spintronic devices due to their ability to couple electronic and magnetic properties. While natural multiferroics including $BaFeO_3$ have been intensely studied for future use, there is a push to develop artificial multiferroics via coupling magnetostrictive materials to piezoelectric substrates. Artifical multiferroics may have an advantage over the traditional multiferroic materials due to their flexibility for optimization for a specific application. In this talk, magnetostrictive materials including Galfenol ($Fe_{100-x}Ga_x$; x=15-25) and Terfenol-D ($Tb_xDy_{1-x}Fe_2$), were coupled to a PMN-PT substrate to allow for voltage control of the ferromagnetic material. Functionality can be extended by exchange coupling the magnetostrictive material to a non-magnetostrictive magnet, including permalloy to allow for quicker switching of the magnetic properties. The work discussed in this talk will include a variety of measurements including voltage-controlled magnetometry and polarized neutron reflectometry (PNR) which demonstrate coherent magnetization rotation with an applied voltage. The results demonstrate a coherent electric field response across tens of nanometers, which is an optimal range for device applications.

9:00 AM

(EMA-S20-017-2025) Ferroelectricity in CuInP2S6 under pressure (Invited)

J. Musfeldt*[1]; S. Shah[1]; P. Mohammadi[2]; S. Cheong[3]; Z. Liu[4]; S. Singh[2]

1. University of Tennessee, Chemistry, USA
2. University of Rochester, Mechanical Engineering, USA
3. Rutgers University, Physics, USA
4. University of Illinois Chicago, Physics, USA

We bring together synchrotron-based infrared absorbtion and Raman scattering with diamond anvil cell techniques, complementary lattice dynamics calculations, and an analysis of the energy landscape to reveal the vibrational properties of CuInP2S6 under pressure. Our objective is to unravel the origin of the recently reported increase in the polarization under compression.

9:30 AM

(EMA-S20-018-2025) Revealing Signatures of Unconventional Superconductivity in Tunneling Andreev Spectroscopy (Invited)

P. Maksymovych*[1]

1. Clemson University, Materials Science and Engineering, USA

Pairing symmetry continues to be a frontier topic with the emergence of new superconductors and their prospects in quantum information. Recently we introduced Tunneling Andreev Reflection (TAR) - a method to detect the probability of Cooper pair injection across an atomic-scale contact. TAR enables STM to directly probe pairing symmetry, magnetism, and topological properties. For example, we used TAR to confirm the sign-changing superconductivity in FeSe, and reveal its suppression along the nematic twin boundaries. However, the trade-off for atomic-scale resolution is the loss of momentum resolution in TAR, necessitating rethinking the origins of specific TAR spectra. Here, based on detailed tight-binding modeling and model experiments, we will reveal the basic mechanisms by which TAR can detect unconventional pairing symmetry. Tunneling Andreev spectra will in general reflect both intrinsic properties of the superconductor as well as those of the tunneling transport - providing a wealth of information to characterize complicated materials and expanding the ability of tunneling spectroscopy to search for exotic quantum materials. Research sponsored by Division of Materials Science and Engineering, BES, US DOE. Experiments carried at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory.

10:30 AM

(EMA-S20-019-2025) Next-Generation Ultralight High-Field Magnets for Higher-Performance Aerospace Applications (Invited)

T. J. Haugan*[1]; T. Bullard[2]; J. Bulmer[2]; C. Kovacs[2]

1. U.S. Air Force Research Laboratory, Aerospace Systems Directorate, AFRL/RQQM, USA
2. UES, Inc., USA

High field magnets that can serve also as inductive energy storage devices are critical components of nearly all high power/energy applications, and with power levels ranging from 100 W to 100 MW. There is a long list of applications that utilize high field magnets (many >2T) for both military and commercial sectors, which can include: i) next-gen electric motors/generators for hybrid-electric propulsion, ii) 'immortal' fluid-free energy storage = 0-40 GJ, iii) magneto-plasma-dynamic (MPD) thrusters for space, iv) fusion power reactors, v) thermal-to-energy conversion; e.g. magnetocaloric power generation (MHD), and many others. The performance of many applications is correlated closely with the exponential strength of the magnetic field (B) controllably achieved, e.g. performance = const*B^n, with n = 1-4. Using SOA technologies of metal-wires or permanent magnets, B = 2.2 T is the 'hard' practical limit achievable for continuous magnet operation. However, with new cryogenic electric conductors and materials developed in the last 10-30 years, continuous B-fields from 2-40 T are practically being achieved. This paper will present the on-going R&D and new materials of this field to design and utilize next-gen magnets 2-40 T. Acknowledgements Support and funding is gratefully acknowledged by AFOSR LRIR's #18RQCOR100, #24RQCOR004 and the Aerospace Systems Directorate (AFRL/RQ).

11:00 AM

(EMA-S20-020-2025) Designing Polar Superconductors through Atomic-Scale Structural and Polarization Analysis (Invited)

S. Salmani-Rezaie*[1]

1. The Ohio State University, USA

The ability to visualize materials at the atomic scale has transformed our understanding of complex quantum phenomena, particularly superconductivity. Electron microscopy, once overlooked in superconductivity studies due to temperature limitations, has now emerged as a powerful tool for examining the intricate atomic and electronic structures that underlie superconducting behavior. This presentation explores electron microscopy's strengths in revealing polarization and structural intricacies that influence superconductivity, using $SrTiO_3$ and $FeSe/SrTiO_3$ as model systems. By investigating the normal state structures of materials near ferroelectricity, we emphasize how atomic-scale polarization and correlated lattice distortions impact the emergence and stability of superconductivity. Focusing on interfaces and structural features, we demonstrate how these insights connect experimental observations with theoretical models, offering a comprehensive understanding of the interplay between atomic-scale structure and superconducting phenomena. Integrating electron microscopy with complementary techniques, we aim to establish a framework for designing superconductors by harnessing atomic-level insights into polarization and structural interactions. This work highlights the transformative potential of electron microscopy in tailoring quantum materials for enhanced superconducting performance.

11:30 AM

(EMA-S20-021-2025) Structural, Electronic, and Magnetic Properties of Reactively Sputtered Heteroepitaxial Candidate Altermagnet RuO_2 (Invited)

S. Fields*[1]; S. Bennett[1]; C. Cress[2]; J. Prestigiacomo[1]; O. van 't Erve[1];
D. Wickramaratne[1]; N. Combs[2]; M. Currie[3]; P. Callahan[1]

1. US Naval Research Laboratory, Materials Science and Technology, USA
2. US Naval Research Laboratory, Electronics Science and Technology Division, USA
3. US Naval Research Laboratory, Optical Sciences, USA

Conventionally developed as an oxygen blocking electrode layer in ferroelectric computing applications and as an oxygen evolution catalyst, conductive rutile RuO_2 has witnessed renewed interest within the spintronics community as a proposed antiferromagnet and altermagnet. Moreover, this material has also been recently revealed to display superconductivity in the presence of sufficient crystal strain. Toward investigating these functional applications, this talk describes the characterization of the structural, electronic, and magnetic properties RuO_2 thin films, grown heteroepitaxially on TiO_2 substrates with several orientations. Through this industrially-applicable, high-temperature reactive sputter deposition process, all investigated TiO_2 substrate orientations are shown to successfully template single crystal RuO_2 films, where the quality of each expectedly depends on the match of the in-plane lattice parameters. Materials prepared using this process are subsequently patterned and incorporated into multilayers to investigate the electronic and magnetic properties of RuO_2 thin films, where interfaces and strain may play key roles in functional properties and future devices.

12:00 PM

(EMA-S20-005-2025) Spin-lattice entanglement and spin-electronic interactions in quasi-2D antiferromagnet $CoPS_3$ (Invited)

M. A. Susner*[1]; R. Rao[2]; B. Conner[1]; T. Mai[1]

1. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA
2. Air Force Research Lab, USA

In this study, we present a detailed study of the strong spin and lattice coupling in $CoPS_3$, a layered magnetic material. We find dramatic and sudden changes in the Raman spectra at temperatures far below the antiferromagnetic transition. These changes, which includes mode repulsion and a magnetic scattering continuum, indicate substantial coupling between lattice and spin excitations. The reduction in phonon lifetimes well below $T_N \approx$ 119K indicates that the lattice degree of freedom is strongly coupled to the spin fluctuation, and vice versa. We believe the orbital moment of the Co^{2+} ions causes such coupling via the spin-orbit effect. We also report the results of a T-dependent reflection spectroscopy study, across a wide energy range (~0.01 to 3 eV), of unsubstituted and 40% Zn substituted for Co. We observe a transition from a paramagnetic to antiferromagnetic state with a $T_N \sim$ 119 K that is completely suppressed in Zn-substituted samples. At 300 K we identify four narrow IR active phonon modes while at 70 K we observe that the low-energy phonons, dominated by Co motion, resolve into two asymmetric modes, indicating coupling to a broad electronic continuum. The temperature-dependent spectral changes indicate strongly correlated behavior between the IR active lattice vibrations, the electronic excitations, and magnetism in unsubstituted $CoPS_3$.

12:30 PM

(EMA-S20-023-2025) Understanding Bulk Nickelates Superconductivity: Impact of Pressure, Strain and Electron Correlation

B. Samanta*[1]; A. Georgescu[1]

1. Indiana University Bloomington, Chemistry, USA

The discovery of superconductivity in bulk nickelates under moderate pressure in 2023, having a transition temperature around 80 K, has reignited interest in exploring superconductivity across the nickelate family. Although the application of stress and strain has been linked to the onset of superconductivity in these materials, the precise atomistic mechanism driving superconductivity at certain stress levels remains unresolved. Since the d^9 configuration, crucial in cuprates, is absent in nickelates, previous theoretical frameworks are inadequate for explaining this phenomenon in nickelates. Thus, to investigate why a Ni-O-Ni straight bond develops a superconductivity in $La_3Ni_2O_7$, we performed a first-principles study to explore the interplay between electronic and crystal structure transitions in these materials under various stresses. Using standard DFT parameters, we accurately capture the transition pressure of 15 GPa, which is in agreement with experimental results reported to date. Further, $La_3Ni_2O_7$ is recognized as a strongly correlated material. Thus, we explored the influence of electronic correlations on the transition pressure and structure by varying the applied Hubbard parameter (U_{eff}). U_{eff} and pressure compete to control the magnetic moment. A lower U_{eff} promotes the dimerization required for superconductivity while a higher U_{eff} promotes electron localization.

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*** Denotes Presenter**

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