

**The American Ceramic Society**

**Materials Challenges in Alternative and  
Renewable Energy 2021 Virtual  
and  
4th Annual Energy Harvesting Society  
Meeting 2021 Virtual**

**ABSTRACT BOOK**

**July 19–22, 2021**

# Introduction

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This volume contains abstracts for over 200 presentations during the Materials Challenges in Alternative and Renewable Energy 2021 Virtual and 4th Annual Energy Harvesting Society Meeting 2021 Virtual. The abstracts are reproduced as submitted by authors, a format that provides for longer, more detailed descriptions of papers. The American Ceramic Society accepts no responsibility for the content or quality of the abstract content. Abstracts are arranged by day, then by symposium and session title. An Author Index appears at the back of this book. The Meeting Guide contains locations of sessions with times, titles and authors of papers, but not presentation abstracts.

## How to Use the Abstract Book

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

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Monday, July 19, 2021

## KIChE Plenary

### Opening Remarks and Plenary Speaker 1

Session Chair: Yoon-Bong Hahn, Chonbuk National University

9:40 AM

#### (KIChE-PLEN-2021) Chemistry for Nano, and Nano for Medicine and Energy

T. Hyeon\*<sup>1</sup>

1. Seoul National University, School of Chemical and Biological Engineering, Republic of Korea

For the last 20 years, I have been focused on designed synthesis, assembly and medical & energy applications of uniform-sized nanocrystals and related nanomaterials. Recently, we have focused on the architecture engineering of nanomaterials for their applications to fuel cell electrocatalysis, lithium ion battery, and photocatalysis. We present a synthesis of highly durable and active electrocatalysts based on ordered fct-PtFe nanoparticles and FeP nanoparticles coated with N-doped carbon shell. The effect of porous structures on the electrocatalytic activity of N-doped carbon is studied by using electrochemical analysis techniques, and the results are applied to synthesize highly active and stable Fe-N-C catalyst for oxygen reduction reaction (ORR). We also report on the design and synthesis of highly active and stable Co-N<sub>4</sub>(O) moiety incorporated in nitrogen-doped graphene (Co<sub>1</sub>-NG(O)) that exhibits a record-high kinetic current density (2.84 mA cm<sup>-2</sup> at 0.65 V vs. RHE) and mass activity (277.3 A g<sup>-1</sup> at 0.65 V vs. RHE) with unprecedented stability (>110 h) for electrochemical hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) production. We report on the design and synthesis of highly active TiO<sub>2</sub> photocatalysts incorporated with site-specific single copper atoms (Cu/TiO<sub>2</sub>) that exhibit reversible & cooperative photoactivation process, and enhancement of photocatalytic hydrogen generation activity.

### EHS S5: Special Symposium - Celebrating 20 Years of Energy Harvesting

Session Chair: Shashank Priya, Pennsylvania State University

10:30 AM

#### (EHS-001-2021) An emerging magnetic energy harvesting technology with magnetoelectrics (Invited)

J. Ryu\*<sup>1</sup>

1. Yeungnam University, Republic of Korea

The deployment of wireless sensor networks (WSNs) for the internet of things (IoT) and remote monitoring devices has made tremendous progress in the last few years. At the same time, energy harvesters are also being developed to satisfy the power requirement of WSNs and other low power consumption electronics. Among various resources for energy harvesting, the magnetic noise produced by power transmission infrastructures are ubiquitous energy sources that could be converted into electricity by high efficiency energy conversion materials or devices. In this presentation, the current status and prospects of an emerging magnetic energy harvesting technology, the so-called magneto-mechano-electric (MME) generators, are reviewed. MME generators utilize the magnetoelectric (ME) coupling in composites of piezoelectric and magnetostrictive materials and interaction between the proof magnet mass and magnetic field. Since the piezoelectric phase in the composite also responds to mechanical vibration directly, an ME-based energy harvester can harness energy from both mechanical vibrations and magnetic fields simultaneously. The MME generator can be a ubiquitous power source for

WSNs, low power electronic devices, and wireless charging systems by harvesting energy from the tiny magnetic fields present as parasitic magnetic noise in an ambient environment.

11:00 AM

#### (EHS-002-2021) Experimental investigations of the parameter influences on the usable bandwidth of passive self-tuning vibratory energy harvesters (Invited)

J. Twiefel\*<sup>1</sup>

1. Leibniz Universität Hannover, Institut for Dynamics and Vibration Research, Germany

In the field of piezo-based vibration energy harvesters, the question of usable bandwidth is essential for a wide range of applications. An exciting technology that was successfully demonstrated for the first time a few years ago is the passive self-tuning harvester. This is usually a beam clamped on both sides, which is equipped with a freely movable mass/slide along the beam direction. One or two piezoelectric elements applied to the beam provide the energy conversion. When this structure is excited with a harmonic oscillation via the two clamping points, the carriage moves so that the oscillation amplitude in the beam is maximized. However, this only works if some parameters are within the appropriate range. These parameters include the vibration amplitude of the excitation, the ratio of the carriage mass to the beam mass, the clearance between carriage and beam. If the parameters are outside this range, other interesting operating points may be found. In this thesis the influences of the different parameters are investigated experimentally. From the results an operation map is derived, which shows how easy or difficult these parameters can be set. In addition, the extent to which operation with non-monoharmonic excitations is also possible is investigated. Based on the results, an evaluation of the practical feasibility is given.

11:30 AM

#### (EHS-003-2021) Ocean Energy Harvesting and Powering the Blue Economy (Invited)

L. Zuo\*<sup>1</sup>

1. Virginia Tech, Mechanical Engineering, USA

There is vast but untapped energy from ocean, including the ocean waves, tidal current, and ocean current. Together with the riverine current, they are called as Marine and Hydrokinetic (MHK) energy. For ocean wave energy alone, the total wave energy potential along the US coastline is 64% of the electricity generated from all resources in the USA, and the power flux is 10-100 KW/m. Although the first patent was in 1799, the ocean energy is still in the early R&D stage. In this talk, we will first review the MHK energy converter technologies and the existing challenges, then discuss our recent efforts in the ocean energy, including the power takeoff design, hydrodynamics, power electronics, control system, tank test and ocean trials. We will emphasize the innovative mechanical motion rectifier (MMR) and active MMR for ocean wave energy conversion and hybrid wave-current energy conversion. Since the levelized cost of energy (LCOE) of the MHK technologies is still relatively high compared with other energy technologies, we also look into low-risk high-impact innovations for off-grid applications - to power the blue economy. To this end our efforts include to power maritime communication, ocean monitoring, sea water desalination, underwater vehicle charging and more.

12:00 PM

## (EHS-004-2021) Powering the Internet of Things: Perspectives on Energy Harvesting from Motion and Vibrations (Invited)

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

1. University of Utah, Mechanical Engineering, USA

The last 20 years has seen an impressive growth of energy harvesting for wireless sensors. While significant progress has been made in areas such thermal and RF energy harvesting, this talk will focus on energy harvesting from vibration and motion. Early research focused on understanding the limits of power generation focusing first on resonant harvesters using piezoelectric, electromagnetic, and electrostatic transducers. In order to overcome the narrow bandwidth of resonant harvesters, a significant research effort explored both tunable and nonlinear wideband harvesters. At present, the limits of harvesting power from vibrations are quite well known, reliable mathematical models have been published, and exceedingly many designs are available in the literature. The next logical step for the research field was to apply the theory and general prototypes to real-world applications. Powering wireless sensors in large industrial plants, rail transport, and automotive applications are a few prominent examples. While briefly covering these other applications, this talk will focus on energy harvesting from human motion, especially for devices worn on the arms as an example application. The talk will conclude with a discussion of the current state of research and potential opportunity areas.

## MCARE S1: Photocatalysts for Hydrogen Evolution Reaction

Session Chair: Yung-Jung Hsu, National Chiao-Tung University

10:30 AM

## (MCARE-001-2021) Comparison of g-C<sub>3</sub>N<sub>4</sub> and Its Heteronanocomposites for Their Hydrogen Production Activities

S. Odabasi Lee\*<sup>1</sup>; K. Yong<sup>1</sup>

1. Pohang University of Science and Technology, Chemical Engineering, Republic of Korea

ZnO/g-C<sub>3</sub>N<sub>4</sub> composite structure has Z-Scheme heterojunction on the interface of these materials. Z-Scheme heterojunction helps to decrease recombination of photogenerated electron hole pairs. g-C<sub>3</sub>N<sub>4</sub> was synthesized by thermal treatment of melamine and g-C<sub>3</sub>N<sub>4</sub>/ZnO was synthesized by a low temperature hydrothermal method. Due to the enhanced charge separation between ZnO and g-C<sub>3</sub>N<sub>4</sub>, the photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub> was enhanced and it further increased by using gold nanoparticles as electron mediator.

10:45 AM

## (MCARE-002-2021) Facile introduction of oxygen vacancy to BiVO<sub>4</sub> photoanode and its enhanced STH efficiency with perovskite solar cell

M. Lee\*<sup>1</sup>; K. Yong<sup>1</sup>

1. POSTECH, Chemical Engineering, Republic of Korea

Photoelectrochemical water splitting is one of the promising hydrogen production strategy but it needs additional extra bias voltage for operation. BiVO<sub>4</sub> is low cost and efficient transition metal oxide material for PEC photoanode. In this study, facile introduction of oxygen vacancy control to BiVO<sub>4</sub> was conducted to enhance photoelectrochemical property, and the PEC photoanode was integrated with perovskite solar cell to fabricate unassisted PV-PEC system that could operate only with solar light. Post treatment with hydrogen gas made surface oxygen vacancy on BiVO<sub>4</sub> and enhanced properties were characterized through UV-vis spectroscopy, XPS, EIS, and Mott-Schottky measurements. The integrated PV-PEC system showed a highly increased operating current and STH efficiency than pristine BiVO<sub>4</sub> case.

11:00 AM

## (MCARE-003-2021) Preparation of hierarchical g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> hollow spheres with highly enhanced photocatalytic activity

H. Moon\*<sup>1</sup>; K. Yong<sup>1</sup>

1. POSTECH, Chemical engineering, Republic of Korea

The g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterostructured hollow spheres were successfully prepared. The developed g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterojunction photocatalyst has a spherical hollow structure with diameters about 700 nm and shell thickness of 35-40 nm. The well designed structure is beneficial for the photocatalytic reaction in terms of large surface area, efficient charge separation and efficient light absorption. The as-prepared samples showed improved solar light and visible light induced photocatalytic activities by hydrogen evolution. The greatly enhanced activity can be attributed to the well-designed heterojunction and the hollow structure of g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub>.

## MCARE S1: General Photocatalysts

Session Chair: Yuanbing Mao, Illinois Institute of Technology

11:45 AM

## (MCARE-004-2021) 2D-Ni(Co,Fe)P/1D-WO<sub>x</sub> Electrocatalysts for Overall Efficient Water Splitting

D. Kim\*<sup>1</sup>; K. Yong<sup>1</sup>

1. POSTECH, Republic of Korea

Designing efficient nano-electrocatalysts is desirable for hydrogen/oxygen evolution reactions (HER/OER), which are major bottleneck of H<sub>2</sub> production in water splitting systems. In this study, we demonstrate novel hierarchical electrocatalysts for alkaline water splitting. Our catalyst has a unique structure consisting of Ni(Co,Fe)P nanosheet (NS) and WO<sub>x</sub> nanowire (NW). The WO<sub>x</sub> NW effectively transport charges (e<sup>-</sup>/h<sup>+</sup>) to the Ni(Co,Fe)P NS through a 1D directional structure. The ultrathin 2D Ni(Co,Fe)P NS grown on the WO<sub>x</sub> NW provide an abundance of active sites for splitting water molecules into H<sub>2</sub> and O<sub>2</sub>. As a result, our hierarchical 2D-NS/1D-NW-structured NiCoP-WO<sub>x</sub> (HER) and NiFeP-WO<sub>x</sub> (OER) catalysts demonstrate excellent activities, requiring low overpotentials of 49 and 270 mV, respectively, to generate a current density of 10 mA/cm<sup>2</sup>. Additionally, they exhibit high electrochemical stability for over 60 h in 1 M KOH. These catalytic activity are outstandingly low among other reported transition metal phosphide catalysts. The interfacial nano-engineering presented provides not only efficient electrocatalysts but also a promising, useful strategy to develop functional 1D/2D hierarchical materials for advanced energy applications.

12:00 PM

## (MCARE-005-2021) Nitrate Reduction over Nickel Phosphide Nanocatalysts (Invited)

J. Vela\*<sup>1</sup>

1. Iowa State University, Chemistry, USA

Burgeoning demand for agricultural products and increasing usage of synthetic nitrogen fertilizer have resulted in significant nitrate (NO<sub>3</sub><sup>-</sup>) accumulation in groundwater. Here, we explore the NO<sub>3</sub><sup>-</sup> hydrogenation over nanoscale Ni<sub>2</sub>P. Ni<sub>2</sub>P is the first non-noble metal-based catalyst that hydrogenates NO<sub>3</sub><sup>-</sup> to NH<sub>4</sub><sup>+</sup> under near ambient conditions (1 atm H<sub>2</sub>, 60 °C) with very high selectivity (96%). It can be recycled for at least 4 cycles without significant loss of activity. NO<sub>2</sub> and NO intermediates are also hydrogenated. Next, we prepare and explore Ni<sub>2</sub>P/Ta<sub>3</sub>N<sub>5</sub>, Ni<sub>2</sub>P/TaON, and Ni<sub>2</sub>P/TiO<sub>2</sub> heterostructures for the photocatalytic reduction of NO<sub>3</sub><sup>-</sup>. Ni<sub>2</sub>P/Ta<sub>3</sub>N<sub>5</sub> and Ni<sub>2</sub>P/TaON display 79% and 61% NO<sub>3</sub><sup>-</sup> conversion at the rate of 196 μmol g<sup>-1</sup>h<sup>-1</sup> and 153 μmol g<sup>-1</sup>h<sup>-1</sup>, respectively. We propose two possible migration pathways of photo-generated electrons. The dominant one is the electron-hole separation on the semiconductor

induced by light, followed by electron injection into Ni<sub>2</sub>P, which upshifts the Fermi level of the Ni<sub>2</sub>P and provides the driving force for the reduction. Finally, we test NO<sub>3</sub><sup>-</sup> hydrogenation over nickel phosphide clathrates ANi<sub>2</sub>P<sub>4</sub> (A = Ba, Sr) that contain Ni<sub>8</sub>P<sub>16</sub> cages. ANi<sub>2</sub>P<sub>4</sub> (A = Ba, Sr) achieve up to 82% NO<sub>3</sub><sup>-</sup> conversion with 100% selectivity for NH<sub>4</sub><sup>+</sup>. We find that decreasing particle size through grinding increases reduction activity, likely due to the introduction of surface defects.

**12:30 PM**

**(MCARE-006-2021) Polymer Passivated Cell Showing Exceptionally High Light-to-Current Conversion Efficiency (Invited)**

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

1. University of Texas Rio Grande Valley, Chemistry, USA

Fiber shaped dye sensitized solar cells are very promising technology due to their light weight and flexibility making them suitable for use in military and textile applications. With the proper use of TiO<sub>2</sub>, quantum dots, bulk heterojunction polymer layer and a liquid polysulfide electrolyte a high open circuit voltage of 0.75V has been achieved. The TiCl<sub>4</sub> annealing of the oxide layer resulted into a uniformly coated smooth but rough surface that facilitated efficient transfer of the photogenerated excitons. The chemical bath deposition technique was used to deposit different layers. A plasma sputtering system was used to fabricate the counter electrode. The photoelectric performance was evaluated at different cell length and a 3.5cm cell length gave the highest light-to-current conversion efficiency of 8.30%. When the cells were connected in series a high open circuit voltage of 1.5 V has been achieved. Future study can be conducted in this field to understand the role of a liquid electrolyte in obtaining high performance flexible solar cells.

**MCARE S5: Materials for Upconversion, Downconversion / Quantum Cutting, Luminescent Downshifting - I**

Session Chair: Eva Hemmer, University of Ottawa

**10:30 AM**

**(MCARE-007-2021) Lanthanide-Based Luminescent Materials for Waveguide and Lasing (Invited)**

T. Sun\*<sup>1</sup>; F. Wang<sup>2</sup>

1. Sun Yat-sen University, School of Chemical Engineering and Technology, China
2. City University of Hong Kong, Department of Materials Science and Engineering, Hong Kong

In the past decades, miniaturized waveguides and lasers have attracted great attention because of their advantages of low noise, good monochromaticity, and high output power. Due to low content of gain media in waveguides and lasers of small sizes, luminescent materials with high optical gains are typically required in these applications. In search of more effective gain materials in waveguide and lasing applications, lanthanide-doped materials have captured increasing interests in recent years. In this talk, I will focus on our recent effort in making upconversion waveguide and lasing. Examples will also be given to demonstrate the design and synthesis of gain materials, as well as the realization of lasing emission especially in the ultraviolet region.

**11:00 AM**

**(MCARE-008-2021) Measuring the Upconversion Luminescence of Ensemble and Single Particle Lanthanide-Based Upconversion Nanocrystals (Invited)**

U. Resch-Genger\*<sup>1</sup>; F. Frenzel<sup>1</sup>; C. Wuerth<sup>1</sup>; B. Grauel<sup>1</sup>; T. Hirsch<sup>2</sup>; M. Haase<sup>3</sup>

1. BAM Federal Institute for Material Research and Testing, Germany
2. University of Regensburg, Institute of Analytical Chemistry, Germany
3. University of Osnabrueck, Institute of Chemistry/New Materials, Germany

Lanthanide-based upconversion nanoparticles (UCNPs) like hexagonal β-NaYF<sub>4</sub> UCNPs doped with Yb<sup>3+</sup> and Er<sup>3+</sup>, which efficiently convert 976 nm light to ultraviolet, visible, and near infrared photons, offer new strategies for luminescence-based sensing, barcoding, and imaging. Their upconversion (UC) luminescence (UCL) features like UCL intensity, quantum yield, relative spectral distribution / UCL luminescence color, and luminescence decay kinetics are, however, strongly influenced by particle size, dopant ion concentration, particle architecture, surface chemistry including presence and thickness of surface passivation and shielding shells, microenvironment/presence of quenchers with high energy vibrations, and excitation power density (P). We present here a comprehensive study of the influence of excitation power density on the UCL features of different types of UCNPs, focusing on Yb<sup>3+</sup> and Er<sup>3+</sup> co-doped NaYF<sub>4</sub> core-only and core-shell nanostructures with different sizes and doping ion concentration, which underlines the importance of P-dependent optimum dopant concentrations for UCNPs performance and the potential of P-tuning of UCL.

**11:30 AM**

**(MCARE-009-2021) Employing anhydrous molecular precursors as a strategy to enhance up-conversion efficiency in Ln<sup>3+</sup>-doped MM'F<sub>4</sub> (M = Li, Na; M' = Y, Gd) (Invited)**

S. Mishra\*<sup>1</sup>; B. Purohit<sup>1</sup>; E. Jeanneau<sup>2</sup>; G. Ledoux<sup>3</sup>; M. Joubert<sup>3</sup>; C. Dujardin<sup>3</sup>; Y. Guyot<sup>3</sup>; D. Amans<sup>3</sup>; B. Mahler<sup>3</sup>

1. University of Lyon1, Institut de Recherches sur l'Environnement et la Catalyse de Lyon (IRCELYON), France
2. Centre de Diffractométrie Henri Longchambon, France
3. Institut Lumière Matière, France

A major challenge in the field of upconverting (UC) nanomaterials is to enhance upconversion luminescence. In comparison to conventional luminophores, quantum yields of lanthanide-doped UC nanoparticles are extremely low (typically less than 1%) and, in general, about an order of magnitude lower than those of corresponding UC bulk materials. It is well-known that -OH defects in the nanocrystals are the primary cause of upconversion quenching. We have employed designed anhydrous molecular precursors as a synthetic strategy to enhance up-conversion efficiency in Yb<sup>3+</sup> and Tm<sup>3+</sup> co-doped MM'F<sub>4</sub> nanocrystals (M = Li, Na; M' = Y, Gd). The bottom-up synthesis not only facilitates a better control over the composition, structure and morphology of the nanomaterials,<sup>5</sup> but anhydrous conditions also minimize -OH functionality on the surface of the upconverting NPs. A detailed up-conversion studies reveal that the uniform nanoparticles obtained from these anhydrous single source precursors had i) superior up-conversion intensity than the UC materials produced from the hydrated inorganic salts, and ii) a comparable efficiency with bulk materials of the same composition. The applications of these nanomaterials in the field of photocatalysis will be described.

12:00 PM

## (MCARE-010-2021) Photonic glass ceramics for frequency conversion (Invited)

L. Tran<sup>1</sup>; K. Startek<sup>2</sup>; O. Sayginer<sup>1</sup>; S. Varas<sup>1</sup>; C. Armellini<sup>1</sup>; A. Chiappini<sup>1</sup>; A. Carpentiero<sup>1</sup>; M. Bollani<sup>3</sup>; F. Scotognella<sup>4</sup>; M. Ferrari<sup>1\*</sup>; G. C. Righini<sup>5</sup>; P. Gluchowski<sup>6</sup>; A. Lukowiak<sup>6</sup>; A. Chiasera<sup>1</sup>

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5. MiPLab, IFAC-CNR, Italy
6. Institute of Low Temperature and Structure Research, PAS, Poland

Frequency conversion is an important mechanism driving the relaxation dynamics in rare earth doped materials with lots of applications in photonics. Among them, photovoltaics is one of the preeminent ones. The key is to control the absorption of the solar radiation, by shifting the unabsorbed wavelengths toward 980 nm, i.e., close to the band gap of crystalline silicon. It is recognized that glass ceramic systems are crucial for the tailoring of energy transfer mechanism. In this talk, we introduce the transparent glass ceramics and some highlights extracted from the current literature on frequency converters. The fundamentals of the energy transfer process between rare earth ions will be presented. An overview is presented on the use of rare earth activated luminescent materials in solar spectrum conversion, focusing the attention on the different couples of lanthanide ions, the host materials, and the quantum cutting mechanism that allow to properly choose the doping ions and therefore to improve the quantum efficiency. The specific role played by the host material is also discussed. Finally, linear and nonlinear energy transfer mechanisms are discussed in looking at HfO<sub>2</sub>, SiO<sub>2</sub> based nanoceramics.

## MCARE S7: Advanced Materials and Nanodevices for Sustainable and Eco-friendly Applications I

Session Chair: Yeon Ho Im, Chonbuk National University

10:30 AM

## (MCARE-011-2021) Functional Electronic and Photonic Devices Integrated with Hybrid Heterostructures based on Two-dimensional Materials (Invited)

S. Baek<sup>1</sup>; C. Shin<sup>1</sup>; H. Son<sup>1</sup>; H. Choi<sup>1</sup>; S. Choi<sup>1</sup>; S. Lee<sup>1\*</sup>

1. Sungkyunkwan University, SAINT, Republic of Korea

Two-dimensional (2D) material families have been attracting extensive interest with the aim to impose new functionalities for electronic, photonic, optoelectronic device applications owing to their unique properties in a wide range of attributes. These attributes involve optical, electromagnetic, and mechanical parts, such as ultra-fast mobility of graphene and black phosphorus, strong light-matter interaction from transition metal dichalcogenides, high transparency, and flexibility for overall 2D materials with atomic-thickness. An extensive library of atomic 2D materials with selectable material properties exists and it is rapidly expanding, with which it is possible to construct hybrid or heterostructures that display novel properties with unique functionalities. Such heterostructures adding a degree of freedom to carriers in the third direction provide interesting possibilities for the design of functional novel devices. In this presentation, recent progresses reported from our group in the areas of synthesis and properties of new-functional hybrid heterostructures based on 2D materials will be discussed, along with their potential applications toward next-generation electronic and photonic devices.

11:00 AM

## (MCARE-012-2021) Electrospun Ta<sub>3</sub>N<sub>5</sub>-(O) fibers as advanced electrocatalysts for hydrogen evolution reaction

R. Mukkavilli<sup>1\*</sup>; A. Ichangi<sup>2</sup>; G. Thiyagarajan<sup>1</sup>; L. Neelakantan<sup>1</sup>; S. Christiansen<sup>3</sup>; S. Mathur<sup>2</sup>; R. Kumar<sup>1</sup>

1. Indian Institute Of Technology, Madras, Metallurgical and Materials Engineering, India
2. University Of Cologne, Inorganic and Materials chemistry, Germany
3. 1. FhG IKTS Dresden, Dresden, Germany. 2. Fraunhofer IKTS, Dresden, Saxony, Germany., Germany

Novel Electrospun Ta<sub>3</sub>N<sub>5</sub>-(O) fibers were synthesized through the combination of electrospinning tantalum ethoxide/PVP mixture followed by high-temperature ammonolysis (1073K, 1173K, 1273K). The obtained fibers exhibited a variation in O/N ratio as a function of temperature. Fiber morphology and structure were studied using scanning electron microscopy, Transmission electron microscopy, X-ray photoelectron spectroscopy, and X-ray diffraction. The obtained fibers were investigated for electrocatalytic HER in 0.5 M H<sub>2</sub>SO<sub>4</sub> & 0.1 M KOH. Compared to oxide fibers @ 1073K, nitride fibers obtained at high temperatures (1173K, 1273K) exhibited a low overpotential of 250 mV @ 10 mA/cm<sup>2</sup> in acidic media. However, a decrease in reaction kinetics was observed for the sample pyrolyzed at 1273 K. This was attributed to higher O/N content and an increase in crystallite size as exemplified through XPS and TEM studies. Further electrochemical impedance spectroscopy also confirmed an increase in charge transfer resistance of the fibers pyrolyzed at 1273 K compared to 1173 K. For the first time, the best performing nitride was later chosen for study in a full cell water electrolyzer in both acidic and alkaline medium and the mechanisms are discussed.

11:15 AM

## (MCARE-013-2021) Biosynthesis of inorganic nanomaterials and their energy harvesting and storage applications

Y. Choi<sup>1\*</sup>; T. Park<sup>2</sup>; D. Lee<sup>3</sup>; S. Lee<sup>1</sup>

1. Korea Advanced Institute of Science and Technology, BioProcess Engineering Research Center, Republic of Korea
2. Chung-Ang University, Department of Chemistry, Republic of Korea
3. Korea Advanced Institute of Science and Technology, Department of Chemical and Biomolecular Engineering, Republic of Korea

Nanomaterials are mostly synthesized by chemical and physical methods, but biological synthesis is also receiving great attention. Recently, wild-type and genetically engineered microorganisms have been harnessed for the biosynthesis of inorganic nanomaterials under mild and environmentally friendly conditions. Microorganisms such as microalgae, fungi and bacteria, as well as bacteriophages, can be used as biofactories to produce various inorganic nanomaterials. Here we report biosynthesis of 60 different inorganic nanomaterials by employing a recombinant *Escherichia coli* strain co-expressing metallothionein and phytochelatin synthase. The periodic table was scanned to select 35 suitable elements using the recombinant *E. coli* cell, followed by biosynthesis of their nanomaterials. Based on the Pourbaix diagram analyses, the initial pH of reactions was changed from 6.5 to 7.5, resulting in biosynthesis of crystalline nanomaterials of those previously amorphous or not synthesized ones. The strategy described in this study allows biosynthesis of inorganic nanomaterials with various properties, providing a new platform for manufacturing diverse nanomaterials in environmentally friendly manner. Moreover, we highlight the applications in energy harvesting and storage of biogenic nanomaterials using microbial cells and bacteriophages.



11:30 AM

**(MCARE-014-2021) MOCVD formation and study of AuNPs-decorated Pd and Pt coatings**D. E. Tryakhov\*<sup>1</sup>

1. NIIC, Russian Federation

The noble metals are in the focus of many investigations concerning of advanced materials for medicine, catalysis, and fuel industry. The AuNPs-decorated Pt coatings attract attention as promising functional materials of medical implants. The Pd containing coatings are suitable materials for membranes for hydrogen separation. The Metal-Organic Chemical Vapor Deposition (MOCVD) and related gas-phase methods are universal for obtaining wide range of materials from ultrafine particles to thick coatings (1 micron) on various substrates. During MOCVD implementation, target materials form at the decomposition of vapor of metalorganic precursors, whose physical and chemical properties predetermine parameters of MOCVD process. In this work, we present results of MOCVD formation of AuNPs-decorated Pd and Pt coatings on Si, Ti, and steel substrates using novel fluorinated precursors of Pd, Pt. The series of high volatile fluorinated beta-diketonate derivatives of Pd(II), Pt(IV) were synthesized in high yields, and their structural features and thermal properties were studied. The AuNPs are deposited on top of Pd or Pt coatings from dimethylgold compounds using a pulse-MOCVD technique. The composition, structure, and morphology of Pd, Pt coatings with/without AuNPs are studied using XRD, XPS, and microscopy methods. This work was funded by the Russian Science Foundation, project No. 20-15-00222

11:45 AM

**(MCARE-015-2021) MOCVD of noble metal film materials onto medical implants: microstructure and biocompatibility of iridium- and gold-based coatings**K. Karakovskaya\*<sup>1</sup>; E. Vikulova<sup>1</sup>; I. Korolkov<sup>1</sup>; T. Koretskaya<sup>1</sup>; I. Asanov<sup>1</sup>; A. Tsygankova<sup>1</sup>; E. Maksimovskii<sup>1</sup>; N. Morozova<sup>1</sup>; E. Chepeleva<sup>2</sup>; Y. Lantsukhay<sup>2</sup>; A. Zheravin<sup>2</sup>; E. Marchenko<sup>3</sup>

1. Nikolaev Institute of Inorganic Chemistry, Russian Federation
2. Meshalkin National Medical Research Center, Russian Federation
3. Kuznetsov Siberian Physical-Technical Institute, Russian Federation

Titanium and titanium nickelide (TiNi) alloy are characterized as ideal materials for fabrication of the implants and other devices for orthopedics and reconstructive surgery. Nevertheless, a special functionalization of these materials' surfaces by coatings of noble metals (Ir, Pt, Au) are promising to improve the biocompatible characteristics of devices. The aim of this work was to develop an approaches to obtain such coatings on Ti and TiNi substrates by metal-organic chemical vapor deposition (MOCVD). We have been focused on formation of Ir films with developed morphology and subsequent discrete Au coatings. Iridium was deposited in the oxidizing atmosphere using volatile precursor [Ir(cod)(acac)] (cod = cyclooctadiene-1,5, acac = acetylacetonate-anion). The influence of the deposition temperature (290-350°C) and reagent gas flow (2-8 l·h<sup>-1</sup>) on the morphology and composition of the sample was studied. A discrete Au coatings onto a pre-deposited iridium layer were obtained using [(CH<sub>3</sub>)<sub>2</sub>Au(thd)] precursor at a deposition temperature of 240°C in oxygen presence. To assess the biocompatibility, the toxicity of the samples in relation to human embryonic stem cell line Man-1 was examined in dynamics. The results obtained were explained based on the coating microstructures. *This work was financially supported by RSF (research project No. 20-15-00222).*

**MCARE S16: Solar Energy Harvesting I**

Session Chair: Sanjay Mathur, University of Cologne

10:30 AM

**(MCARE-016-2021) Highly Stable and Efficient Perovskite Solar Cells with Functional Composites (Invited)**Y. Hahn\*<sup>1</sup>

1. Jeonbuk National University, School of Semiconductor and Chemical Engineering, Republic of Korea

For practical use of perovskite solar cells (PSCs) the instability issues of devices, attributed to degradation of perovskite molecules by moisture, ions migration, and thermal- and light-instability, have to be solved. Furthermore, most of presented high efficiency PSCs utilize halogenated antisolvents such as toluene and chlorobenzene to assist perovskite crystal growth with large grain-size and high uniformity, but they are toxic and detrimental to environment. To solve such issues, we developed simple methods for production of functional nanocomposites such as Ag-rGO, perovskite-NiO, perovskite/Ag-rGO, NiO-carbon-graphite, Al<sub>2</sub>O<sub>3</sub>/graphene, etc and utilized them for the fabrication of highly stable and efficient PSCs. We report highly efficient and stable PSCs based on perovskite/Ag-reduced graphene oxide (Ag-rGO) and mesoporous Al<sub>2</sub>O<sub>3</sub>/graphene (mp-AG) composites. Compared to the mp-TiO<sub>2</sub> ETL based cells, the champion device based on perovskite/Ag-rGO and SrTiO<sub>3</sub>/mp-AG composites showed overall a best performance. More importantly, the champion device without encapsulation exhibited not only remarkable thermal- and photo-stability but also long-term stability with retaining 97-99 % of the initial values of photovoltaic parameters with sustaining ~ 93% of initial PCE over 300 days under ambient conditions.

11:00 AM

**(MCARE-017-2021) Fully-ambient-air Processed Perovskite Solar Cells with Perovskite-based Composites and Interface Engineering (Invited)**Y. Wang\*<sup>1</sup>

1. Jinan University, Institute of New Energy Technology, China

Due to poor-stability of lead-halide perovskite materials in ambient condition, often high-quality perovskite films require controlling fabrication and annealing atmosphere. Here we developed solution-processed perovskite-NiO based-composite films in ambient condition. Firstly, we reported an air-stable, hole-conductor-free (HCF), and high photocurrent PSCs with MAPbI<sub>3</sub>-NiO NPs composite. Furthermore, we used MAPbI<sub>3-x</sub>Cl<sub>x</sub>-NiO NPs composites and a simple and effective interfacial engineering with metal oxide nanoparticles, resulting in a high PCE of 18.10 % and a remarkable air-stability over 210 days. Subsequently, we achieved fully-ambient-processed stable and mesoscopic semitransparent PSCs by non-continuous islands-structure-MAPbI<sub>3-x</sub>Cl<sub>x</sub>-NiO NPs composite and interface engineering. Recently, we developed carbon-graphite-Cu:NiO-perovskite and FA<sub>x</sub>MA<sub>1-x</sub>PbI<sub>3-y</sub>Cl<sub>y</sub>-Cu:NiO based composites through antisolvent-free and fully-ambient-air processes for highly stable and efficient PSCs. The improved performance and air stability of perovskite-NiO composites and interface engineering-based PSCs are attributed to the enhanced charge carrier transportation via improving photo-absorption and fast hole-conduction by NiO NPs, and strong chemical interaction between NiO and MAPbI<sub>3</sub> or MAPbI<sub>3-x</sub>Cl<sub>x</sub> molecules, and the lower interface defects.

11:30 AM

### (MCARE-018-2021) Improved Optical and Photoelectrochemical Properties of Surface Patterned Titanium Indium Oxide Thin Film via Sol-Gel Based Soft Lithography

H. Khan<sup>\*1</sup>; S. Kwon<sup>1</sup>

1. Pusan National University, School of Materials Science and Engineering, Republic of Korea

Metal oxide semiconductor (MOS) thin films always draw special interest to the materials researchers for their advanced applications in diverse areas. Moreover, nanopatterning onto the MOS thin film surfaces is a novel technique to boost the efficiency of different optoelectronic devices by enhancing light absorption/trapping. Surface patterned films can increase the effective optical path length of incident light inside the film matrix by light trapping or scattering. Herein, 1-dimensional (1D) nanoprism and 2-dimensional (2D) nanocone shaped surface patterned titanium indium oxide thin films were fabricated by sol-gel based soft lithography technique. Structural, microstructural and optical properties of fabricated films were studied systematically and correlated with photoelectrochemical (PEC) properties. Significant improvement in photocurrent density (PD) of 2D patterned film was observed under visible light. The improved structural, microstructural and optical properties were responsible for enhancing PD. Thus, the mesoporous film with periodic nanocone shaped structure could be used as an efficient photoanode for water oxidation in PEC cell. This facile technique could create an avenue for fabrication of complexed periodic surface structures for improving PEC efficiency.

11:45 AM

### (MCARE-019-2021) SrTiO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub>-Graphene Electron Transport Layer for Highly Stable and Efficient Composites-Based Perovskite Solar Cells with 20.6 % Efficiency

T. Mahmoudi<sup>\*1</sup>; Y. Hahn<sup>1</sup>

1. Chonbuk National University, Chemical Engineering, Republic of Korea

For practical use of perovskite solar cells (PSCs) the instability issues of devices, attributed to degradation of perovskite molecules by moisture, ions migration, and thermal and light instability, have to be solved. Herein, we report highly efficient and stable PSCs based on perovskite/Ag-reduced graphene oxide (Ag-rGO) and mesoporous Al<sub>2</sub>O<sub>3</sub>/graphene (mp-AG) composites. The mp-AG composite was conductive with one-order of magnitude higher mobility than mp-TiO<sub>2</sub> and used for electron transport layer (ETL). Compared to the mp-TiO<sub>2</sub> ETL based cells, the champion device based on perovskite/Ag-rGO and SrTiO<sub>3</sub>/mp-AG composites showed overall a best performance. More importantly, the champion device without encapsulation exhibited not only remarkable thermal- and photo-stability but also long-term stability with retaining 97-99 % of the initial values of photovoltaic parameters with sustaining ~ 93% of initial PCE over 300 days under ambient conditions.

12:00 PM

### (MCARE-020-2021) Hybrid Seeded Growth SnO<sub>2</sub> Nanowires for Heterostructure Electrodes with Enhanced Photoelectrochemical Performance

S. Bera<sup>\*1</sup>; S. Kwon<sup>1</sup>

1. Pusan National University, School of Materials Science and Engineering, Republic of Korea

Rutile nanowires (NWs) hold great promises for numerous applications due to their variety of tunable physicochemical properties, but to the date, their direct synthesis onto versatile conducting substrates remains a significant challenge. Herein, orientation engineering of rutile SnO<sub>2</sub> NWs on a variety of substrates by atomic layer deposition (ALD) seeding have been investigated. Seed layers onto carbon cloth produces high surface area SnO<sub>2</sub> NWs, which would show efficient electrochemical CO<sub>2</sub> reduction. In addition,

hierarchical architecture resulted from seeded growth of NWs on SnO<sub>2</sub> nanosheets allows thin layers of BiVO<sub>4</sub>, forming a heterojunction photoanode, which shows enhanced photoelectrochemical performance. This study illustrates that such a versatile interfacial engineering effort for a heterogeneous system by the ALD technique would benefit a wide range of practical applications.

### MCARE S1: Photocatalysts for Water Splitting

Session Chair: Yuanbing Mao, Illinois Institute of Technology

1:30 PM

### (MCARE-021-2021) Inhibition of charge recombination by combining WO<sub>x</sub> and g-C<sub>3</sub>N<sub>4</sub> : Analysis of charge transfer by PL, TRPL

I. Hong<sup>\*2</sup>; K. Yong<sup>1</sup>

1. Engineering Ceramics Research, Korea Institute of Materials Science, Chemical Engineering, Republic of Korea
2. Engineering Ceramics Research, Korea Institute of Materials Science, Republic of Korea

Graphitic carbon nitride(g-C<sub>3</sub>N<sub>4</sub>) is suitable candidate material for photocatalysts that can produce hydrogen energy in an eco-friendly way through water decomposition. However, a single g-C<sub>3</sub>N<sub>4</sub> has a limitation of photocatalytic activity due to fast recombination of photogenerated electron-hole pairs. Many researchers have been studied to solve this problem with doping, depositing noble metals and so on. We tried to enhance the charge transfer by forming heterojunction with g-C<sub>3</sub>N<sub>4</sub> and tungsten suboxide(WO<sub>x</sub>). The analysis of the charge transfer improvement was carried out with photoluminescence(PL) and the charge carrier life time was confirmed by Time-resolved photoluminescence(TRPL). From the TRPL data, calculated PL decay lifetimes transformed into the charge transfer constant. It was confirmed that the photocatalytic hydrogen production activity was improved by inhibiting rapid recombination of charge carriers.

1:45 PM

### (MCARE-022-2021) Fields Matter: Better Water Splitting Through Magnetic Field-Assisted Processing of Hematite Thin Films

D. Stadler<sup>1</sup>; M. Pyeon<sup>1</sup>; V. Rauch<sup>1</sup>; M. Gürsoy<sup>3</sup>; M. Deo<sup>1</sup>; Y. Gönüllü<sup>1</sup>; T. Fischer<sup>\*1</sup>; T. Hwang<sup>2</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Institute of Inorganic Chemistry, Germany
2. Korea Institute of Industrial Technology (KITECH), Republic of Korea
3. Selçuk Üniversitesi, Turkey

We report the magnetic field influence during plasma enhanced chemical vapor deposition (PECVD) of hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) nanostructures. Hematite films grown from iron precursors showed pronounced changes in crystallographic textures depending upon whether PECVD was performed with or without the influence of external magnetic field. Static magnetic fields created by rod-type (RTMs) or disk-type magnets (DTMs) resulted in hematite films with anisotropic or equiaxed grains, respectively. Using RTMs, a superior photoelectrochemical (PEC) performance was obtained for hematite photoanodes synthesized under perpendicularly applied magnetic field (with respect to substrate), whereas parallel magnetic field resulted in the most efficient hematite photoanode in the case of DTM. Our experimental data on microstructure and functional properties of hematite films showed that application of magnetic fields parallel and perpendicular have a significant effect on the crystallite size and texture with preferred growth and/or suppression of grains with specific texture in  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> films. Investigations on the water splitting properties of the hematite films in a photoelectrochemical reactor revealed that photocurrent values of hematite photoanodes were remarkably different for films deposited with (0.659 mA/cm<sup>2</sup>) or without (0.484 mA/cm<sup>2</sup>) external magnetic field.

2:00 PM

**(MCARE-023-2021) Effect of dipole moments built in bilayer interfaces on photo-electrochemical water splitting (Invited)**H. Lee<sup>\*1</sup>; V. Nahrstedt<sup>1</sup>; H. Choi<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Germany

Efficient photo-induced electrocatalyst design is in huge demand to develop sustainable energy resource. As a result of this, a number of researches have proceeded to improve oxygen evolution rate in a photo-induced electrochemical (PEC) system and a variety of electrocatalysts have been released. Among these tremendous efforts, even though charge separation is one of the most important factors in a PEC reaction, application of fundamental theory from understanding of charge separation is barely mentioned. Particularly, separating photo-generated charges is crucial to a PEC system because unless photo-induced charges transfer toward reactants, the charges are going to recombine immediately. Therefore, a PEC system is need of applicable strategies. Herein, a dipole moment formation in a bilayer catalyst is suggested to induce internal electric field by means of improving charge separation and consequently to enhance oxygen generation. In this work,  $\text{MgFe}_2\text{O}_4/\text{Fe}_2\text{O}_3$  and  $\text{NiFe}_2\text{O}_4/\text{Fe}_2\text{O}_3$  are fabricated as bilayer catalysts to form Mg-Fe and Ni-Fe dipole moments at each interfaces of these catalysts. Electrochemical performances of the bilayer catalysts and single layer  $\text{Fe}_2\text{O}_3$  are compared to investigate how the dipole moments affect photo-electrocatalysis and effect of selection of cation to form a dipole moment.

2:30 PM

**(MCARE-024-2021) Formation of polarons and their electronic structures within oxide-based photo-electrocatalysts (Invited)**M. N. Huda<sup>\*1</sup>

1. University of Texas at Arlington, Department of Physics, USA

Hydrogen production from water splitting via the photo-electrochemical (PEC) process remains to be the most potential green technology. The key material for this technology is photo-electrocatalyst that are required to absorb sunlight, excite and transport charge carriers efficiently towards the liquid-semiconductor interface to split water molecule. Metal-oxides are thought to be the most stable materials under intense interfacial reactive conditions. However, the overall solar to hydrogen production efficiencies are not as high as expected, even for those with near-suitable bandgap energies. One of the main reasons is attributed to the poor transport properties in metal-oxides, especially in the 3d transition metal-oxides where electrons are strongly correlated. In this presentation, representative metal-oxides photo-catalysts will be considered to demonstrate the polaron formation mechanism. From detailed electronic structure calculations by density functional theory (DFT) based methods, these oxides' polaronic states will be depicted. It will also be shown how these polaronic states affect the transport properties and the open-circuit voltages of the PEC cell. We will also discuss how well these computational results compare with the recent experimental outcome. Computations were performed at Texas Advanced Computing Center (TACC).

**MCARE S1: Photocatalysts for Oxygen Evolution****Reaction**

Session Chair: Zhenxing Feng, Oregon State University

3:00 PM

**(MCARE-025-2021) Boosting effect in 3d metal oxygen evolution electrocatalysts investigated using in situ soft X-ray absorption spectroscopy (Invited)**D. Drevon<sup>2</sup>; V. Sikolenko<sup>3</sup>; D. Ojwang<sup>1</sup>; M. Valvo<sup>1</sup>; M. Risch<sup>4</sup>; H. Dau<sup>3</sup>; M. Görlin<sup>\*1</sup>

1. Uppsala University, Chemistry - Ångström laboratory, Sweden
2. Helmholtz Zentrum Berlin, Institute for Solar Fuels, Germany
3. Free University of Berlin, Physics, Germany
4. Helmholtz Zentrum Berlin, Young Investigator Group Oxygen Evolution Mechanism Engineering, Germany

To generate hydrogen ( $\text{H}_2$ ) from water is of great interest in the production of zero-carbon fuels, and can be combined with light-harvesting materials. This however requires efficient catalysts for the anodic half-reaction of water splitting, the oxygen evolution reaction (OER). The interest in transition metal oxides is steadily growing since they can effectively oxidize water at low overpotentials in alkaline electrolyte. An understanding of the electronic and chemical processes at the electrolyte interface of the catalysts is crucial for general strategic design principles. Here we investigate commonly employed transition metal oxides of Ni, Fe, Co, and Mn electrocatalytically. There is a known boosting effect in the bimetallic catalysts, which all exhibit higher turnover rates compared to the monometallic catalysts. We employ in situ X-ray absorption spectroscopy (XAS) at the metal L- and oxygen K-edges to gain information on the mixing between metal 3d states and oxygen 2p states (M-O covalency). This has recently been in focus since redox activity on oxygens (ligand holes) are thought to play an important role. We find that the boosting effect in the bimetallic catalysts can be explained by a low level of M-O covalency, which challenges the emerging rationale that redox-activity on oxygen ligands is a key process for efficient catalysis.

3:30 PM

**(MCARE-026-2021) Layered Double Hydroxides for Oxygen Evolution Reaction in Water Electrolysis (Invited)**S. Chen<sup>\*1</sup>

1. University of Houston, Physics, USA

Hydrogen gas produced by water electrolysis is considered a clean and renewable fuel, especially when the power of electrolyzers is provided by solar and wind energy. To improve the efficiency of water electrolyzers, electrocatalysts are required for both cathodic hydrogen evolution reaction (HER) and anodic oxygen evolution reaction (OER). Owing to a four-electron transfer reaction, OER is more sluggish than HER. Thus the electrocatalysts for OER have attracted intensive research interest. In this presentation, I will focus on layered double hydroxides (LDHs) as a promising OER electrocatalyst, especially self-supported nickel, iron, and cobalt based LDHs. I will present our efforts on fabrication, characterization, and mechanistic understanding of the materials and device performances. For example, our recent B-Co<sub>2</sub>Fe LDH can drive current densities of 10 and 100 mA cm<sup>-2</sup> at overpotentials of 205 and 246 mV, respectively, in 1 M KOH, along with a small Tafel slope of 39.2 mV dec<sup>-1</sup>.

4:00 PM

## (MCARE-027-2021) Cost effective PV-EC system combining NiMP (M = Fe, Mo, Co, V) nanowire and perovskite solar cell

H. Roh\*<sup>1</sup>; K. Yong<sup>1</sup>

1. POSTECH, Republic of Korea

NiMP (Fe, Mo, Co, V) nanowire is fabricated by cation exchange of ZnO nanowire and phosphorization. NiMP retain nanowire structures during synthesis process. NiMP is cheap and sustainable transition metal based electrocatalyst. These catalysts show high hydrogen evolution reaction (HER) and oxygen evolution reaction activity (OER). NiMoP has especially high HER activity as low overpotential because of defect on surface. NiFeP has the best OER activity with low overpotential and high stability. Unassisted PV-EC system is fabricated by combining NiMP nanowire on Ni Foam and 2 series perovskite solar cell. This system can produce hydrogen by 14 % solar to hydrogen (STH) efficiency.

## MCARE S5: Materials for Upconversion, Downconversion / Quantum Cutting, Luminescent Downshifting - II

Session Chair: Jose Marques-Hueso, Heriot-Watt University

1:30 PM

## (MCARE-028-2021) Sol-gel Derived Up-Conversion Materials for Solid State Lighting (Invited)

R. M. Almeida\*<sup>1</sup>

1. Instituto Superior Técnico, Engenharia Química / CQE, Portugal

White light emitting diodes (WLEDs) based on Ln-doped phosphors (phosphor-converted WLEDs) still have efficiency limitations, namely because the Stokes shift from UV/blue LED excitation to the emitted lower frequency visible light converts some of the pump energy into heat. However, if white light generation (WLG) is achieved through IR-pumped UC instead, the cost of the LED lamp will be reduced, while the energy loss from Stokes shift can be minimized and UV/blue light leaks may be avoided. SG synthesis of Ln-doped phosphors both in bulk and film form for UC in Solid State Lighting has been achieved and the different materials have been characterized by XRD, SEM, Ellipsometry, Raman and photoluminescence (PL) spectroscopies. The SG-derived matrix was either aluminosilicate glass, titania or yttrium fluoride. The active Ln elements were Yb (as a sensitizer for 980 nm pump absorption), Er (red and green emitter), Tb (green emitter) and Tm (blue/red emitter), to obtain the right proportions of the three primary colors, based on the CIE chromaticity diagram coordinates. The color temperature and color rendering index have also been calculated. UC assisted by photonic crystals (PCs) like Bragg mirrors or Fabry-Perot microcavities has also been studied and compared with results from reference samples without PC structures.

2:00 PM

## (MCARE-029-2021) Direct Photoluminescence Quantum Yield (PLQY) Measurement with Temperature for Downshifting and Upconversion Using a Modified Integrating Sphere

C. M. Jones\*<sup>1</sup>; N. Panov<sup>2</sup>; A. Zhakeyev<sup>1</sup>; E. Hemmer<sup>2</sup>; J. Marques-Hueso<sup>1</sup>

1. Heriot-Watt University, Institute of Signals, Sensors and Systems (ISSS), United Kingdom
2. University of Ottawa, Department of Chemistry and Biomolecular Science, Canada

Photoluminescent nanothermometers have great application potential due to their thermal sensitivity, size, and non-invasive detection mechanism. However, characterising the photoluminescence quantum yield (PLQY) of these materials with respect to temperature is uncommon due to limited equipment availability. In this

presentation, direct PLQY characterisation data at various temperatures is discussed through the implementation of an affordable integrating sphere modification to give it temperature controlling capabilities. Both downshifting quantum dots and various upconversion materials are studied. Next, the investigation deepens into the influence of effects such as scattering, inner-filter effects, sample geometry, self-absorption, and excitation induced thermal effects, for maximising the PLQY in UC composites. Due to the significance of these effects and the issues they raise around UC PLQY measurements, the reliability of the method is then examined.

2:15 PM

## (MCARE-030-2021) Hyperspectral imaging and optical trapping: Complimentary tools for assessing direction-dependent polarized emission from upconverting microparticles

N. Panov<sup>1</sup>; D. Lu<sup>2</sup>; E. Ortiz-Rivero<sup>2</sup>; E. Martinazzo Rodrigues\*<sup>1</sup>; P. Haro<sup>2</sup>; D. Jaque<sup>2</sup>; E. Hemmer<sup>1</sup>

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada
2. Universidad Autónoma de Madrid (UAM) and Ramon y Cajal Biomedical Research Institute (IRYCIS), Spain

Single-particle fluorescent probes with the capacity to infer specific intracellular conditions, for instance, have great application potential in the realm of biomedicine. Imaging techniques that improve our understanding of the fluorescence processes at a single-particle level are thus instrumental in actualizing this potential. This study demonstrates the importance of implementing synergistic single-particle spectroscopic techniques to gain a more comprehensive understanding of the optical anisotropy exhibited by upconverting LiYF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> microparticles. More specifically, optical trapping and single-particle polarized emission spectroscopy is herein leveraged to provide a plausible explanation for the spatial emission intensity distribution variation exhibited by LiYF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> microparticles during hyperspectral imaging. By probing the polarized emission stemming from a single, optically trapped LiYF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> microparticle, it was possible to find evidence that the emission intensity anisotropy exhibited by the respective microparticles during hyperspectral imaging arises as a consequence of the selection rules governing the emission probability in rare-earth (RE<sup>3+</sup>) ions doped into a uniaxially birefringent host matrix such as LiYF<sub>4</sub>.

2:30 PM

## (MCARE-031-2021) Engineering an Alkaline-earth Host Lattice for Efficient Luminescence at the Single Particle Limit (Invited)

D. F. Swearer\*<sup>1</sup>; S. Fischer<sup>1</sup>; D. Angell<sup>1</sup>; J. Dionne<sup>1</sup>

1. Stanford University, Material Science and Engineering, USA

While the relative energy alignment of 4f orbitals from trivalent lanthanides (Ln<sup>3+</sup>) remains relatively independent of the local environment, the host-lattice into which lanthanides are doped can play an important role in the complex energy-transfer pathways that occur prior to luminescence. Here, we will discuss the synthesis of a family of alkaline-earth rare-earth fluoride host lattices (M<sub>1-x</sub>Ln<sub>x</sub>F<sub>2+x</sub>) and its development as a robust platform for cathodoluminescence (CL) spectroscopy. Using solvothermal decomposition of trifluoroacetate (TFA) precursors in the presence of coordinating solvents allows for the generation of over thirty novel host-lattices. Ten optically unique nanophosphor were characterized with CL spectroscopy at the ensemble and single-particle level within a transmission electron microscope (TEM). Using time-resolved CL capabilities built into a conventional TEM, time-resolved measurements reveal distinctions between CL lifetimes of different lanthanide dopants, as well as individual 4f-4f transitions measured by spectrally filtered CL. Pushing this technique to measure CL lifetimes beyond the ensemble and to the single-particle limit will be a unique tool for measuring the complex energy transfer pathways that exist in lanthanide-doped ceramics and to quantify particle-to-particle variations influenced by small changes induced by the host-lattice.

## MCARE S7: Advanced Materials and Nanodevices for Sustainable and Eco-friendly Applications II

Session Chair: Praveen Sekhar, Washington State University, Vancouver

1:30 PM

### (MCARE-032-2021) Electrochemical process for energy application (Invited)

J. Lim\*<sup>1</sup>

1. Gachon, Republic of Korea

Semiconducting V–VI compounds have many applications such as piezoelectric, thermoelectric, and photovoltaic fields. Electrochemical processes have many advantages including low-cost, rapid deposition rate, and ease of control their microstructure and crystallinity by adjusting electrodeposition parameters. In this work, we demonstrated cost-effective high throughput fabrication of unique hierarchical nanostructures To improve the thermoelectric properties. Bi-Te, Sb-Te, and hybrid organic/inorganic thermoelectric composite were selected as proof of concept materials because they possess unique electrical and thermoelectric properties which lead to many potential applications including thermoelectric and sensors. In addition, we synthesized kerf-less Si solar cell substrate and electrode for high thermal conductive substrate. More details will be presented.

2:00 PM

### (MCARE-033-2021) Photonic multilayer structure induced high near-infrared (NIR) blockage as energy-saving window

J. Kim\*<sup>1</sup>; S. Baek<sup>1</sup>; J. Park<sup>1</sup>; K. Kim<sup>2</sup>; J. Lee<sup>1</sup>

1. Pohang University of Science and Technology (POSTECH), Pohang, Korea, Materials Science and Engineering, Republic of Korea
2. Pusan National University, Busan, Korea (the Republic of), Materials Science and Engineering, Republic of Korea

Blocking near-infrared (NIR) is indispensable for saving energy consumed to maintain an interior temperature in buildings. However, simultaneously enhancing visible transmittance and NIR reflection remains challenging. Here, we demonstrate a TiO<sub>2</sub>/Ag/TiO<sub>2</sub>/SiO<sub>2</sub>/TiO<sub>2</sub> multilayer film on a glass substrate to block the entire NIR (800 ≤ λ ≤ 2500 nm) while maintaining high visible transmittance. We first design and optimize the thickness of a TiO<sub>2</sub>/Ag/TiO<sub>2</sub> structure; the metal layer reflects NIR and the dielectric layers increase visible transmittance with zero reflection condition. To further enhance NIR-blocking efficiency, we implement a TiO<sub>2</sub> back reflector with a SiO<sub>2</sub> spacer to TiO<sub>2</sub>/Ag/TiO<sub>2</sub> structure. TiO<sub>2</sub> layer with high refractive index sandwiched between glass substrate and SiO<sub>2</sub> with low refractive indices can induce additional Fresnel reflection without sacrificing transmittance in visible light. The optimal photonic multilayer film shows solar energy rejection 89.2% (reflection 86.5%, absorption 2.7%) in NIR, visible transmittance 69.9%. Furthermore, the blocking capability in NIR of the designed multilayer film is maintained over a wide range of incident angles of light.

2:15 PM

### (MCARE-034-2021) Robust Heat Resistant Superhydrophobic Coatings fabricated by functionalized Nanoparticles

A. K. Schmidt-Verma\*<sup>1</sup>; T. Fischer<sup>1</sup>; S. Mathur<sup>1</sup>

1. Universität zu Köln, Germany

The technology of superhydrophobic ceramic coatings with self-cleaning properties gained strong attention during recent years, especially for industrial applications. Impurities on treated materials are easier removed compared to untreated materials which leads to reduced maintenance costs and offers a green alternative to the usage of aggressive cleaning agents. In this regard, control over surface properties and chemical structure is mandatory for the development

of new eco- and user-friendly materials. Although the potential of commercial products is immense and their market truly global, the wide range of possible application is limited by the low temperature and mechanical stability of employed coatings. In this work, a route for the preparation of a superhydrophobic coating with mechanical and thermal stability was fabricated on glass substrates by spin-, and spray coating method. The coating was formed in a solution containing various nanoparticles such as SiO<sub>2</sub>, TiO<sub>2</sub> and ZrO<sub>2</sub> and silicic acid, in which the ratio of silicic acid was varied to tune the roughness of the coating. For receiving superhydrophobicity, subsequent and in-situ functionalization with low surface energy material have been performed. After surface functionalization, robust thermally stable films with contact angle close to 180° was preserved even after temperature treatments up to 350 °C and mechanical tests.

2:30 PM

### (MCARE-035-2021) LiTaO<sub>3</sub> Piezoelectric Devices

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

1. University of Cologne, Germany

Electromechanical energy demands on homogenous thick films of piezoceramics with sufficiently large piezoelectric constant and reproducible performance. Single-phase LiTaO<sub>3</sub> films deposited by sol-gel processing have been fabricated as cantilevers to investigate the interdependence of dielectric and piezoelectric properties as a function of film thickness. Phase pure LiTaO<sub>3</sub> films with varying thickness in the range of 2.07-4.37 μm on stainless steel substrates were obtained after calcination of samples at 650°C. Various physical, and chemical properties were evaluated with respect to the thickness of material. As both ferroelectric and piezoelectric properties of LiTaO<sub>3</sub> films are dependent on film thickness, an optimal energy conversion efficiency was obtained for a thickness of ~3 μm. Furthermore, these devices were tested up to a temperature of 150°C for voltage generation. Given the need for lead-free piezoelectric materials for environmental applications, these LiTaO<sub>3</sub> cantilevers are very promising for vibrational energy harvester (VEH) applications primarily due to their cost effectiveness, small size, stability at higher temperatures, and repeatable properties, which makes them suitable for MEMS devices for industrial applications.

2:45 PM

### (MCARE-036-2021) Magnetic Field-Assisted Chemical Vapor Deposition: New Pathways for Functional Materials

D. Stadler<sup>1</sup>; T. Fischer\*<sup>1</sup>; I. Gessner<sup>1</sup>; S. Mathur<sup>1</sup>

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

Temperature is the key parameter for controlling the phase and film morphology during chemical vapor deposition (CVD), since precursor decomposition, growth rate and obtained phases are depending on the very same. Anyhow, far from equilibrium phases and morphologies are not accessible solely by temperature but also by the application of external electric and magnetic fields. While electric fields often result in additional heating of the specimen, static magnetic (DC) fields do not lead to additional temperature gradients inside the samples and thus offer additional control on phase and morphology of the as-obtained films. Here, magnetic field-assisted CVD (mfCVD) will be presented as new tool for the phase selective deposition of (magnetic) transition metal oxides. The field-matter interplay at various temperatures and field strengths will be highlighted for transition metal oxides and their physical, morphological and chemical properties will be discussed. Electron microscopy will demonstrate changes in morphology, while X-ray diffraction and absorption measurements will reveal changes in the obtained phase evolution and chemical surrounding. Electric, magnetic and catalytic property measurements of oxide films formed in different field environments will finally show the potential of mfCVD as additional manufacturing technique for the synthesis of functional materials.

3:00 PM

### (MCARE-037-2021) A Piezo-Triboelectric Hybrid Energy Film Comprised of KNN/PVDF/MWCNT Composites for Energy Harvesting and Sensory Applications

A. Abdullah<sup>2</sup>; M. Sadaf<sup>\*1</sup>; A. Chowdhury<sup>1</sup>; M. Uddin<sup>1</sup>

1. University of Texas Rio Grande Valley, Chemistry, USA
2. University of Texas Rio Grande Valley, Mechanical Engineering, USA

Triboelectric and Piezoelectric materials have been widely used for harvesting mechanical energy from the ambient environment as well as for sensory applications. In this work, a Potassium Sodium Niobate (KNN) based Energy film has been developed for utilizing mechanical energy through triboelectric and piezoelectric mechanisms. The KNN particles were synthesized using wet ball milling technique and incorporated into Poly(vinylidene fluoride) (PVDF) matrix along with Multiwalled Carbon Nanotubes (MWCNT). The film was used to develop a Piezoelectric Nanogenerator (PENG) with Copper electrodes. The piezoelectric output of the film was further tested with Copper electrodes at variable tapping frequencies (1Hz to 4Hz) and pressures (10 to 40psi). The open-circuit voltage increased with the increase of both tapping frequency and pressure. The maximum piezoelectric output voltage was observed to be 26V while the maximum current was noted as 5.8 $\mu$ A. The films also showed unique output signals for different types of finger motions. The film was further utilized to build a Piezo-triboelectric hybrid nanogenerator. This film was integrated with conventional electronic components (bridge rectifiers, resistors, and capacitors), and results showed the potential of the KNN based energy film for force, pressure, and motion sensing as well as energy harvesting.

3:15 PM

### (MCARE-038-2021) Glycothermal synthesis and photoluminescence of Mg-Si modified Ce:YAG nanophosphors

S. Peter<sup>\*1</sup>; M. Fitzpatrick<sup>2</sup>; A. Kitai<sup>1</sup>

1. McMaster University, Engineering Physics, Canada
2. McMaster University, McMaster Analytical X-Ray Diffraction Facility, Canada

The absorption spectrum of Ce in a YAG based host grown using the glycothermal method was modified using the addition of Mg-Si pairs. Photoluminescence intensity was dramatically improved by increasing the reaction temperature to 315 °C instead of the conventionally used 300 °C. It was found that Mg acetate and tetraethylorthosilicate (TEOS) are suitable as precursors for the glycothermal process, as EDS elemental mapping showed their homogeneous inclusion in the final product. Their addition only slightly modified the emission spectrum of Ce:YAG. It was found that increasing the reaction temperature to 315 °C yielded nanoparticles 56  $\pm$  16 nm in size with a 3.3x enhancement in absorption and 3.7x enhancement in emission intensities compared to samples synthesized at 300 °C, and an increase in photoluminescence quantum yield from 32% to 48%. Reaction kinetics of the precursors and a proposed route for post-synthesis surface functionalization are discussed.

## MCARE S16: Solar Energy Harvesting II

Session Chair: Heechae Choi, University of Cologne

1:30 PM

### (MCARE-039-2021) Nanostructured complex oxides by solution chemistry (Invited)

G. Westin<sup>\*1</sup>

1. Uppsala University, Sweden

There is an increasing demand for complex multi-functional materials of high elemental and structural complexity, often hierarchically structured with sizes down to a few nm. These structures also have to be of high quality and be produced at low cost, which means few and fast processing steps why it is anticipated that molecular based solution processes will be the main route for fabrication. Although the last decade has seen a rapid development of solution based processing routes there is still a strong need for new molecular based processes, where there is a strong connection between the target composition and micro-structure and the precursor structure and process steps in-between. By using low temperature synthesis and suitable molecules there are also great possibilities to achieve far from thermodynamically stable doping levels, composites and inorganic materials built with memory of the molecular precursor structures. Here we will describe solution processes to complex oxide, metal, and metal-in-ceramic composites in a wide range of microstructures including thin and ultra-thin films, coatings, nano-powders, and sponges. The processes have been studied with a large range of techniques including; TG, DSC/DTA, XRD, XPS, SEM-EDS, TEM-EDS, and IR and Raman spectroscopy.

2:00 PM

### (MCARE-040-2021) A-site cation engineering in bismuth perovskite-inspired materials for solar cells

F. Uenlue<sup>\*1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Chemistry Department, Germany

Lead halide perovskites have made a huge step towards highly efficient emergent photovoltaic technology with already 25.2% power conversion efficiency. Stability and reproducibility problems are tackled by A-site cation engineering, in which organic and inorganic cations are mixed to obtain tunable, stable and efficient multiple-cation lead halide perovskites ( $A_{1-x}A'_xPbX_{3-2x}X'_2$ ). However, one of the major problems encountered with Pb halide perovskites, apart from structural and chemical stability, is the toxicity associated with heavy metal lead. Potentially less toxic bismuth (Bi) halide perovskites were reported to possess promising optoelectronic properties including a high absorption coefficient and can be processed from solution using a variety of wet chemical deposition techniques and additives. In this work, the A-site cation approach was applied by varying the A-site of the  $A_3Bi_2I_9$  with organic cations like  $CH_3NH_3^+$  (methylammonium, MA),  $CH(NH_2)_2^+$  (formamidinium, FA),  $(CH_3)_2NH_2^+$  (dimethylammonium, DMA), (guanidinium,  $NH_2)_3^+$  (GA), and alkali metal cations for photovoltaic application. Furthermore, double-cation bismuth perovskite-inspired materials based on MA and Cs were fabricated and tested in solar cells. Among all the possible compositions studied,  $Cs^+/MA^+$  double-cation based bismuth perovskite-inspired device shows enhancement in the device power conversion efficiency up to 1.5%.

2:15 PM

**(MCARE-041-2021) Volatile Mono and Di-hydrido Compounds of Aluminium**C. K. Amadi\*<sup>1</sup>; S. Mathur<sup>1</sup>

1. Institute of Inorganic Chemistry, Chemistry, Germany

Aluminum hydrides have found applications as hydrogen storage materials, precursors for chemical vapor deposition, and fundamental applications as catalysts. In this work, two structures of mono  $[\text{AlH}(\text{TfB-TBA})_2]$  and di-hydrido  $[\text{Al}_2\text{H}(\text{TfB-TBA})_2]$  compounds of aluminium has been synthesized and elucidated accordingly. The chemical environment of the compounds were unambiguously established in the solid state by single-crystal x-ray diffraction, showing square pyramidal shape and a dimeric shape respectively. The bond distances between the Al and N atoms suggests that the interaction between Al and N atoms is stronger in the mono-hydride than in the di-hydrido dimeric compound. The presence of the hydrides remains invincible owing to low electron density. The presence of the hydrides were further detected using IR spectroscopy. The sublimation temperatures of the hydrides made them promising and potential single source precursors for  $\text{Al}_2\text{O}_3$ .

2:30 PM

**(MCARE-042-2021) Materials characterization – where modelling meets experiment (Invited)**K. Hermansson\*<sup>1</sup>

1. Uppsala University, Uppsala, Sweden, Department of Chemistry-Angstrom, Sweden

Complex metal oxide materials and their surfaces and interfaces, be they for example catalysts, sensors or solid-electrolyte interfaces in lithium-ion batteries, play crucial roles in our society and in the development of new technologies. For surface and interface systems, new powerful experimental characterization techniques have emerged in the last decades. Despite this progress, the understanding (and thus the tuning) of structure-activity relationships of complex interfaces is still in its infancy. Fortunately, experimental characterisation can receive valuable assistance from computational modelling. Comparison with computer-simulated images and spectra makes it possible to analyse key functions and structural features in detail, e.g. at the electronic or atomistic levels. The overall result is (in good cases) unprecedented information and insight. However there are still many barriers to overcome on the computational side although large breakthroughs have been achieved also here. Mimicking complex “realistic enough” scenarios is a challenging undertaking and the computational scientist needs to make wise and shrewd decisions about both the choices of structural model and computational methods. I will discuss ongoing efforts of our own and in other laboratories concerning the use of computer modelling for the characterisation of complex materials (especially metal oxides).

3:00 PM

**(MCARE-043-2021) Small yet bright lanthanide-based nanoparticles via rapid microwave-assisted synthesis (Invited)**E. Hemmer\*<sup>1</sup>

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

Based on their optical properties, lanthanide-based compounds are suggested for a wide range of applications including biomedicine, optoelectronics, and solar energy conversion. Our favorite nanomaterials are lanthanide-based fluorides ( $\text{MLnF}_6$ , M = alkali metal, Ln = lanthanides + Yttrium), and our research addresses challenges in their synthesis and establishment of structure-property relationships. The growing attention toward such optically active materials has prompted the development of novel synthesis methods for a more reliable and efficient access. In this vein, microwave-assisted routes provide advantages over traditional solvothermal methods,

namely, significantly shorter reaction durations, more rigid reaction conditions, and thus a higher degree of reproducibility. Upon control of multiple physico-chemical reaction parameters – including the choice of precursors, the reaction temperature, and time –  $\text{MLnF}_6$  materials of tailored crystalline phase and size at the sub-10 nm realm can be obtained. Such control is crucial for the understanding of fundamental structure-property relationships and when aiming for the design of next-generation energy converters. For instance, the upconverting properties of the obtained nanomaterials render them suitable energy donors when combined with lanthanide-based complexes acting as energy acceptors.

3:30 PM

**(MCARE-044-2021) Unraveling the role of Sn-segregation on hematite photoelectrodes interfaces for solar water splitting (Invited)**F. L. de Souza\*<sup>1</sup>

1. Federal University of ABC, Center of Natural Science and Humanity, Brazil

The poor electronic conductivity of polycrystalline hematite has been challenging the researchers and prevents its application as a photoanode in a photoelectrochemical cell. The present work showed that the Sn-addition enhances the electronic transport of hematite by reduces the grain boundary block effect. A controlled sintering process allowed us to freeze the state of electronic defects, in which the electrical properties of hematite are governed by the grain boundary and Sn segregation. Electrical measurements showed that the current flows preferentially through the grain boundary with the presence of Sn-segregated. Sn-addition probably leads to a decrease in grain boundary resistance. Atomic force microscopy and electric force microscopy measurements confirm the results of the impedance analysis. These present findings opened a new avenue for comprehending the charge transport mechanism in a polycrystalline oxide-based semiconductor. In fact, the engineering of grain boundaries seems to create a preferential pathway facilitating the electron transport through the material boosting their electronic conductivities. This result will have a direct influence on the sunlight-induced water splitting performance of the hematite photoanode.

**ON-DEMAND POSTERS**

9:00 AM

**(MCARE-ODP001-2021) Understanding the dynamic nature of acid sites on  $\text{TiO}_2$ -supported vanadia catalysts under SCR-relevant conditions**I. Song<sup>1</sup>; D. Kim\*<sup>1</sup>

1. Seoul National University, Republic of Korea

The mechanisms of the selective catalytic reduction (SCR) of  $\text{NO}$  with  $\text{NH}_3$  are under debate, especially in terms of the participation of Brønsted and Lewis acid sites on  $\text{V}_2\text{O}_5/\text{TiO}_2$  catalyst. In this work, the origin and nature of acid sites on  $\text{V}_2\text{O}_5/\text{TiO}_2$  were investigated by using DFT calculations combined with in situ DRIFT experiments. It was found that the Brønsted acidity of vanadia catalyst is related to the charge transfer between  $\text{TiO}_2$  support and  $\text{VO}_x$ , which was considered as an origin of V-OH formation. Computational results showed that  $\text{V}^{5+}$  site can act as weaker Lewis acid sites instead of  $\text{Ti}^{4+}$  site on surface. Furthermore, we elucidated the dynamic nature of transformation between Brønsted and Lewis sites on  $\text{V}_2\text{O}_5/\text{TiO}_2$  occurring in SCR-relevant conditions. The reversible change between the two acid sites occurred not only by hydration in the presence of water but also by changing the redox state of the catalyst. The reducing environment enriched the surface with Lewis sites, while the oxidizing environment gave the catalyst surface more Brønsted sites. As a result, the equilibria between the two acid sites changes sensitively with the reactants contained in the reaction gas.

Our observations highlight the importance of understanding the nature of acid sites and the variability of Brønsted/Lewis acidity in real conditions when measuring rates of SCR reaction.

### (MCARE-ODP002-2021) Structure-Activity Relationship of $\text{VO}_x/\text{TiO}_2$ Catalysts for Mercury Oxidation: A DFT Study

D. Shin<sup>\*1</sup>; W. Yeo<sup>1</sup>; M. Kim<sup>2</sup>; J. Han<sup>1</sup>

1. POSTECH, Republic of Korea
2. Daegu University, Republic of Korea

Elemental mercury ( $\text{Hg}^0$ ), mostly from coal combustion, poses a critical threat to ecosystems and the health of human beings, as it causes several fatal human diseases. Thus, there has been an effort to strengthen regulations around the world. Catalytic oxidation of  $\text{Hg}^0$  into  $\text{HgCl}_2$  is considered an economical and practical option, and selective catalytic reduction catalysts such as titania-supported vanadia ( $\text{VO}_x/\text{TiO}_2$ ) have been shown to also oxidize  $\text{Hg}^0$  to  $\text{Hg}^{2+}$ . Herein, based on density functional theory (DFT) calculations, we demonstrate the relationship between the coordinative environment of V in the  $\text{VO}_x/\text{TiO}_2$  catalyst and the catalytic activity towards  $\text{Hg}^0$  oxidation, as well as the effect of hydroxylation. We mechanistically estimated the  $\text{Hg}^0$  oxidation activity of several  $\text{VO}_x/\text{TiO}_2$  models using previously reported mechanisms. We also explored the temperature (T)- and pressure (p)-dependent thermodynamic stabilities of the  $\text{VO}_x/\text{TiO}_2$  catalyst models by calculating the Gibbs free energy of formation ( $\Delta G^{\text{form}}$ ). Finally, the thermodynamic (T, p) conditions that favor high activity of the  $\text{VO}_x/\text{TiO}_2$  catalyst are suggested.

### (MCARE-ODP003-2021) Challenges with Creating High Capacity Porous $\text{CaFe}_2\text{O}_4$ Anodes

J. Strimaitis<sup>\*1</sup>; S. Danquah<sup>1</sup>; C. Denize<sup>1</sup>; C. E. Bonner<sup>1</sup>; S. Pradhan<sup>1</sup>; M. Bahoura<sup>1</sup>

1. Norfolk State University, USA

Porous  $\text{CaFe}_2\text{O}_4$  (pCFO), an environmentally-friendly conversion-type anodic material, has a low voltage discharge plateau (<1 V vs.  $\text{Li}/\text{Li}^+$ ), strong cyclic stability, and high specific capacities at high rates of charge/discharge (300 – 800 mAh/g from 1000 – 50 mA/g), leaving it well suited to meet the performance demands of next generation lithium-ion batteries (LIBs) and hybrid supercapacitors (HSCs). However, recent attempts at synthesis and electrochemical testing demonstrate that pCFO cannot reach these high specific capacities without appropriate preparation. Common pitfalls, such as poor slurry mixing, lithium metal oxidation, and coin cell orientation, are investigated and ruled out as contributing factors to the low capacities. Analysis with scanning electron microscopy (SEM) suggests, instead, that the fault may lie in the disconnected morphology of pCFO prepared via solution combustion synthesis (SCS) with low levels of fuel. Methods of increasing capacity via direct contact prelithiation, high fuel SCS, or alternative fuel SCS are examined further with promising insights

### (MCARE-ODP004-2021) Improved OMS-2 catalysts for low temperature PM oxidation

M. Kim<sup>\*1</sup>; J. Lee<sup>1</sup>; E. Lee<sup>1</sup>; K. Lee<sup>1</sup>

1. Korea University, Republic of Korea

Petroleum-based vehicles (e.g., diesel, gasoline, NG, LPG) emit various hazardous materials including carbon monoxide (CO), nitric oxide (NO), hydrocarbon (HC), and particulate matter (PM). Accordingly, automobile exhaust regulations have been reinforced to remove the harmfulness of the pollutants in recent years and development of emission purification catalysts which are active in low temperature for high fuel efficiency and low emission vehicle. PM is composed of carbonaceous materials and adsorbed hydrocarbons. Without oxidation catalyst, high ignition temperature is required due to the stable structure of PM compared with CO and hydrocarbon. Especially, low oxidizing agents in gasoline direct injection engine (GDI) resulted in high combustion temperature to

regeneration of PM filter. Hence, PM oxidation catalyst which can generate highly active oxygen species is necessary and cryptomelane-type octahedral molecular sieve (K-OMS-2) can be applied due to high oxygen mobility. In addition, the potassium cation can be substituted with other cations like alkali, transition metal, and noble metal for promoting effect. In this study, various ion doped OMS-2 catalysts were prepared by ion exchange method for soot oxidation. Soot oxidation activities were evaluated and correlated with catalyst characterizations.

### (MCARE-ODP005-2021) Exsolved Metal-Boosted Active Perovskite Oxide Catalyst for Stable Water Gas Shift Reaction

R. Huang<sup>\*1</sup>; C. Lim<sup>1</sup>; M. Jang<sup>1</sup>; J. Hwang<sup>1</sup>; J. Han<sup>1</sup>

1. Pohang University of Science and Technology, Dept. of Chemical Engineering, Republic of Korea

We designed a Ni-exsolved perovskite catalyst for the high-temperature water-gas shift reaction. The perovskite particle has the formula of  $\text{La}_{0.9}\text{Fe}_{0.95}\text{Ni}_{0.05}\text{O}_3$  and has metal nanoparticles (NPs) exsolved on its surface after reduction treatment. XRD, SEM, HR-TEM and XPS analysis were used to confirm the existence of the exsolved Ni metal NPs. This catalyst provided higher CO conversion and H<sub>2</sub> yield, and exceptionally better catalytic stability than the commercial catalyst. Temperature-programmed desorption and reduction measurements revealed the active sites for the enhanced activity. Density functional theory calculations and DRIFT results elucidated the reaction mechanism on this catalyst. We believe that our results can increase the possibility of achieving an effective and economical catalyst for gas-phase reactions.

### (MCARE-ODP006-2021) Metal-organic framework-derived synthesis of $\text{CoS}_x@/\text{NiCo}_2\text{S}_4@/\text{Fe-PPY}$ core-shell nanocages and their application for electrochemical reactions

H. Q. Nguyen<sup>\*1</sup>; J. Kim<sup>1</sup>

1. Kyunghee University, Chemical Engineering, Republic of Korea

Electrochemical separation of water to generate hydrogen from renewable energy sources has been considered a green and efficient strategy for the production of virgin hydrogen. Recently, many MOF-derived functional materials have been reported as electrical catalysts for excessive potential reductions for HER and OER, two of the half-critical reactions to water separation. Herein, we designed a novel yolk shell/conductive polymer consisting of polypyrrole (PPy) and  $\text{Co}_9\text{S}_8@/\text{NiCo}_2\text{S}_4$  formulated through simple hydroxylation and sulfide steps using ZIF-67 as preforming precursors ( $\text{CoS}_x@/\text{NiCo}_2\text{S}_4@/\text{PPy}$ ). Conductive polymers, polypyrrole (PPy) have great potential as catalysts due to their good stability, high electrical conductivity, and abundant nitrogen content and can also be used as a substrate for combining metal catalysts.  $\text{CoS}_x@/\text{NiCo}_2\text{S}_4@/\text{Fe-PPy}$  could be used as electrocatalyst for both OER and HER. To achieve a current density of 10 mA  $\text{cm}^{-2}$ ,  $\text{CoS}_x@/\text{NiCo}_2\text{S}_4@/\text{Fe-PPy}$  only requires a low excess potential of 260 and 240 mV, respectively, for HER and OER. The excellent electrocatalytic activity of  $\text{CoS}_x@/\text{NiCo}_2\text{S}_4@/\text{Fe-PPy}$  can be assigned to a combination of transition metal (Fe, Ni, Co) and heteroatom (N, S) doping and in particular due to polypyrrole's high electrical conductivity.

### (MCARE-ODP007-2021) Boosting the Photocatalytic Hydrogen Production from Glucose Using $\pi$ -conjugated Molecule Capping on Hybrid $\text{CdS-Pt}$ Nanoplatelet

P. Lu<sup>\*1</sup>; D. Lee<sup>1</sup>

1. Korea Advanced Institute of Science and Technology, Republic of Korea

Photocatalytic hydrogen production from biomass, such as glucose, is attracting enormous interest, driven by the promise of addressing both energy supply and storage. Colloidal hybrid nanostructures have been at the forefront of these efforts owing to their light-induced spatial charge separation. The efficiency of the photocatalysts is often limited by the slow hole transfer for subsequent oxidation reactions, ensuing high charge recombination rates. Here we



propose that employing a  $\pi$ -conjugated molecular shell to efficiently relay the hole from the semiconductor to the scavenger leads to a marked increase in the  $H_2$  evolution rate. The efficient hole transfer opens new pathways to improve the oxidation side of photocatalysis.

**(MCARE-ODP008-2021) Synthesis of Fe-N-C electrocatalyst from EDTA-modified zirconium based MOF-808**

Y. Kim<sup>\*1</sup>; K. Im<sup>1</sup>; H. Kwon<sup>2</sup>; J. Kim<sup>1</sup>

1. Kyung Hee university, Republic of Korea
2. Pukyong National University, Republic of Korea

Metal-organic framework (MOF) forms one to three-dimensional crystal structure by strong bonding between metal clusters and organic ligands. MOF is a new class of porous crystalline materials with high crystallinity, micro/mesopores, and a large specific surface area. Zr-MOF-808 is composed of Zr-SBUs connected to six 1,3,5-benzenetricarboxylate (BTC) linkers to form a 3D porous framework containing two different types of pores. These two pores increase mass transfer and can be used well as electrocatalyst support. In this study, we synthesized EDTA-MOF-808 through solvent-assisted linker exchange method. Formate linkers in MOF-808 were exchanged with EDTA ligands by this method. By assuming that all the N atoms come from loaded EDTA molecules, the EDTA content in MOF was estimated to be as high as 33%. EDTA can bind to various heavy metal species. When Fe species were added to EDTA-MOF-808, Fe species and N in EDTA were bonded, resulting in Fe-N-C electrocatalyst after carbonization. This catalyst was characterized by HR FE-SEM, HR TEM, XRD, BET and XPS.

**(MCARE-ODP009-2021) Silver mediated Z-scheme electron transfer in  $MoO_3/C_3N_4$  for efficient visible light photocatalytic degradation of pharmaceutical pollutant ofloxacin**

S. Adhikari<sup>1</sup>; D. Kim<sup>\*1</sup>

1. Chonnam National University, Chemical Engineering, Republic of Korea

Ofloxacin is an emerging pharmaceutical pollutant, which remains quite stable in the released waste-water bodies. These pollutants have potential in exercising biological effects to aquatic organisms affecting both the ecosystem and water system. Photocatalysis has come up as a fast technique in treatment of these waste-water systems through various combinations of nanostructured materials. It is necessary to take action in removal of these harmful pollutants via visible light active nanostructured materials. In this work, a z-scheme structure  $MoO_3/C_3N_4$  is more channelized through deposition of silver for fast and efficient photocatalytic reactions. The combination of different catalysts with favorable band positions enables the catalysts for enhanced generation of redox radicals. The catalysts were designed through simple hydrothermal and metal borohydride reduction process. A detailed photocatalytic studies were performed in pursuit of achieving higher catalysis of ofloxacin under optimum conditions with silver mediated  $MoO_3/C_3N_4$  photocatalyst. Detailed mechanistic studies have also been carried out to deduce the radicals involved in the catalytic process. The presented strategy implies that such designed nanostructure could be exploited in environmental remediation through photochemistry.

**Tuesday, July 20, 2021**

**EHS Plenary**

**EHS Plenary Speaker**

Session Chair: Shashank Priya, Pennsylvania State University

**9:05 AM**

**(EHS-PLN-2021) Thermoelectrics for Distributed Cooling and Energy Harvesting**

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1. Northwestern University, Department of Material Science and Engineering, USA

Thermoelectric semiconductors provide a quiet, refrigerant-free alternative to traditional vapor compression cycles for cooling or energy harvesting. Distributive Cooling using thermoelectrics can heat or cool only where it is needed and when it is needed. Only the uncomfortable occupant needs heating or cooling, not the entire room, vehicle or building. Such a system level efficiency improvement could revolutionize the way we think about HVAC and provide disruptive technologies that make a real difference to global energy use and climate change. Temperature gradients and heat flow are omnipresent in natural and human-made settings and offer the opportunity to scavenge energy from the environment. This talk will also discuss the design principles for thermoelectric generators using an effective thermal conductivity approach. Such design principles provide good estimates of the power that could be produced and the size and complexity of the thermoelectric generator that would be required.

**Poster Session 1A (live presentations) also available in on-demand session**

**10:00 AM**

**(EHS-P-001-2021) Surface modification by dielectric nanosheets for high power lithium micro-batteries**

H. Yim<sup>\*1</sup>; J. Choi<sup>1</sup>

1. Korea Institute of Science and Technology, Republic of Korea

The lithium micro-batteries have been developed for wearable electronics, micro-sensors, and micro-robot because of its great energy output from dense electrode film, small self-discharges, no explosion hazard, and a reduction in the net volume of the devices<sup>1</sup>. However, it is difficult to use for practical application due to the poor electrochemical performance because of the huge charge transfer resistance at the solid electrolyte/electrode interface. Therefore, in order to modify the electrolyte/electrode interface, we deposited  $Sr_2Nb_3O_{10}$  dielectric nanosheets on the electrode surface. We successfully fabricated all-solid-state  $LiNi_{0.5}Mn_{1.5}O_4/Sr_2Nb_3O_{10}$  dielectric nanosheet/LiPON/Li structure batteries using RF magnetron sputtering, Langmuir-blodgett method, and thermal evaporation. The electric dipoles in dielectric layer are arranged and affect to  $Li^+$  ions distribution. Structural properties and electrochemical properties were investigated by XRD, SEM and WBC3000 battery cyclor in voltage range of 3.0 to 4.9 V with different C-rates.

## (EHS-P-002-2021) Porous organic filler for the high-temperature difference of Bi<sub>2</sub>Te<sub>3</sub>-based thermoelectric module

S. Jung<sup>1</sup>; J. Shin<sup>\*1</sup>; S. Lim<sup>1</sup>; B. Kwon<sup>1</sup>; S. Baek<sup>1</sup>; H. Park<sup>1</sup>; H. Song<sup>1</sup>; C. Kang<sup>1</sup>; J. Kim<sup>1</sup>

1. Korea Institute of Science and Technology, Electronic material research center, Republic of Korea

A flexible thermoelectric module has attracted great attention for renewable energy harvesters and electronic coolers. The device performance critically substantially depends on the internal temperature difference between the thermoelectric legs. However, since most of the flexible fillers have high thermal conductivity, the legs surrounded by the pads lose their thermal energies, thereby weakening the thermoelectric performance of the module. Thus, an ideal thermoelectric module requires a thermally insulating filler with flexibility. Herein, we newly designed a flexible module, comprising the porous PDMS (polydimethylsiloxane) filler and Bi<sub>2</sub>Te<sub>3</sub>-based thermoelectric legs. The porous PDMS brought about the relatively low thermal conductivity (0.08 W/m-K) than that of dense PDMS (0.20 W/m-K) for the module so that the internal temperature difference was increased. Additionally, thanks to a novel structural change of the module, the thermoelectric properties were significantly enhanced with high durability; the power density increased by 34% at 8 K of external temperature difference with outstanding figure-of-merit (0.75), compared to those of the PDMS-based flexible generators. Thus, Our approach will be a promising insight to design flexible electronic devices.

## (MCARE-P-003-2021) All-Solid-State Transparent Thin Film Lithium Ion Batteries with LiFePO<sub>4</sub> cathode

Y. Hwang<sup>\*1</sup>; J. Choi<sup>1</sup>

1. Center for Electronic Materials, Korea Institute of Science and Technology, Seoul, Korea (the Republic of), Republic of Korea

Transparent devices have been fabricated for various applications. These transparent electrochemical energy storage devices have attracted extensive attention for the power supply of next-generation. However, the production of transparent batteries is difficult to fabricate since the materials acceptable in Lithium Ion Batteries are not transparent except electrolyte. Therefore, we increased the transparency through patterning. Silicon's high capacity of 3579mAh/g makes it an attractive choice for use as negative electrodes in lithium-ion batteries. However, cathode material LiFePO<sub>4</sub> (LFP) has a large difference in capacity with Si, and if it is made with full cell based on capacity ratio, it will be difficult to operate it. In this study, we have devised a new structure, reducing the gap between Si and LFP to make it possible to operate. Full cell was fabricated with LFP cathode and Si anode, LiPON with radio frequency (RF) sputter. Using ITO/Glass substrate, we created a cell with a total thickness of 1.5μm excluding substrate. The physical properties were analyzed by XRD, SEM. Transparency is measured by UV-Vis spectroscopy. EIS test is taken to check the ionic conductivity of electrolytes. Electrochemical properties of full cell were analyzed by beaker cell test, checking charge/discharge profiles with 100 cycles.

## (MCARE-P-004-2021) Uniform amorphous FePO<sub>4</sub> nanospheres as cathode for sodium ion batteries

L. Zhang<sup>\*1</sup>; K. Kim<sup>1</sup>

1. Pusan National University, Republic of Korea

To feed the increasing demand of large-scale energy storage applications, Sodium ion batteries (LIBs) have attracted increasing interest in the energy storages due to abundant sodium resources. The olivine phase NaFePO<sub>4</sub> as cathode for sodium ion batteries is not stable and cannot be synthesized by conventional synthetic routes due to its thermodynamically instability nature. Therefore, Its analogue FePO<sub>4</sub> becomes a candidate as cathode for sodium ion batteries. Now Uniform amorphous FePO<sub>4</sub> nanospheres were synthesized now through a simple hydrothermal method. X-ray

diffraction (XRD) analyses show that FePO<sub>4</sub> is amorphous phase. And after annealing process in Ar atmosphere, XRD analyses of the sample showed the crystal FePO<sub>4</sub> phase without any impurities or second phases. Scanning electron microscopy (SEM) analyses show that the amorphous FePO<sub>4</sub> nanospheres with the diameter about 220 nm have a good dispersibility and uniformity. Though testing its electrochemical performance tests, the uniform amorphous FePO<sub>4</sub> nanospheres exhibited an outstanding sodium ion storage performance.

## (MCARE-P-005-2021) Effect of upconversion nanoparticles on photocatalytic activity of ZnFe<sub>2</sub>O<sub>4</sub>/TiO<sub>2</sub>

S. Lee<sup>1</sup>; Y. Lim<sup>2</sup>; U. Sim<sup>2</sup>; Y. Park<sup>\*1</sup>

1. Chonnam National University, School of Chemical Engineering, Republic of Korea
2. Chonnam National University, Department of Materials Science & Engineering, Republic of Korea

We designed a novel heterojunction photoelectrode using upconversion nanoparticles (UCNPs) with near-infrared (NIR) light absorption to improve the solar absorption efficiency. UCNPs convert NIR to UV and visible light, which is beneficial for photochemical O<sub>2</sub> evolution in the photoelectrode. We fabricated an UCNP-decorated ZnFe<sub>2</sub>O<sub>4</sub>/TiO<sub>2</sub> photocatalyst (UCNPs-ZFO/TiO<sub>2</sub>) using a two-step process. First, TiO<sub>2</sub> nanopillars were grown on a transparent fluorine-doped tin oxide substrate by a hydrothermal method and, second, ZFO nanoparticles and UCNPs were sequentially drop-cast on the TiO<sub>2</sub> nanopillars. UCNPs-ZFO/TiO<sub>2</sub> exhibits a significantly higher photocurrent density compared with ZFO/TiO<sub>2</sub> and pristine TiO<sub>2</sub>. The applied bias photon-to-current efficiency of UCNPs-ZFO/TiO<sub>2</sub> was calculated to be 4.1 times higher than that of TiO<sub>2</sub>. The UCNPs-ZFO/TiO<sub>2</sub> photoanode also showed the lowest charge transfer resistance and the highest charge density among the four types of tested electrodes. Therefore, the combination of UCNPs and ZFO on the TiO<sub>2</sub> photoanode is an effective strategy to significantly improve photoelectrochemical performance owing to the synergetic utilization of NIR light by UCNPs and visible light by the ZFO nanoparticles.

## (MCARE-P-006-2021) Out-of-plane piezoelectric response of MoS<sub>2</sub> sheets on a flexible plastic substrate by highly controlled chemical vapor deposition

Y. Lim<sup>2</sup>; H. Kim<sup>2</sup>; C. Jeong<sup>\*1</sup>

1. Jeonbuk National University, Division of Advanced Materials Engineering, Department of Energy Storage/Conversion Engineering of Graduate School, Republic of Korea
2. Jeonbuk National University, Department of Energy Storage/Conversion Engineering of Graduate School, Republic of Korea

Two-dimensional (2D) layered materials have unique electromechanical properties in contrast to their bulk materials. Specially, the out-of-plane piezoresponse of 2D layered materials is still veiled according to their properties and mechanisms, while the in-plane piezoelectricity has been well identified. Here, a largearea MoS<sub>2</sub> monolayer was deposited on a SiO<sub>2</sub>/Si substrate by chemical vapor deposition, and subsequently, it was transferred to a flexible plastic substrate. The number of MoS<sub>2</sub> layers (1L, 2L, and 3L) was controlled by the synthesis time (10, 20, and 30 min). The layer number of MoS<sub>2</sub> was identified using Raman and photoluminescence spectra. We observed the surface morphology of the MoS<sub>2</sub> monolayer consisting of both large-corrugated and small-corrugated regions using atomic force microscopic characterization. Piezoresponse force microscopic measurements represented that the out-of-plane surface charge distribution of the MoS<sub>2</sub> monolayer was attributed to the corrugation of the MoS<sub>2</sub> layer. Further, the local piezoresponse of the MoS<sub>2</sub> showed that the out-of-plane piezoelectric effect can be induced by flexoelectric effects. This study shows the possibilities of producing the synthesis and piezoelectricity of largearea 2D materials for piezoelectric applications.

**(MCARE-P-007-2021) The high power density of water droplet-based triboelectric nanogenerator**S. Yun<sup>\*1</sup>; K. Yong<sup>1</sup>

1. POSTECH, Chemical engineering, Republic of Korea

Triboelectric nanogenerator (TENG) is considered a sustainable power source that converts mechanical energy into electric energy. Water droplet-based TENGs (WD-TENGs) harvest energy from triboelectrification between water and solid. This work suggests materials and structures for improving the power density of WD-TENGs. WD-TENG are simple structures in which layers of insulators are placed directly in contact with droplets on the electrodes. We prepared PTFE and PDMS with high electron-withdrawing capability as an insulator layer in various ways. Open-circuit voltage was also measured for structures with free-standing mode and one electrode placed on top of the insulator layer to compare TENG performance. This TENG shows a maximal open-circuit voltage of 30 V per droplet. This work provides a method for optimizing the WD-TENG structure to achieve a higher power density compared to conventional WD-TENGs.

**(MCARE-P-008-2021) Indium phosphide quantum dot-mediated bacterial infection treatment for drug-resistant bacteria inactivation**I. Lee<sup>\*1</sup>; D. Lee<sup>1</sup>

1. Korea Advanced Institute of Science and Technology, Chemical and Biomolecular Engineering, Republic of Korea

Antibiotic-resistant bacterial cell infection is a serious problem in many countries. Reactive oxygen species (ROS), which is toxic to bacterial cells, is one of reactive species responsible for the photoactivity of semiconductor nanoparticles. In this study, we have prepared highly efficient antimicrobial colloidal semiconductor quantum dots (QDs). The bandgap energy of indium phosphide quantum dots (InP QDs) was tuned by quantum confinement effect. The InP QDs were treated to gram positive (drug-resistant *Bacillus cereus* and *Staphylococcus aureus*) and gram negative (drug-resistant *Escherichia coli*) bacteria and the bacterial viability was analyzed to confirm the QD-induced bacterial cell death. The InP QDs efficiently attacked and growth-inhibited the bacterial cell, but had less effect on the mammalian cells (COS-7 and fibroblast). The InP QDs could be used for clinical phototherapy to care the bacterial infections.

**(MCARE-P-009-2021) Photocatalytic Activity of Colloidal Core-Position Controlled CdSe/CdS Nanorods**G. M. Kim<sup>\*1</sup>; D. Lee<sup>1</sup>

1. Korea Advanced Institute of Science and Technology, Chemical and Biomolecular Engineering, Republic of Korea

Colloidal CdSe/CdS dot-in-rod structure, which consists of CdSe core in CdS nanorod, has attracted great attention in the view of photocatalysis because of its advantages, such as size-dependent absorption properties, long exciton lifetime, slow exciton recombination and high photocatalytic activity. However, there are still lack of investigation about dot-in-rod structure effects to photocatalytic activities. Some study shows the effect of CdS nanorod length and CdSe core size to the electronic structure and exciton dynamics and finally photocatalytic activity, but the effect of relative core position parameter in CdS nanorod is still unknown. Recently, our group reported core-position (seed-position) control in CdS nanorods with modifying relative growth rate of each axial direction. In this work, we synthesized core-position controlled CdSe/CdS nanorods and CdS nanorods, and utilized these structures to photocatalytic hydrogen generation reaction. Results showed that as relative core position moved toward CdS nanorod center, photocatalytic activity increased.

**Poster Session 1B (live presentations) also available in on-demand session**

10:30 AM

**(MCARE-P-010-2021) NiSb nanoparticles anchored in 3D carbon nanosheet networks for advanced Lithium-ion battery**L. Yu<sup>\*1</sup>

1. Pusan National University, Republic of Korea

The 3D carbon networks with hollow structure and high surface area have attracted tremendous attention on advanced energy materials. Herein we successfully designed and synthesized the NiSb alloy nanoparticles anchored in 3D carbon nanosheet networks (NiSb@3DCNNs) by a facile galvanic replacement reaction. By a simple annealed treatment, the macromolecule organic polyvinyl pyrrolidone was chosen as the carbon source and self-assembled the 3D nanosheet networks via an improved metal nitrate-assisted polymer-blowing process. The electroactive NiSb alloy nanoparticles anchored in carbon networks inheriting the super advantages of hollow structure stability, high surface area and excellent electrical conductivities which could contribute to endow abundant active sites for Li<sup>+</sup>, decrease the pathway for fast ion diffusion and synthesized the stable SEI film on the outside carbon nanosheets. Accordingly, NiSb@3DCNNs perform outstanding electrochemical performance including large specific capacity (659.5 mA h g<sup>-1</sup>), remarkable rate capability (656.9, 593.4, 526.4, 468.6, 428.9 and 385 mA h g<sup>-1</sup> at 50, 100, 200, 500, 1000 and 2000 mA g<sup>-1</sup>, respectively) and long cycle life (222.1 mA h g<sup>-1</sup> after long 2500 cycles at 2000 mA g<sup>-1</sup>) as Lithium-ion battery anodes.

**(MCARE-P-012-2021) The electro-catalyst composed with N-doping CNT and Bismuth Oxide for Nitrogen fixation**C. Lim<sup>\*1</sup>; K. Yong<sup>1</sup>; Y. Jeung<sup>1</sup>

1. POSTECH, Republic of Korea

Ammonia has received a lot of attention as a raw material for artificial fertilizers and fine chemicals, and in recent years, it has become more important as the possibility of using it as a hydrogen storage and carrier. However, the Haber-Bosch process, a representative method of producing ammonia, has problems of requiring large energy due to its high temperature and high pressure process and emitting large amount of carbon dioxide due to the usage of high purity hydrogen. To overcome these issues, the electrochemical nitrogen reduction process has great attention because it is eco-friendly and requires less energy compared to the Haber-Bosch process. In this study, an electrocatalyst composed of carbon nanotube (CNT) and bismuth oxide was developed to increase the efficiency of such electrochemical nitrogen reduction catalysts. We can synthesize CNT by annealing melamine and deposit bismuth oxide on the CNT by electrodeposition method. The synthesized nitrogen reduction reaction catalyst has high selectivity and high productivity.

**(MCARE-P-015-2021) Synthesis and characterization of HKUST-1 derived from hollow Cu<sub>2</sub>O**Y. Lee<sup>\*1</sup>, K. Im<sup>1</sup>, J. Kim<sup>1</sup>

1. Kyung Hee University, Chemical Engineering, Republic of Korea

Nanomaterials are still receiving a lot of attention due to their excellent properties and various applications. Among them, metal-organic framework (MOF) can be applied in various ways such as gas separation, storage, and catalysis. In this work, we synthesized hollow Cu<sub>2</sub>O, followed by conversion to HKUST-1 in organic linker solution, maintaining the hollow structure. As a result, the HKUST-1 was formed in a spherical structure. Then, the HKUST-1 particles were characterized by XRD, FE-SEM, and BET.

### (MCARE-P-017-2021) Synthesis of Mo & Ru doped Zr-MOF(UiO-67) as stable and efficient electrocatalyst support for electrochemical reactions

Y. Koo<sup>\*1</sup>, K. Im<sup>1</sup>, J. Kim<sup>1</sup>

1. Kyunghee University, Chemical Engineering, Republic of Korea

Development of highly active and durable electrocatalysts for efficient oxygen evolution reaction (OER) or Hydrogen evolution reaction (HER) in acidic media remains important challenge for high-performance electrochemical conversion and storage applications such as fuel cells and metal-air batteries. Doping with a transition metal was recently shown to greatly boost the activity and durability of Ru based electrocatalysts for the OER or HER. Molybdenum phosphide exhibits high activity towards the HER in both acid and alkaline media even in bulk form. UiO-67 is a Zr-based MOF which can provide the oxygen-vacancy required for the reverse water gas shift reaction and can be used as a support for highly dispersed nanostructured catalysts to prevent nanoparticles from sintering and aggregation at high temperature, maintaining its catalytic activity. In this study, we synthesized Mo doped UiO-67 using microwave-assisted synthesis method as efficient and stable electrocatalyst support, followed by Ru impregnation for HER or OER. The synthesized catalysts were analyzed by BET, XRD, FE-SEM and electrochemical experiment.

### (MCARE-P-018-2021) Design of an Ultrastable and Highly Active Ceria Catalyst for CO Oxidation by Rare-Earth- and Transition-Metal Co-Doping

H. Kim<sup>\*1</sup>; D. Shin<sup>1</sup>; J. Han<sup>1</sup>

1. Pohang University of Science and Technology (POSTECH), Department of Chemical Engineering, Republic of Korea

Developing a catalyst that can be applied to various applications requires excellent stability beyond simply high activity. To satisfy these needs, a co-doping was introduced to enhance the intrinsic effects of the catalyst, and a model system of CO oxidation was used to validate the fundamental properties. We selected CeO<sub>2</sub> with high oxygen storage capacity (OSC), and the goal was achieved by the co-incorporation of rare earth metal (RE) and transition metal (TM). The role of RE dopant in (RE, Cu)-DC was demonstrated to stabilize the catalyst surface, and TM dopant induced an increase in defect concentration by low vacancy formation energy ( $E_{vf}$ ). Resultingly, despite the harsh condition for ~700 h (1 cycle: 900 °C, 24 h → cooling at room temperature → target °C, 24 h), the (RE, Cu)-DC proved a strong resistance to deactivation. Also, the catalyst had improved activity at low temperatures. This approach of ultra-stable catalyst will be able to overcome the problems facing deactivation in a variety of applications.

## Poster Session 1C (live presentations) also available in on-demand session

11:00 AM

### (MCARE-P-020-2021) HC trap with Cu-ZSM-5 and correlation between Cu ions and hydrocarbon adsorption properties

J. Kim<sup>\*1</sup>

1. Korea University, Chemical and Biological Engineering, Republic of Korea

Various wt.% of Cu were impregnated on commercial ZSM-5 (Si/Al ratio of 11.5). And resulted Cu-ZSM-5 were applied to CST (cold-start test) as a HC (hydrocarbon) trap which is complement of TWC (three-way catalyst) in gasoline automobile at low temperature exhaust gas. In CST, the resulting Cu-ZSM-5 could not only adsorb propene and toluene in the exit gas stream with 10 vol.% of water vapor, but also act as an active oxidizer of propene and toluene. Furthermore, we could find the optimal amount of

Cu wt.% at Cu-ZSM-5 for the most effective HC trap. To illuminate the relationship between Cu ions and hydrocarbon adsorption properties of Cu-ZSM-5 in CST performances, we conducted H<sub>2</sub>-TPR, CO-adsorbed FT-IR, and NO adsorbed FT-IR measurements. From H<sub>2</sub>-TPR results, each of Cu<sup>+</sup>, Cu<sup>2+</sup>, and CuO was quantified. Additionally, each of CO-adsorbed and NO-adsorbed FT-IR spectra results show relative amount of Cu<sup>+</sup> ions and relative amount of Cu<sup>+</sup>, Cu<sup>2+</sup>, and CuO in Cu-ZSM-5 samples, respectively. With these experiment results and propene adsorption properties from CST, we could find proportional relationship between relative quantity of Cu<sup>+</sup> and amount of adsorbed propene on Cu-ZSM-5.

### (MCARE-P-024-2021) Particle dynamics in coating and drying processes for bidisperse particulate suspension systems

B. Chun<sup>1</sup>; J. Park<sup>1</sup>; J. Yun<sup>1</sup>; H. Jung<sup>\*1</sup>

1. Korea University, Chemical and Biological Engineering, Republic of Korea

Functional liquids used in coating industries are often polydispersed particulate suspensions to make the coating products with demanded characteristics such as wear resistance, optical properties, thermal and electrical conductivities, and catalytic performance. Evenly distributed particles in the coating films or substrates are mostly desirable. However, such situation cannot be not always achievable even though well-dispersed raw materials are supplied. In coating processes, for instance, the inhomogeneity in particle distribution can be encountered inside the narrow slit channel flow at high shear rate regime and in drying operation at relatively high Peclet number. We have numerically studied the migration and segregation phenomena of bimodal spherical particles suspended in a Newtonian simple shear flow, employing the mesoscale lattice Boltzmann method (LBM). Also, transient development of concentration of bimodal colloids during vertical drying, whether small-on-top or large-on-top depending on drying conditions, has been elucidated using the fluctuating LBM with thermal fluctuation and hydrodynamic interaction.

### (MCARE-P-025-2021) Development of non-precious metal passive NO<sub>x</sub> adsorber based on layered double hydroxides

Y. Choi<sup>\*1</sup>; K. Lee<sup>1</sup>

1. Korea university, Department of Chemical and Biological Engineering, Republic of Korea

Nitrogen oxides (NO<sub>x</sub>) can cause serious environmental issues and human diseases, thus the regulations of NO<sub>x</sub> emission from vehicles have been tightened. Selective catalytic reduction with ammonia (NH<sub>3</sub>-SCR) has been used for vehicle NO<sub>x</sub> reduction system. However, current SCR system is not efficient for NO<sub>x</sub> removal during 'cold-start' period due to the decreased catalytic activity of SCR catalyst and kinetic limitation of urea decomposition into NH<sub>3</sub> at low temperatures. In this regard, passive NO<sub>x</sub> adsorber (PNA) was suggested as supplementary low-temperature deNO<sub>x</sub> technology. PNA temporarily stores NO<sub>x</sub> at low temperatures and releases the adsorbed NO<sub>x</sub> once the exhaust temperature reaches the operating temperature (200 °C). Subsequently, released NO<sub>x</sub> is reduced in downstream NH<sub>3</sub>-SCR system to achieve high NO<sub>x</sub> removal efficiency. Most of PNA materials are based on precious metal (Pt, Pd or Ag) on amorphous oxides supports or crystalline zeolites. In this study, new type of PNA material based on layered double hydroxides (LDHs) was developed. Mixed metal oxides from LDHs exhibited high NO<sub>x</sub> storage performance, and also efficiently released the adsorbed NO<sub>x</sub> as soon as the temperature reached 200 °C. Furthermore, NO<sub>x</sub> adsorption and desorption behaviors of the developed LDHs-based PNA material were investigated under various conditions to ensure that it could be applied in vehicle exhaust system.

### (MCARE-P-026-2021) Enhanced oxygen transport by PVPA contents at cathode of the high temperature proton exchange membrane fuel cells

E. Lee<sup>1</sup>; D. Kim<sup>1</sup>; C. Pak<sup>\*1</sup>

1. Gwangju Institute of Science and Technology, Republic of Korea

Polyvinylphosphonic acid (PVPA) is polymeric acid that is reported to form hydrogen networks with phosphoric acid groups and provide proton pathways, and it bounds to polybenzimidazol (PBI) via multipoint acid-base reactions. It was found that the hydrogen bonding network of PVPA was sufficient to carry proton via the Grötthuss mechanism. In this study, the PVPA is impregnated onto the catalyst layer instead of phosphate to enhance the MEA performance. Cathode gas diffusion electrodes (GDEs) was made by a bar coating method. PVPA solution was sprayed on the cathode GDE and the amount of coated PVPA was 0.5, 1.0, 2.0 and 3.0 mg/cm<sup>2</sup>, respectively. The PVPA content was required for reaching a satisfactory performance. When the loading of PVPA was 1 mg/cm<sup>2</sup>, it had the highest peak power density and the lowest R<sub>ct</sub> value. The PVPA enhanced the proton conductivity but high PVPA contents covered Pt surfaces, which made the triple phase boundary reduced. The comparison with the MEA using the GDE coated by phosphoric acid and nothing. The MEA using PVPA coated GDE had higher performance and lower R<sub>ct</sub> value than using phosphoric acid. Adding phosphoric acid increased amount of free phosphoric acid in electrode and then it interrupted the pores which were used by oxygen pathways. However, adding PVPA reduced free phosphoric acid and thus the oxygen mass transports enhanced.

### (MCARE-P-027-2021) Enhancement of catalytic activity and operation durability of biocatalyst by using thiol-maleimide cross linking bond

Y. Chung<sup>\*1</sup>; H. Jeon<sup>1</sup>; J. Ji<sup>2</sup>; H. An<sup>1</sup>; Y. Kwon<sup>2</sup>

1. Korea National University of Transportation, Department of Chemical and Biological Engineering, Republic of Korea
2. Seoul National University of Science and Technology, Department of Chemical and Biomolecular Engineering, Republic of Korea

Hydrophilic cross linking bond using thiol-maleimide conjugation is introduced to produce an aggregate to enhance the activity and durability of glucose oxidase (GOx) based biocatalyst. 1,8-Bismaleimido-diethyleneglycol (BMPEG) is adopted to use as an alternative to *γ*-glutaraldehyde (GA), which can reduce catalytic activity of GOx. The catalyst using BMPEG based enzyme aggregate ([RGO/FePc]/[GOx-BMPEG]) showed high sensitivity (62.4 μW mM<sup>-1</sup> cm<sup>-2</sup>) and long duration, though the immobilized amount of enzyme was around half that on GA used ([RGO/FePc]/[GOx-GA]). This phenomenon was caused by the hydrophilicity of the BMPEG based bridges, which improve the mass transfer of glucose substrate that is generally hindered by hydrophobic bridges when using GA, and the protection of the thiol end groups near FAD (flavin adenine dinucleotide) of GOx by the thiol-maleimide reaction of BMPEG. Thus, enzyme aggregate using GOx-BMPEG is a superior alternative to conventional cross linking method (GOx-GA) for use in implantable bioelectronics such as biofuel cell and biosensor. This work was supported by grant from the academic research program of Korea National University of Transportation (KNUT) in 2020.

### (MCARE-P-028-2021) Fabrication of Transdermal Delivery Enhanced Nanofiber patch (PMSEA-SA/PCL-MTA) for Wound Dressing

S. H. Choi<sup>\*1</sup>; S. Hong<sup>1</sup>; K. Yoon<sup>1</sup>

1. Hannam University, Chemistry, Republic of Korea

Dimethyl sulfoxide (DMSO) was one of the important solvents in biological and as medicine for transdermal delivery enhancers. PolyDMSO has inspired by the good biological properties of DMSO, like a highly hydrophilic, and good transdermal delivery. Sodium alginate (SA) of linear polysaccharide was widely used for biological

application fields because of specific properties such as biocompatible, biodegradability, and non-toxicity. We study has focused on delivery enhancers and antimicrobial properties of fabricated nanofiber patch. First, poly(2-(methylsulfinyl)ethyl acrylate)/sodium alginate (PMSEA/SA) nanofibers predicted transdermal delivery enhanced properties because PMSEA was analogs of DMSO properties. Second, the poly( $\epsilon$ -caprolactone)/[2-(methacryloyloxy)ethyl] trimethylammonium (PCL/MTA) nanofibers expected to protect the wound site against external infection. Finally, transdermal delivery enhanced nanofibers (PMSEA-SA/PCL-MTA) were confirmed mechanical tests, Fourier-transform infrared spectroscopy (FT-IR), <sup>1</sup>H Nuclear Magnetic Resonance (<sup>1</sup>H-NMR), Field-emission Scanning Electron Microscopy (FE-SEM), water contact angle, Differential Scanning Calorimetry (DSC), Thermogravimetric analysis (TGA), and antimicrobial test.

### (MCARE-P-029-2021) Bimetallic metal organic frameworks mediated loading of Co and Fe catalysts on In<sub>2</sub>O<sub>3</sub> nanofibers: Design of highly sensitive ethanol sensors

S. Lee<sup>\*1</sup>; T. Kim<sup>1</sup>; Y. Jo<sup>1</sup>; K. Kim<sup>1</sup>; J. Lee<sup>1</sup>

1. Korea University, Republic of Korea

The metal oxide catalysts have been loaded on the oxide chemiresistors to enhance the response, selectivity, and responding/recovering speeds. When two or more different nano-catalysts are co-loaded on the sensing materials in order to achieve synergistic catalytic promotion, the uniform mixing and distribution of catalysts are difficult since the nanoparticles tend to agglomerate. Herein, we used bimetallic zeolitic imidazolate frameworks as the template to load two different catalytic materials on sensing materials uniformly. For this, In/PVP solution containing Co, Fe bimetallic zeolitic imidazolate were electrospun, then heat-treated to synthesize Co<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub>-loaded In<sub>2</sub>O<sub>3</sub> nanofibers. The gas characteristics of synthesized nanofibers were evaluated toward 5 ppm of ethanol, p-xylene, toluene, benzene CO and H<sub>2</sub> at 250 – 400 °C. The Co<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub>-loaded In<sub>2</sub>O<sub>3</sub> nanofibers showed ultra-high response (resistance ratio - 1 = 210) to 5 ppm ethanol at 250 °C. Furthermore, the synthesized nanofibers exhibited high selectivity toward ethanol at 250 °C over other interference gases. The enhanced gas characteristics of Co<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub>-loaded In<sub>2</sub>O<sub>3</sub> nanofibers were discussed in association with synergistic catalytic effect of Co<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub> and the electronic sensitization due to the formation of heterojunction between p-(Co<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub>) and n-(In<sub>2</sub>O<sub>3</sub>).

### EHS S4: Thermoelectric Energy Harvesting I (Joint with MCARE Symp 3)

Session Chair: Bed Poudel, Pennsylvania State University

12:30 PM

#### (EHS-005-2021) High Power Factor Versus High zT in Thermoelectric Materials and Generators (Invited)

A. Feldhoff<sup>\*1</sup>; M. Wolf<sup>1</sup>; R. Hinterding<sup>1</sup>

1. Leibniz University Hannover, Institute of Physical Chemistry and Electrochemistry, Germany

Starting with a simple transport equation for entropy and electrical charge, the power conversion and its efficiency are deduced for a single thermoelectric material apart from a device. The material's performance is discussed on the material's voltage-electrical current curve, which is presented in a generalized manner by relating it to the electrically open-circuited voltage and the electrically closed-circuited electrical current. Particular working points on the material's voltage-electrical current curve are deduced. It is shown that optimizing a thermoelectric material in generator mode for maximum electrical power output - based on the power factor - or optimizing it for maximum efficiency - based on the figure-of-merit - are different tasks. A similar behavior of a deviation between

maximum efficiency and maximum electrical power output can be found for the optimization of thermoelectric generators. Here, the vast number of various material classes makes it difficult to maintain an overview of the best candidates for a specific task. For this purpose, Ioffe plots are revitalized, which facilitate the clear comparison of thermoelectric properties of different materials to either access high electrical power output or high conversion efficiency.

**1:00 PM**

### **(EHS-006-2021) Enhancement of thermoelectric performance in non-toxic CuInTe<sub>2</sub>/SnTe coated grain nanocomposite**

J. Hwang<sup>\*1</sup>; M. Lee<sup>1</sup>; M. Han<sup>1</sup>; S. Kim<sup>1</sup>; S. Kim<sup>1</sup>

1. Ewha Womans university, Chemistry, Republic of Korea

Coated grain nanostructure has significant advantages for thermoelectricity because of energy filtering and effective coherent phonon scattering by coated grain boundary. Coated grain nanocomposites consist of CuInTe<sub>2</sub>/SnTe with eco-friendly coating layer of CuInTe<sub>2</sub> covering the grain of SnTe matrix. The coated grain nanostructure was synthesized using the cation exchange process on SnTe particles. For the effective coating agent we considered following factors: the hard soft acid base (HSAB) concept, the thermodynamic factor, and crystal structure similarity. The Seebeck coefficient was increased by 40% due to energy filtering through CuInTe<sub>2</sub> coating layer. The coherent phonon scattering by coating layer effectively reduces the lattice thermal conductivity to almost the minimum value. The thermoelectric figure of merit ( $zT$ ) for the CuInTe<sub>2</sub>/SnTe nanocomposite was 1.68 at 823 K, which is significant high value for bulk eco-friendly thermoelectric materials. The average  $zT$  of 0.76 in wide temperature range from 373 K to 823 K was recorded, which is beneficial advantage for practical application.

**1:15 PM**

### **(EHS-007-2021) Thermoelectric Cooling Technology in Electronics Heat Management**

B. Poudel<sup>\*1</sup>; A. Nozariasbmarz<sup>2</sup>; W. Li<sup>1</sup>; H. Kang<sup>1</sup>; H. Zhu<sup>1</sup>; S. Priya<sup>1</sup>

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

Thermoelectric coolers are solid state heat pumps moving heat energy by applying electric current. These devices can be used in electronic components cooling to maintain a safe operation temperature thereby extending the lifetime and performance reliability of such components. This cooling technology has also attracted lots of interest where temperature stabilization or cooling the electronics components to below ambient temperature is required such as Laser diodes or IR detectors. In this work, we will discuss desired materials characteristics and device design that impacts the cooling performance significantly instead of the traditionally used commercial materials and modules. We will further discuss the comparison of passive cooling such as heat pipes and heat sinks with the active cooling technology such as thermoelectric cooling to understand the suitability of each technology in particular applications. This work aims at providing comprehensive review and recommendation of materials and device technology for viable electronic cooling solution.

**1:30 PM**

### **(EHS-008-2021) Bismuth Telluride/half-Heusler Segmented Thermoelectric Modules Provide Record 12% Conversion Efficiency**

W. Li<sup>\*1</sup>; B. Poudel<sup>1</sup>; R. Sriramdas<sup>1</sup>; A. Nozariasbmarz<sup>1</sup>; S. Priya<sup>1</sup>

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

The rapid enhancement of the thermoelectric (TE) figure-of-merit ( $zT$ ) in the past decade has opened the opportunity for developing and transitioning solid state waste heat recovery systems. Here a novel TE device architecture is demonstrated in conjunction with heterogeneous material integration that results in record

module-level conversion efficiency of 12% under a temperature gradient of  $\sim 584$  K. This breakthrough is result of success in fabricating bismuth telluride/half-Heusler segmented TE modules using the "Hot-to-Cold" fabrication technique that provides significantly reduced electrical and thermal contact resistances. Extensive analytical and finite element modeling is conducted to provide understanding of the nature of thermal transport and contributions arising from various thermal and physical parameters. Bismuth telluride/half-Heusler based segmented thermoelectric generators (TEGs) can provide higher practical temperature gradient with optimum average  $zT$  across the whole operating range. We believe these results will have immediate impact on the design and development of TEGs and in general design of devices based upon heterostructures that take advantage of gradient in the figure of merit.

**1:45 PM**

### **(EHS-009-2021) High Performance Thermoelectric Modules for Smart Buildings Sensors**

A. Nozariasbmarz<sup>\*1</sup>; B. Poudel<sup>1</sup>; W. Li<sup>1</sup>; H. Kang<sup>1</sup>; H. Zhu<sup>1</sup>; S. Priya<sup>1</sup>

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

Future smart buildings require new technologies that enable to recover wasted energies. Thermoelectrics are environmentally friendly devices that can directly convert heat into electricity and vice versa. Thermoelectric generators and coolers are reliable technologies for waste heat recovery and cooling applications, respectively. Their different applications require specific materials, module and system design to provide the best performance. The external thermal resistance and boundary conditions influence the performance of the thermoelectric devices. Commercial thermoelectric modules are not designed for specific applications when the thermal resistance of the heat source or sink is high such as hot-water pipes and wearables. In this research, we provide fundamental insight on the operation of thermoelectric modules suitable for field deployments by illustrating the combinatory effect of thermoelectric material properties, device boundary conditions, and environmental thermal resistance to achieve the highest performance in such environment. For this goal, we designed and fabricated different thermoelectric modules and tested them under real application condition.

### **EHS S4: Thermoelectric Energy Harvesting II (Joint with MCARE Symp 3)**

Session Chair: Wenjie Li, The Pennsylvania State University

**2:45 PM**

### **(EHS-012-2021) Distributed Transport Properties: Expanded Seebeck Coefficient Range Enables Thermoelectrics With Superior Performance Without Higher ZT Materials (Invited)**

D. Crane<sup>\*1</sup>; B. Madigan<sup>1</sup>; L. Bell<sup>1</sup>

1. DTP Thermoelectrics, LLC, USA

Performance and governing equations of thermoelectric (TE) systems incorporating material with distributed transport properties (DTP) is presented. With the further development of semiconductor production processes, material construction with controlled spatially dependent transport properties (Seebeck coefficient, electrical conductivity and thermal conductivity) has become more commercially feasible. Using numerical analysis and temperature dependent material properties for bismuth telluride, our study demonstrates the feasibility of creating a single-stage TE device operating in cooling mode with a maximum temperature differential exceeding 100C at a 300K hot side temperature, exceeding the state-of-the-art by more than 35%. The enabling technology is the optimization of transport property distribution within the TE legs, including TE material with Seebeck coefficient  $\geq 300 \mu\text{V/K}$  at 300K used at the hot end and  $\leq 180 \mu\text{V/K}$  at 300K used at the cold end of the TE element. We project that coefficient of performance (COP) and cooling power

increase greater than 40% and 100% respectively at high temperature differentials. We will also show that such TE devices will have superior performance under all operating conditions (both nominal and off-nominal) and can require less TE material compared to conventional TE devices.

**3:15 PM**

**(EHS-013-2021) High temperature performance of All-Oxide 2D Layered Thermoelectric Device Fabricated by Plasma Spray**

F. R. Caliarì<sup>\*1</sup>, S. Sampath<sup>1</sup>

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

Harvesting waste energy using thermoelectric (TE) technology increases overall power conversion and efficiency from combustion-based energy generation systems. However, design restrictions of commercially available thermoelectric devices and toxicity of commercial thermoelectric materials currently limit large-scale deployment. Additive and multilayered design and manufacturing of thermoelectric modules are a potential pathway to overcome current design restrictions as it enables to implement the device directly to the engineering structures with direct access to waste heat. Plasma spray is the chosen technology in this work to fabricate such patterned and layered TE devices, using as p-type  $\text{Ca}_2\text{Co}_2\text{O}_5$  and the surrogate n-type material  $\text{La}(\text{Sr})\text{MnO}_3$ . Specially designed uncouple TE devices were tested at 1000°C, owing the high temperature capability of such oxides.

**3:30 PM**

**(EHS-014-2021) Thermoelectric System Economics - The Apex: New Paradigms in Manufacturing and Interface Performance Driving System Cost Optimizations (Invited)**

T. J. Hendricks<sup>\*1</sup>

1. NASA-Jet Propulsion Laboratory/California Institute of Technology, Propulsion, Thermal, & Materials Engineering, USA

Recent research in thermoelectric system economics (TSE) has revealed new integrated cost-performance relationships elucidating new cost optimization design paradigms for thermoelectric (TE) systems. New cost-performance relationships show critical tradeoffs between key TEG component costs (heat exchangers, TE materials and manufacturing costs) and performance, and allow one to differentiate competing cost and performance effects. New design paradigms and relationships demonstrate a holistic approach enhancing understanding of crucial interrelationships between component costs, TE design parameters and material properties, heat exchanger design parameters, and interface heat flux in minimizing TEG system costs. New work extends the integrated cost-performance analysis to include critical thermal and electrical interface contact resistance effects into key relationships, extends insight into the effects of manufacturing cost-sensitivities on TE element design, and provides broader insight into cost-optimized TE design to expand new TSE paradigms. We will discuss optimized TE element design for minimizing TEG cost and design guidelines associated with thermal and electrical contact resistance effects and TE manufacturing sensitivities. Key non-dimensional design parameters will be presented showing critical design-driving interdependencies.

**4:00 PM**

**(EHS-015-2021) High performance thermoelectric device fabrication and their stability**

B. Poudel<sup>\*1</sup>, A. Nozariasbmarz<sup>1</sup>; W. Li<sup>1</sup>; S. Priya<sup>1</sup>

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

Thermoelectric generators (TEGs), which are solid state devices converting thermal energy into electrical energy, are promising solution for waste heat recovery. However, there are challenges to realize them in economically viable way such as low conversion efficiency,

lack of reliable high temperature device fabrication process and long-term stability. In order to realize an efficient and reliable thermoelectric power generation, it is critical that in conjunction with high TE materials figure of merit,  $zT$ , there is also a reliable TE module fabrication process. In this presentation, we will discuss the important considerations and techniques that have been successfully applied in reliable and efficient module fabrication. We will discuss the TEG fabrication process that results in low thermal and electrical contact resistances between metal electrodes and TE legs that are compatible to high application temperatures, 600 degrees Celcius. The fabrication approach is demonstrated in Bismuth Tellurides and half-Heusler TE materials systems. High temperature brazing material is used as a filler that enables direct bonding of TE legs to the copper electrode without metallizing legs in half-Heusler TE materials. These results are highly promising for advancing the TE modules in waste heat recovery applications.

**4:15 PM**

**(EHS-017-2021) Oxidation Resistance of Half-Heusler Alloys for High Temperature Sustainable Thermoelectric Generators in Air**

H. Kang<sup>\*1</sup>; U. Saparamadu<sup>1</sup>; A. Nozariasbmarz<sup>1</sup>; W. Li<sup>1</sup>; B. Poudel<sup>1</sup>; H. Zhu<sup>1</sup>; S. Priya<sup>1</sup>

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

Thermoelectric (TE) energy harvesting is one of the rapidly growing fields to enable us to utilize a tremendous amount of wasted heat energy. Half-Heusler (hH) alloy is one of the leading TE materials for medium to high temperature applications as it exhibits high TE performance and good mechanical strength at the temperature as high as 973 K. The oxidation resistance of the TE materials is a critical factor in implementing practical applications for extreme environments without a vacuum sealing. Here, the most promising and well-developed hH alloys of  $\text{MNiSn}$ ,  $\text{MCoSb}$ , and  $\text{NbFeSb}$  system ( $M = \text{Hf, Zr, and Ti}$ ) have been studied to figure out their potential for high temperature thermoelectric generator (TEG) application in air. The n-type  $\text{MNiSn}$  and p-type  $\text{NbFeSb}$  compounds are found to show excellent oxidation resistance at a high temperature of 873 K for 72 hours, whereas  $\text{MCoSb}$  compounds do not exhibit a similar level of stability. The oxidation-resistance is derived from the presence of the intermetallic Ni-Sn layer for  $\text{MNiSn}$  and Nb-TiO<sub>2</sub> double layer for  $(\text{Nb,Ti})\text{FeSb}$ , which blocking oxygen diffusion out of the oxide phase. An uni-couple TEG, fabricated from developed thermally stable materials, demonstrated stable performance for more than 150 hours at 873 K in air. These results are very promising for the deployment of TE materials in waste heat recovery systems in air.

**MCARE S5: Materials for Upconversion,**

**Downconversion / Quantum Cutting, Luminescent Downshifting - III**

Session Chair: Jose Marques-Hueso, Heriot-Watt University

**12:30 PM**

**(MCARE-045-2021) Amplifying the prospects of upconverting nanoparticles (Invited)**

J. Schuck<sup>\*1</sup>

1. Columbia University, USA

Though their unique optical properties are proving advantageous for numerous applications, an ongoing challenge facing upconverting nanoparticles (UCNPs) remains achieving satisfactory upconverted signal and quantum yield while illuminating at low fluences. Here, I will describe the pros and cons of various strategies used to improve UCNP signals and efficiencies, which are pushing UCNP brightness to unprecedented levels. Of particular note here are advances in dye-sensitized UCNPs, high-lanthanide-content compositions, exploitation of stimulated emission, and, most recently, the realization of photon avalanching lanthanide-based nanoparticles. The

impact of these concepts is now being widely felt in fields spanning deep-tissue imaging, optogenetics, remote sensing, anti-counterfeiting, and solar light harvesting.

**1:00 PM**

**(MCARE-046-2021) Using Eu3+ as a versatile probe for local and long-range chemistries (Invited)**

J. Dorman<sup>\*1</sup>

1. Louisiana State University, Chemical Engineering, USA

Rare earth elements play a significant role in the global economy due to their unique luminescent, catalytic, and magnetic properties resulting from their f electrons. Of these rare earths, Eu is commonly used as a luminescent center due to its temperature and structural responses and its ability to electronically couple with transition metal ions. However, the luminescent host must be carefully designed in order to take advantage of these unique properties as atomic and long-range chemical probes. Using a combination of synthetic methods (molten salt, sol-gel, hydrothermal), we are able to spatially control dopant ions within core-shell nanoparticles. When these nanoparticles are exposed to different external stimuli (temperature, magnetic fields, chemical environments) the characteristic Eu luminescent spectrum undergoes unique changes, which we can model to extract the local and long-range chemical environments. In this presentation, I will discuss our research using Eu to design new nanostructures and their dynamic luminescent signal for ferroelectric, catalytic, and biological sensing applications. By engineering these nanostructures, we have been able to improve the temperature and concentration sensitivities using non-invasive, low-cost approaches.

**1:30 PM**

**(MCARE-047-2021) Luminescent Pyrochlore Metal Oxide Nanoparticles**

Y. Mao<sup>\*1</sup>

1. Illinois Institute of Technology, Department of Chemistry, USA

Designing lanthanide doped luminescent materials especially nano-materials with multifunctional applications is highly challenging and demanding. The chemistry and structure of the host materials for lanthanide ions are critical in the selection of known phosphors and in the discovery of new phosphor materials for being used for the applications. Materials with  $A_2M_2O_7$  pyrochlore composition recently have displayed a variety of advanced applications in solid oxide fuel cells, photocatalysis, thermographic phosphor, thermal barrier coating, X-ray scintillator, photoluminescence, and nuclear waste host, etc. In the past few years, we have focused on the studies of pyrochlore  $A^{III}_2M^{IV}_2O_7$  nanoparticles (NPs, where A = trivalent heavy element ions of both lanthanides and actinides, and M =  $Zr^{4+}$ ,  $Hf^{4+}$ , etc.) useful for solid-state lighting, X-ray scintillators, thermometry, and bioimaging. We have achieved substantial tunability of their particle size, crystal phase, and more importantly, luminescence properties. We have gained a clear understanding of the influences of synthesis conditions, particle morphology and composition on their photoluminescence and radioluminescence. The tunable luminescence properties of these lanthanide doped pyrochlore NPs indicate their great application potentials in solid-state lighting and multicolor luminescence devices.

**1:45 PM**

**(MCARE-048-2021) Luminescent Solar Concentrators based on Quantum Dots and Carbon Dots (Invited)**

D. Benetti<sup>\*1</sup>; F. Rosei<sup>1</sup>

1. Institut National de la Recherche Scientifique, Énergie Matériaux Télécommunications, Canada

Luminescent solar concentrators (LSCs) are an emerging solar technology that allows to harvest and concentrate sunlight in various medium to large scale applications such as building integrated photovoltaics (BIPV) and greenhouses. Among various types of luminescent particles suitable for LSCs, inorganic quantum dots (QDs) are excellent candidates due to their size-tunable optical properties, and high photoluminescence quantum yield (PLQY). In this presentation different strategies will be introduced to achieve cost-effective large-area LSC based on inorganic QDs. Moreover, in order to increase the eco-sustainability of such devices, it will be also explored the possibility to replace semiconductor QDs with organic nano-emitters such as carbon dots (Cdots). Compared to semiconductor QDs, Cdots contain exclusively non-toxic elements (C, O, H and N) and can be synthesized in large quantities at low cost, allowing the preparation of eco-friendly LSC devices.

**MCARE S5: Multifunctional Spectral Conversion**

**Materials: Applications Beyond the Energy Sector**

Session Chair: Eva Hemmer, University of Ottawa

**2:45 PM**

**(MCARE-049-2021) Porous SiC electroluminescence from p-i-n junction (Invited)**

A. Kitai<sup>\*1</sup>; S. Bawa<sup>1</sup>; T. Zhang<sup>1</sup>; L. Dow<sup>1</sup>; S. Peter<sup>1</sup>

1. McMaster University, Engineering Physics/Materials, Canada

Electroluminescence of porous silicon carbide is achieved in a forward-biased SiC p-i-n junction. A broad green spectral feature centered at approximately 510nm is shown to arise from porous SiC. A large SiC surface area in the vicinity of the junction is created by diamond cutting followed by an electrochemically enhanced hydrogen fluoride etch that produces a layer of porous SiC. Photoluminescence is shown not to be responsible for the green emission. This supports the model of carrier recombination at the porous region. A lateral bipolar diffusion model is presented in which mobile carriers diffuse laterally from the junction towards the porous SiC surface region driven by a lateral carrier concentration gradient. A lateral bipolar diffusion mechanism is proposed as a means to achieve high quantum efficiencies in future SiC p-n homo-junction or double heterojunction light emitting diodes. Competing recombination processes and associated ideality factors in 4H SiC diodes are also examined. The interdigitated structure of PIN SiC devices is discussed.

**3:15 PM**

**(MCARE-050-2021) Toward Biosourced Materials for Electrochemical Energy Storage: The Case of Melanin Biopigments and Tannins (Invited)**

C. Santato<sup>\*1</sup>

1. Ecole Polytechnique de Montreal, Canada

Sustainable electrochemical energy storage solutions are needed to efficiently exploit renewable intermittent energy sources. In principle, redox active biosourced (natural) molecules deposited on the surface of carbon materials allow for an increase in the energy density of corresponding electrochemical capacitors, since faradaic processes add to electrostatic ones. Herein, we report on melanins and tannins as possible redox active molecules for sustainable electrochemical capacitors operating in aqueous electrolytes. Further,



we will discuss the possibility to integrate the conversion and storage functions within the same multifunctional biosourced material; we identified the redox-active, quinone-based, melanin pigment, featuring a broadband absorption in the UV-vis region, as the ideal candidate for such an exploration. A key element determining our choice to study melanins and tannins is that they can be extracted from forest residues or agricultural biomass and food waste, a clear advantage in terms of sustainability.

**3:45 PM**

**(MCARE-051-2021) Exploration of Lanthanum Hafnate Pyrochlores for Radioactive Waste Containment**

Y. Mao<sup>\*1</sup>

1. Illinois Institute of Technology, Department of Chemistry, USA

High level radioactive waste (HLW) is accumulated with the development of civilian and military nuclear power. Oxide ceramics are considered as alternatives to well-established nuclear waste forms. Pyrochlores with the general chemical composition  $A_2M_2O_7$  can incorporate large amounts of actinides. Moreover, they have attracted considerable attention as inert matrix materials for actinide burning. Along this line, we doped lanthanum hafnate  $La_2Hf_2O_7$  with uranium. We found that U dopant was stabilized at both  $U^{4+}$  and  $U^{6+}$  oxidation states in which the  $U^{+4}$  ions substituted the  $Hf^{4+}$  ions and the  $U^{+6}$  oxidation state existing in octahedral uranate  $UO_6^{6-}$  form resided at the  $La^{3+}$  sites. We also observed their structural phase transformation with increasing U doping level. In another work, we investigated the effect of U concentrations on the structural and optical properties of  $RE_2Hf_2O_7:U$  ( $RE = Y, Gd, Nd, \text{ and } Lu$ ). This work deepened our understanding of the behavior of uranium ions doped in different  $RE_2Hf_2O_7$  host matrices. In another relevant study, we exposed  $RE_2Hf_2O_7:Eu^{3+}$  ( $RE = Y, La, Pr, Gd, Er, Lu$ ) to highly energetic gamma-ray irradiation. Some of them underwent a structural phase transition from pyrochlore to fluorite. Ultimately, we expect to identify a type of HLW hosts with long term stability, high resistance against radiation and corrosion, desirable chemical stability and high waste loading.

**4:00 PM**

**(MCARE-052-2021) Persistent Luminescence properties of Doped Spinel Metal Oxide Nanoparticles**

Y. Mao<sup>\*1</sup>

1. Illinois Institute of Technology, Department of Chemistry, USA

Persistent Luminescent materials have been attracting significant attention among scientific community owing to their tremendous potentials in the areas of bioimaging, solid state lighting, security applications, etc. Spinel  $ZnGa_2O_4$  has been explored as a favorable host with properties such as high chemical and thermal stability and wide band gap. To improve the persistence luminescence of  $ZnGa_2O_4:Cr^{3+}$  (ZGOC) and make it more commercially viable, we have hydrothermally synthesized ZGOC nanoparticles (NPs) by fine-tuning their nucleation kinetics and crystal size through (i) controlled precipitation using urea as participant, (ii) adjusting Zn/Ga precursor ratio, and (iii) the addition of ammonium nitrate. Deep red emitting ZGOC NPs with higher PL and PerL luminescence have been realized when compared with the counterparts synthesized using precipitants of NaOH and  $NH_4OH$ . Also, to take advantages of NIR excitation with its high penetration depth, low autofluorescence and high damage threshold to tissues, we co-doped the ZGOC NPs judiciously with  $Yb^{3+}$  and  $Er^{3+}$  to form ZGO-YEC NPs. Excitingly, these ZGO-YEC NPs emit bright singular red emission under 980 nm excitation. Overall, our studies provide new pathways for optical scientists to design high quality luminescent materials for multifunctional applications in the areas of health, energy, security and environment.

**MCARE S16: Solar Energy Harvesting III**

Session Chair: Feray Uenlue, University of Cologne

**12:30 PM**

**(MCARE-053-2021) Single-Source Precursors for Controlled Gas Phase Deposition of Iridium-based Catalytic Coatings for Water Splitting Applications**

M. Frank<sup>\*1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Inorganic Chemistry, Germany

Investigation of the interplay of metal-organic chemistry will enrich the state-of-the-art of chemical vapor deposition (CVD) and atomic layer deposition (ALD) technology and open new possibilities for the applications of new Ir-based materials. Therefore, new heteroleptic Janus-typed compounds exhibiting high volatility and defined thermal decomposition under CVD and ALD conditions are reported to elaborate the precursor chemistry – materials synthesis – functional property chain. The new precursors unify both reactivity and sufficient stability through its heteroleptic constitution to provide a precise control over compositional purity in CVD and ALD deposits. CVD- and ALD-grown materials were tested towards their (electro)catalytic applications, particular in the oxygen evolution reactions. In this work functional characterization of deposited materials will be reported and their catalytic behavior is examined. The deposition on various substrate materials without the need of additional reactant gases underlines the potential of this heteroleptic precursor class for CVD and ALD of metallic thin films. The presented CVD data opens new possibilities in the vapor phase synthesis of materials facilitating the application of such films, for example, as electro- or photocatalyst in oxygen evolution reactions (OER).

**12:45 PM**

**(MCARE-054-2021) Superhard Conductive Rhenium Nitride Thin Films via Magnetic Field-Assisted CVD from Volatile Rhenium Precursors**

Z. Aytuna<sup>\*1</sup>; M. Frank<sup>1</sup>; S. Mathur<sup>1</sup>

1. Institute of inorganic Chemistry, Department of Chemistry, Germany

Rhenium nitride is a promising candidate as superhard conductor. Different rhenium-to-nitrogen ratios and several phases result in challenging synthetic strategies for phase pure rhenium nitride. Novel heteroleptic rhenium(I) compounds, [fac-Re(I)(CO)3(L)] (e.g., L= tfb-dmpda, (N,N-(4,4,4-trifluorobut-1-en-3-on)-dimethyl propylene diamine)), containing preformed Re-N bonds act as efficient precursors for selective growth of polycrystalline rhenium nitride (ReN) films by vapor phase deposition. This is the first known access to synthesize phase pure rhenium nitride by single source precursor approach without the need of additional gases. Interdependence of materials strength and thin film orientation is strongly influenced by external magnetic fields. Deposition of ReN films in presence of an external magnetic field showed an orientation effect with preferred growth of crystallites along  $\langle 100 \rangle$  direction.

**1:00 PM**

**(MCARE-055-2021) Size-dependent properties of nanostructured metal oxides (Invited)**

P. Broqvist<sup>1</sup>; J. Kullgren<sup>\*1</sup>

1. Uppsala University, Department of Chemistry-Ångström Laboratory, Sweden

Nanostructured metal oxide materials are important in many technologically relevant applications. One reason for this is that their chemical and physical properties can be tuned merely by controlling their sizes, shapes, and stoichiometries at the nanoscale. Experiments alone are often too obtuse to allow us to make the connection between the local atomic structure and wanted properties. Here, theory can have an important role to fill by providing

tools for determining the often very delicate chemistry governing the materials' functionalities. In this presentation, I will show the use of our in-house developed multiscale modeling tools applied to two different cases concerning nanostructured metal oxides: (i) size-dependent redox-activity of nanoceria, and in particular, the understanding of its large photovoltaic and oxygen storage activities measured for very small ceria nanoparticles ( $d < 5$  nm), and (ii) clustering of Eu in Eu-doped ZnO nanosponges. In particular, I will address the added value of using an integrated theoretical and experimental approach which allows for a deeper understanding of the fundamental chemical processes at play.

**1:30 PM**

### **(MCARE-056-2021) Molecular Level Synthesis of InFeO<sub>3</sub> and InFeO<sub>3</sub>/Fe<sub>2</sub>O<sub>3</sub> Nanocomposites**

V. Nahrstedt<sup>\*1</sup>; D. Stadler<sup>1</sup>; T. Fischer<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Germany

New heterometallic In-Fe alkoxides [InFe(O<sup>t</sup>Bu)<sub>4</sub>(PyTFP)<sub>2</sub>] (1), [InFe<sub>2</sub>(O<sup>nco</sup>Pen)<sub>9</sub>(Py)] (2) and [InFe<sub>3</sub>(O<sup>nco</sup>Pen)<sub>12</sub>] (3) were synthesized and structurally characterized. The arrangement of metal centers in mixed-metal framework was governed by the In:Fe ratio and the coordination preferences of Fe(III) and In(III) centers to be in tetrahedral and octahedral environments, respectively. Thermal decomposition studies of compounds 1-3 under inert conditions with subsequent powder diffraction studies revealed the formation of Fe<sub>2</sub>O<sub>3</sub> and In<sub>2</sub>O<sub>3</sub> in case of 3 and 2, whereas 1 intriguingly produced elemental In and Fe. In contrary, thermal decomposition of 1-3 under ambient conditions produced a ternary oxide, InFeO<sub>3</sub>, with additional Fe<sub>2</sub>O<sub>3</sub> present as a secondary phase in different stoichiometric ratio predetermined through In:Fe ratio in 2 and 3. The intimate mixing of different phases in InFeO<sub>3</sub>/Fe<sub>2</sub>O<sub>3</sub> nanocomposites was confirmed by transmission electron microscopy of solid residues obtained after the decomposition of 1 and 2. The pure InFeO<sub>3</sub> particles demonstrated ferromagnetic anomalies around 170 K as determined by temperature-dependent field-cooled and zero-field-cooled magnetization experiments. A first order magnetic transition with an increase in the ZFC measurements was explained by temperature induced reduction of the Fe-Fe distance and the corresponding increase in super-exchange.

**1:45 PM**

### **(MCARE-057-2021) Limited Drift Distance of Photoexcited Minority Carrier in Surface Space Charge region (Invited)**

H. Choi<sup>\*1</sup>

1. University of Cologne, Germany

A theory model for limited drift distance of photoexcited carrier was established being motivated by the huge number of recent research works devoted to designing solar-energy conversion materials and unclear explanations on optimum doping/defect concentrations. Many of recent experimental evidences have proven that built-in electric field in surface charge depletion region plays the key role to separate and transport photoexcited charge carriers. This study was initiated by raising the possibility that only a small part of charge depletion layer near surface can deliver photogenerated minority carrier within lifetime on the contrary to the conventional assumptions. Using electrostatics, we derived theoretical maximum distance of photoexcited minority carrier drift within the surface space charge region. According to our newly derived theory model, the drift distance of heavy hole semiconductor materials can have only finite drift length within the charge depletion region, and it is the origin of the optimum doping/defect concentration existences. The recently reported existences of finite optimum doping concentrations and particle size effects on the activities of photocatalytic materials were successfully explained with our new theory model.

**2:15 PM**

### **(MCARE-058-2021) Enhancing charge delocalization and transport of metal halide perovskite quantum dots using conjugated molecular ligands (Invited)**

J. Z. Zhang<sup>\*1</sup>

1. University of California Santa Cruz, Chemistry and Biochemistry, USA

Metal halide perovskites are highly promising for applications in field including photovoltaics and LEDs due to their unique optoelectronic properties. Perovskite quantum dots (PQDs) afford additional advantages including tunable optical and electronic properties. However, insulating ligands used to stabilize PQDs limit their charge transfer and transport properties in the solid form for device applications. One approach to solving this problem is to use short conductive aromatic ligands that allow delocalization of the electronic wave function from the PQDs and facilitate charge transport between PQDs by lowering the energy barrier. We have demonstrated such approach using methylammonium lead bromide (MAPbBr<sub>3</sub>) and iodine (MAPbI<sub>3</sub>) QDs prepared using various conjugated molecular ligands such as benzylamine (BZA) and benzoic acid (BA) capping ligands. Optimized BZA-BA-MAPbBr<sub>3</sub> QDs are highly stable and show very high photoluminescence (PL) quantum yield (QY). More importantly, the BZA-BA-MAPbBr<sub>3</sub> QD film exhibits higher conductivity and more efficient charge extraction compared to PQDs with insulating ligands based on electrochemical measurements and transient photocurrent and photovoltage spectroscopy. Preliminary data were obtained on prototype LED devices, show encouraging results.

**Wednesday, July 21, 2021**

## **MCARE Plenary**

### **Plenary Speaker 3**

Session Chair: Sanjay Mathur, University of Cologne

**9:05 AM**

### **(MCARE-PLEN-2021) Hybrid Perovskites - Materials Formation and Scaling**

E. Unger<sup>\*1</sup>

1. Helmholtz-Zentrum Berlin für Materialien und Energie, Germany  
unavailable

## **EHS S1: Materials, Components and Devices for Self-powered Electronics I**

Session Chair: Jungho Ryu, Yeungnam University

**10:00 AM**

### **(EHS-018-2021) Precursor's thermodynamics for advanced MOCVD materials**

A. Makarenko<sup>\*1</sup>; K. Zherikova<sup>1</sup>

1. NIIC SB RAS, Russian Federation

Platinum-group element coatings are used in medicine (pacemakers, implants, etc.) and hydrogen energetics. Metal-Organic Chemical Vapor Deposition is the main method to obtain such materials. The first stage of MOCVD is sublimation/vaporization of the precursors, so knowledge about their vapor pressures and sublimation/vaporization thermodynamics is crucial for optimization of the deposition processes. In this case, the precision vapor pressure data are required. From this point of view, thermodynamic model which would allow the predicting of vapor pressures and thermodynamic

characteristics of precursors as well as verification of the existing data is very desired. In this work, metal (Ir, Fe, Sc, etc.)  $\beta$ -diketonates have been considered. For the studied compounds, the thermodynamic literature data have been carefully collected and some new data have been obtained. Also, the approach has been developed to adjust thermodynamic characteristics to the reference temperature. Using verified and unified thermodynamic values, «structure-property» correlations have been established; they help to reveal the changes in chelate thermal properties during both the central atom and the organic ligand variation. The presentation includes data obtained during implementation of the project financially supported by the Russian Science Foundation (N 20-15-00222).

**10:15 AM**

**(EHS-019-2021) Electrically Engaged Undulation System for Hydrodynamic Energy Harvesting**

K. Lu\*<sup>1</sup>

1. Pyro-E, USA

Pyro-E has demonstrated a 5-watt power source to support seafaring devices for ocean observation. The Electrically Engaged Undulation (EEL) system uses electroactive materials to harvest hydrodynamic energy in a manner that is 100-times more powerful than current practice. The target application is for submersible gliders to 1) Improve coverage, 2) Reduce latency, and 3) Mitigate frequent maintenance trips at sea. Here, the incumbent battery technology lacks the duration to make measurements economical, costing as much as ~\$100,000 per kilobyte of data for temperature and salinity. In contrast, EEL can sustain gliders indefinitely via the piezoelectric effect – a material-led phenomenon that converts applied stress into electricity. Notably, the concept uses exponential force amplification to improve performance. For the presentation, new simulation and experimental work were conducted to address the challenges of coupling vortex-induced forces with eel-like undulations for energy harvesting. Also investigated is the tolerance to subsea extremes such as large hydrostatic pressures. Highlights of the innovation include 1) Power capability spanning three orders of magnitude from 0.05 to 5 watts, 2) 75% bandwidth matching the excitation of ocean waves and hydrodynamic forces, and 3) Tunable frequency response without using a proof mass or active electronic feedback.

**10:30 AM**

**(EHS-020-2021) High-power density magnetic field harvester using a two-degree-of-freedom architecture**

R. Sriramdas\*<sup>1</sup>; R. Cruz<sup>1</sup>; M. Kang<sup>1</sup>; S. Priya<sup>1</sup>

1. Pennsylvania State University, USA

Energy harvesting from magnetic fields around current-carrying wires is a promising technology for ubiquitous power supply. Magneto-mechano-electric harvesters provide high power densities for the internet of things (IoT) sensors and systems to prolong the sensing network lifetime. Here we propose a two-degree-of-freedom (2-DOF) magnetoelectric energy harvester that provides enhanced power generation capability from the ambient magnetic fields. The proposed architecture enhances power density by operating in its higher mode. The tuned 2-DOF system in its second mode induces larger strains into the primary structure, thereby increasing the harvested energy. A simultaneous decrease of the secondary magnetic mass displacement further promotes the uniform excitation from the end magnet. The harvester is fabricated using Metglas and piezoelectric macro-fiber composite with 7.5 g magnet tip mass. The harvester generates 3.1 mW from an average magnetic flux of 5 G. The specific power density of the harvester is 0.275 mW/cm<sup>3</sup>/g, which is 600% higher when compared to one-degree-of-freedom

conventional cantilever type energy harvesters. This improvement in power density advances the implementation of magnetic field energy harvesting into IoT systems to provide wireless powering from ambient magnetic fields continuously.

**10:45 AM**

**(EHS-021-2021) An Underwater Acoustic Transmitter Powered by Fish's Swimming Motion**

H. Li\*<sup>1</sup>; J. Lu<sup>1</sup>; M. Myjak<sup>1</sup>; S. Liss<sup>1</sup>; R. Brown<sup>1</sup>; Z. Deng<sup>1</sup>; C. Tian<sup>2</sup>

1. Pacific Northwest National Laboratory, USA

2. Institute of Deep-sea Science and Engineering, Chinese Academy of Sciences, China

Acoustic telemetry is the primary technology to actively track aquatic animals for behavioral studies. However, the small energy capacities of the batteries used in acoustic transmitters have been a main limiting factor for the length of the time period over which the tagged animals can be monitored. To tackle this challenge, we developed a battery-free acoustic transmitter that uses a Macro Fiber Composite (MFC) piezoelectric beam to harvest energy from fish swimming as the power source. Prototypes of the transmitter were successfully implanted into juvenile white sturgeons and the transmission performance of the transmitters were monitored for months. The prototypes were able to emit up to hundreds of transmissions per hour, dependent on the tagged fish's activity level. A benchtop test setup was also used to simulate and understand the energy-harvesting performance of the device in fish by applying test parameters learned from a video study of the fish's swimming behavior. It was discovered that degradation of the PZT material in the MFC under the dynamic stress resulted from the fish's swimming motion gradually reduced the transmission performance of the transmitter over time.

**EHS S6: Special Symposium: European Energy Harvesting Workshop with Special Honor to Professor Pim W.A. Groen**

Session Chairs: Grzegorz Litak, Lublin University of Technology; Yang Bai, University of Oulu

**10:00 AM**

**(EHS-022-2021) A tribute to the work of the late Professor Pim Groen and his contribution to the field of electroceramics and their applications (Invited)**

S. van der Zwag\*<sup>1</sup>

1. Technical University of Delft, Faculty of Aerospace Engineering, Netherlands

For many decades professor Pim (W.A.) Groen has been one of the leading Dutch scientist in the field of electroceramics. First as a researcher at Philips, then at Morgan Electroceramics, then at TNO and finally as professor Smart Ceramics at the TU Delft. He passed away on May 6<sup>th</sup> 2020. In this short presentation I will focus on the work he did on polymer-piezo ceramic composites in which he combined the attractive flexibility of the polymer matrix with the high sensitivity of well aligned piezo ceramic particles. Using this approach he obtained very attractive combinations of properties such as a high sensitivity, a low temperature synthesis, self healing behaviour and many other unusual combinations. I will also address their application in the field of energy harvesting, an application which initially seemed promising, but may be hard to bring to energy-rich devices.

10:30 AM

### (EHS-023-2021) Celebrating the Intellectual and Technological Contributions of Pim Groen (Invited)

C. Randall\*<sup>1</sup>

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

We have all had the pleasure to have worked with Pim on several topics in electroceramics and composites. In this presentation, we will highlight the connections between our own work and these collaborations. Pim's work embraced fundamental materials physics and chemistry and then directed these approaches to provide engineering solutions. The topics that will be discussed include dielectrics, piezoelectrics, and thermistors, put in context to the understanding of the science at that time. In the case of doping high reliable BaTiO<sub>3</sub> dielectrics that can be integrated into base metal capacitors, this involves work on amphoteric Dy<sup>+3</sup>. This work was performed at Philips Research Laboratory (Aachen) and, later, during his time at Yageo Research and production facilities in Taiwan. Also, while at Philips, he also considered the complex defect chemistry and compositional design of these materials; we will point out these insights on the spinel-based structures, as well as his search for new high temperature thermistor materials. In the case of piezoelectrics, he worked on a broad number of problems, including copper cofired actuators, high temperature morphotropic phase boundary piezoceramics, and 0-3 and quasi 1-3 piezocomposites. His broad experience led to a large piezoelectric program in the Netherlands named Smart Pie, and as part of that program, he co-authored a book on piezoelectric ceramic materials.

11:00 AM

### (EHS-024-2021) Early conversations, energy harvesting using ZnO nanostructures (Invited)

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

1. LSBU, Engineering, United Kingdom

My first meeting with Pim was at the ACerS meeting in Florida... we drank beer, ate burgers, walked in the sunshine and talked about energy harvesting. At that time my group was working on understanding how piezoelectrics, mainly for us nanostructured ZnO, could be used to harvest stray vibration and power small devices. Our earlier work developing ZnO as a backbone to photovoltaic or LED devices was morphing towards scavenging kinetic energy. In this talk I will discuss the progress we made in developing an understanding of the interaction with ZnO and the development of diodes in an effort to increase energy harvesting. By varying the diode structure and passivating the surface of the ZnO nanostructures there was a 10 fold increase in energy and power density of the devices. The load resistance also increases with the increase in energy extraction. We explain the improved performance in terms of increased surface screening and reduced losses. This work then led to our work on ZnO photovoltaics and improved performance with acoustic strain. Pim sent me an electronic cutting of the work from a Dutch newspaper and we had some great conversations about future work.

11:30 AM

### (EHS-025-2021) Piezoelectric materials and their role in energy harvesting - Celebrating Prof. Groen's contributions (Invited)

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

1. Pennsylvania State University, USA

Piezoelectric ceramic materials with high piezoelectric constant can generate large strain in response to applied electric field or generate high voltage in response to applied mechanical stress. Piezoelectric ceramics find application in variety of industries covering electronic, communication, imaging, sensing, and electromechanical devices. High energy density and ease of miniaturization are further driving the development of new piezoelectric technologies, such as energy

harvesters for the Internet of Things (IoT) devices. This presentation will highlight Prof. Groen's contributions in the context of two topical areas: lead-free piezoelectric materials and piezoelectric energy harvesting. With regulations driving the restriction on the use of hazardous substances in electronic devices, enormous efforts have been devoted towards the search of lead-free piezoelectric materials. Material systems based upon (Bi<sub>0.5</sub>Na<sub>0.5</sub>)TiO<sub>3</sub>-based (BNT), (K<sub>0.5</sub>Na<sub>0.5</sub>)NbO<sub>3</sub>-based (KNN), BaTiO<sub>3</sub>-based (BT) ceramics, and their solid solutions have attracted significant interests. Using these high-performance piezoelectric materials and their composites, both rigid and flexible energy harvesting devices can be fabricated to capture vibrations available in the surroundings. Examples covering both piezoelectric materials and energy harvesting devices will be presented.

### MCARE S2: Advanced Materials for Energy Storage

Session Chair: Yu (Michael) Zhong, Worcester Polytechnic Institute

10:00 AM

### (MCARE-059-2021) Synthesis of hcp Cobalt Nitrogen doped carbon catalyst through plasma engineering for Oxygen Reduction Reaction

J. Yoon\*<sup>1</sup>; S. Kim<sup>1</sup>; O. H. Li<sup>1</sup>

1. Pusan National University, Materials Science and Engineering, Republic of Korea

Next generation energy storage devices are being studied such as metal-air batteries. catalysts are being used to improve the reaction due to the sluggish oxygen reduction reaction (ORR) at the air cathode. Currently, the main catalysts used are precious metal catalysts such as platinum and palladium. However, due to high prices and low durability, a new catalyst such as the transition metal-doped carbon catalysts attract many attentions due to their economical aspect and high catalytic performance. In this study, cobalt catalyst with hcp crystalline structure was anchored through a plasma engineering uniformly in the nitrogen-carbon structure and maintained a size of 10~20 nm. The synthesized hcp cobalt-nitrogen doped carbon catalyst (Co/NC) showed superior ORR catalytic performance ( $E_{1/2} = 0.851$  V vs RHE) and competitive ORR performance commercial 20 wt.% Pt/C catalyst ( $E_{1/2} = 0.855$  V vs RHE). Finally, Cobalt nitrogen-doped carbon catalyst synthesized by controlling cobalt crystal structure can be an effective way to replace precious catalysts for metal-air batteries.

10:15 AM

### (MCARE-060-2021) TiNb<sub>2</sub>O<sub>7</sub> - a novel and fast-charging anode material for Li-ion batteries

M. Wilhelm\*<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Germany

Carbon-based anode materials in conventional lithium-ion batteries (LiBs) are widely available and dominant in the big market of energy storage systems. Due to some performance limiting leakages of this setup like the formation of a passivating solid-electrolyte interphase (SEI) at a low working potential (~0.1 V vs. Li/Li<sup>+</sup>), it is essential to develop energy storage devices that exhibit besides good cycle stability, high energy and power density. TiNb<sub>2</sub>O<sub>7</sub> (TNO) is reported as a promising alternative anode material for lithium-ion batteries. TNO nanocomposites were in-situ synthesized through a simple, controllable, and scalable sol-gel route. However, the electric and ionic conductivities in bulk TNO electrodes are too poor to support the requirements of power density for commercialization. Incorporating TNO into carbon nanocomposites by the usage of the electrospinning technique increases the electronic conductivity and enhances the Li<sup>+</sup> diffusion coefficient. The synergetic positive effect of the carbon nanocomposites using a unique electrospinning technique and the crystalline phase exhibits benefits in high-rate Li<sup>+</sup> capability. An economical and environmentally friendly promising

alternative anode material for LiBs using TNO and their embedding in carbon nanostructure paves the way for next-generation novel electrodes for electrochemical energy storage.

### 10:30 AM

#### (MCARE-061-2021) A Flexible Free Standing Cathode from $\text{MgIn}_2\text{S}_4$ / Carbon Nanofibers for Magnesium Sulfur Batteries

R. Adam<sup>\*1</sup>; M. Wilhelm<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Inorganic Chemistry, Germany

An ever-expanding demand of more efficient energy storage systems pushes the development of next generation batteries. Among these magnesium-sulfur batteries are a candidate which is not to underestimate. The higher theoretical gravimetric capacity ( $\text{Mg}^{2+}$ : 3459 mAh  $\text{cm}^{-3}$ ,  $\text{Li}^+$ : 2062 mAh  $\text{cm}^{-3}$ ) and higher operational safety are only some benefits this alternative battery design holds against the current state of the art. A higher abundance in the earth crust reduces the materials prices, enables sustainable mining conditions, promoting an eco-friendly future of energy storage systems. However, the sluggish diffusion of the  $\text{Mg}^{2+}$ -ion due to its rather hard nature, complicates its way into the commercial battery market. To counteract the sluggish kinetics the search for potential cathode materials brought up thio-spinels as promising candidates.  $\text{MgIn}_2\text{S}_4$  nanoflowers were used to increase the mobility of the magnesium ions based on high surface area and bigger anions compared to oxygen-containing spinels. A conductive carbon fiber mat was prepared via electrospinning, onto which  $\text{MgIn}_2\text{S}_4$  was deposited via solvothermal methods hence utilizing the high theoretical capacity of the insulating sulfur. The carbon fiber mat maintains its flexibility during the whole process and a conductive cathode material is obtained. A leaf-like phase similar to a flower structure was detected on the carbon fibers.

### 10:45 AM

#### (MCARE-062-2021) Bilayered $\text{NiZn}(\text{CO}_3)(\text{OH})_2$ - $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$ nanocomposites as positive electrode for supercapacitors

D. Lee<sup>\*1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Germany

Open architecture and porous  $\text{NiZn}(\text{CO}_3)(\text{OH})_2$ - $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$  bilayers were fabricated on a nickel foam substrate through a two-step processing of Ni and Zn salts under hydrothermal conditions. The initial layer of  $\text{NiZn}(\text{CO}_3)(\text{OH})_2$  nanosheets, obtained by alkaline hydrolysis of nickel and zinc salts, was clad with a top layer consisting of  $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$  nanowire arrays. This double-decker arrangement offered a higher mechanical stability and enhanced electrochemical performance in  $\text{NiZn}(\text{CO}_3)(\text{OH})_2$ - $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$  electrodes, which showed an excellent maximum specific capacitance of 1168.8 F  $\text{g}^{-1}$  at 3 A  $\text{g}^{-1}$  and superior cycling stability with a capacity retention of ~85.7% after 5000 cycles. Moreover, the asymmetric two-layered  $\text{NiZn}(\text{CO}_3)(\text{OH})_2$ - $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$ /graphene electrodes provided sufficient capacitive energy to turn on a LED light. This superior electrochemical performance is attributed to the hierarchical architecture and large surface area of the composite electrodes that render them in view of facile and scalable synthesis and greater cycling safety as promising candidates for practical applications.

### 11:00 AM

#### (MCARE-063-2021) Free-Standing Carbon Pellicles: Electrospinning Synthesis and Application as Anode for Sodium-Ion Battery (Invited)

Y. Yue<sup>\*1</sup>; D. Austin<sup>1</sup>

1. Delaware State University, Chemistry, USA

Carbon-based anode materials had raised a great deal of interest due to their low-cost, high stability, and light-weight. Among these carbonaceous materials, porous carbon pellicle is a potential anode

material for sodium-ion battery with the advantages of high specific strength, high temperature resistance, and high conductivity. Here, N-doped hierarchically structured carbon pellicles were prepared from the carbonization of zeolitic imidazolate framework/polyacrylonitrile composite fibers which were fabricated by electrospinning technique. As an anode for sodium-ion batteries, the fiber carbon pellicles showed superior reversible capacity (186.2 mAh  $\text{g}^{-1}$ ) at the current density of 1.0 A  $\text{g}^{-1}$  with an excellent cyclic stability. These results indicated that self-supporting porous pellicles obtained by simple electrostatic spinning method are promising anode materials for development of various porous conductive carbon nanomaterials of interest for electrochemical energy storage devices.

### 11:30 AM

#### (MCARE-064-2021) Mixed reduced and bronze-like $\text{Nb}_2\text{O}_5$ phases for hybrid supercapacitor applications

F. R. Caliri<sup>\*1</sup>, J.T. Matshushima<sup>2</sup>, V. Rodrigues<sup>2</sup>, F. Miranda<sup>3</sup>, M. Balcan<sup>2</sup>, S. Sampath<sup>1</sup>

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

2. National Institute of Space Research, Brazil

3. Technological Institute of Aeronautics, Brazil

In-situ synthesis of mixed reduced and bronze-like  $\text{Nb}_2\text{O}_5$  deposit is a potential pathway for the development of hybrid supercapacitors. This can be achieved by promoting the incongruent vaporization and rapid solidification of monoclinic H-  $\text{Nb}_2\text{O}_5$  feedstock using thermal plasma technology, yielding the formation of bronze-like T and TT-  $\text{Nb}_2\text{O}_5$ , along with  $\text{Nb}_{12}\text{O}_{29}$  and  $\text{NbO}_2$ . These phases are distributed in a layered array of metastable phases T- $\text{Nb}_2\text{O}_5$  and TT- $\text{Nb}_2\text{O}_5$  within the splat core and nonstoichiometry phases  $\text{NbO}_2$  and  $\text{Nb}_{12}\text{O}_{29}$  at the splat boundaries, as revealed by Raman spectroscopy, X-ray diffraction and scanning electron microscope. Furthermore, the electrochemical impedance spectroscopy, Li-ion kinetics and power density are described.

### MCARE S5: Development and Synthesis of Novel Optical Materials - I

Session Chair: Jose Marques-Hueso, Heriot-Watt University

### 10:00 AM

#### (MCARE-065-2021) Formation pathway model of Colloidal Semiconductor Compound Magic-Size Clusters and Quantum Dots (Invited)

K. Yu<sup>\*1</sup>

1. Sichuan University, National Engineering Research Center for Biomaterials, China

Colloidal semiconductor binary II-VI metal (M) chalcogenide (E) quantum dots (QDs) and magic-size clusters (MSCs) have been produced together, sometimes. For the past 35 years, the QD synthesis has been carried out largely as an empirical art, with limited knowledge about the pre-nucleation stage known as the induction period (IP). Recently, we proposed a two-pathway model to explain the co-production of QDs and MSCs. One pathway involves the formation of monomers (Mo) and fragments (Fr), which lead to the nucleation and growth of QDs. This pathway can be addressed by the LaMer model of the one-step based classical nucleation theory (CNT). The other pathway, which we identified a couple of years ago, involves the self-assembly of M and E precursors, followed by the formation of the very MSC precursor compound (PC) from each assembly. The non-classical nucleation theory accounts for this PC-enabled pathway. In this presentation, our latest advances will be discussed on the transformation of the PC to ultra-small QDs with enhanced particle yield as well as to alloy MSCs. The transformation pathways will be explained. Our recent advances bring an in-depth understanding of the coproduction of QDs and MSCs, narrow the knowledge gap on the induction period of QDs, and contribute to the promotion of the nanomaterial synthesis from an empirical art to science.

10:30 AM

**(MCARE-066-2021) Anisotropic perovskite nanocrystals, engineering materials for light manipulation and conversion at the atomic level (Invited)**

Y. Bekenstein\*<sup>1</sup>

1. Technion - Israel Institute of Technology, Material Science and Engineering, Israel

New materials pose new challenges. Lead-halide perovskites have emerged as important optoelectronic materials with excellent efficiencies in photovoltaic and light-emitting applications. These physical properties stand in contrast with recent experimental observations of high dynamic disorder, room temperature structural transformation, and questionable material stability. We study halide perovskites at the limit of the smallest crystals we can make using the toolbox of colloidal chemistry. I will show how through synthetic control of cesium lead halide nanocrystal's shape; we control quantum confinement of excitons with atomic precision (in 2D nanoplates) and achieve anisotropic emission (in 1D nanowires). In addition, by changing the anion composition facile band gap tunability at room temperature throughout the visible spectrum is achieved. We were able to induce and image defects into the perovskite crystals and observe their dynamics which teach us of the self-healing properties to these materials. Next steps include growing colloidal heterostructure to better understand how to interface these new materials and harvest energy efficiently out of them. The manifestation of these physical characteristics, facile synthesis and processing pose these fluorophores in an exciting position to address next generation energy challenges.

11:00 AM

**(MCARE-067-2021) Interfacial properties in composite nano-systems for energy harvesting (Invited)**

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

1. Lulea University of Technology, Engineering Sciences & Mathematics, Sweden

Composite nanostructures can be efficiently applied for Sunlight detection and conversion and for energy harvesting and generation of solar fuels. In most of the systems, like photodetectors, excitonic solar cells and (photo)-electrochemical cells, nanomaterials can play a critical role in boosting photoconversion efficiency by ameliorating the processes of charge photogeneration, dissociation and transport. Critical role is played by the structure and quality of the interface. Several strategies can be pursued to maximize energy harvesting and storage, including broadening of light absorbance to reduce light losses, fastening exciton dissociation and charge injection from the photoactive medium to the charge transporting materials. In this lecture, a few examples of application of nanocomposites will be discussed, including all-oxide coaxial p-n junction nanowire photodetectors and solar cells, core-shell quantum dot fluorophores for high-efficiency luminescent solar concentrators, composite sulfides for hydrogen generation, and oriented carbon nanotube forest dispersed in polymer matrix as efficient low-temperature thermoelectric composite. Emphasis will be given to the role of interface engineering in improving the efficiency in different systems, spanning from electric power generation from Sunlight, to chemical fuel production, to conversion of heat lost through thermoelectric materials.

11:30 AM

**(MCARE-068-2021) Nano-crystalline ZnO:Eu sponges; nature of Ln doping (Invited)**

G. Westin\*<sup>1</sup>

1. Uppsala University, Sweden

There is a strong demand for tailored materials for sensors, catalysts, solar-cells and energy storage for renewable energy areas. Typical features of these materials are; a large interface to the surrounding

liquid electrolyte, reaction liquid, or gas phase, surface modification for e.g. band structure and corrosion control, and catalysis. Often a high conductivity is required to get generated electrons out to the surface or electrode which implies materials of high crystalline quality with controlled dopant positioning, as well as a good connectivity though the structure. Here we present a salt-based synthesis route yielding nano-crystalline ZnO:Eu (0-5% Eu) sponges built of ca. 10 nm sized crystallites at temperatures down to 200°C, and describe their phase-development on heating in great detail. For the ZnO:Eu sponges, the doping of large alio-valent Eu<sup>3+</sup>-ions in the ZnO was of particular interest. TEM and XPS studies showed that a homogenous doping of Eu-ions was present up to at least 700-900 °C for 5-0.5% Eu sponges. Further TG, IR and XPS revealed residues of organics at 200-300 °C and carbonate at 300-500 °C. At higher temperatures, Eu<sub>2</sub>O<sub>3</sub> was separated as nano-crystals on the surface of the ZnO sponge.

**MCARE S15: Advances in Fundamental Science and Development of Photovoltaic Materials and Devices**

Session Chairs: Daniele Benetti, Institut National de la Recherche Scientifique; Kelsey Stoerzinger, Oregon State University

10:00 AM

**(MCARE-069-2021) Singlet-Fission Solar Cells: Why So Hard? (Invited)**

O. G. Reid\*<sup>1</sup>; N. A. Pace<sup>2</sup>; G. Rumbles<sup>2</sup>; J. C. Johnson<sup>2</sup>

1. University of Colorado Boulder, Renewable and Sustainable Energy Institute, USA
2. National Renewable Energy Laboratory, Chemistry and Nanoscience, USA

Singlet-fission is one possible route to multiply excited states in solar cells and ultimately exceed the Shockley-Queisser efficiency limit, but producing solar cells that harness this process has proved to be surprisingly difficult. Our team has discovered why this is so. In polyacenes – prototypical singlet fission materials – we find that the rate constant for charge transfer between triplet excitons and molecular electron acceptors is extremely small, even when the Gibbs energy of the reaction is optimal. Moreover, it does not matter whether triplet excitons are generated through singlet fission or via intersystem crossing, implying that this is a fundamental characteristic of triplet states on polyacenes and not related to the presence of correlated triplet pairs after singlet-fission.

10:30 AM

**(MCARE-070-2021) New Sulfides Photoabsorbers by Combining Experiment and Theory (Invited)**

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

1. Helmholtz Zentrum Berlin, Germany, Germany

The development of new energy materials from the mere speculation of their existence up to a working prototype device is an exciting but highly complex, even daunting task. Based on two case studies, I will discuss the lessons learned and the tremendous opportunities offered by an integrated experimental/computational approach to materials development. The first case study is the development of sulfide perovskite (ABS<sub>3</sub>) absorbers for solar cells. The process included an initial computational screening step covering 705 potential compounds, the identification of the 15 most promising materials based on a set of descriptors, the synthesis of the selected compound LaYS<sub>3</sub>, the experiment-theory interplay in the interpretation of characterization results, and finally the fabrication of the first chalcogenide perovskite solar cell. The second case study is the design of new quaternary photoabsorbers inspired by Cu<sub>2</sub>ZnSnS<sub>4</sub> – a compound once regarded as highly promising but whose fundamental limitations have now become apparent. Here, the combination of experiment and theory was instrumental to understanding property trends over a wide chemical space. These new

insights have led to the development of a unified theory of defects and tail states in Cu-based quaternary sulfides.

11:00 AM

**(MCARE-071-2021) Ionic compounds enable efficient and durable perovskite photovoltaics (Invited)**

Y. Lin\*<sup>1</sup>

1. University of Oxford, Physics, United Kingdom

Hybrid organic-inorganic metal-halide perovskites stand out as obvious candidates for solar energy generation and photovoltaic applications owing to their much-heralded material property trio: remarkable absorption coefficients, long-lived photocarriers and tuneable bandgaps. After introducing the solid-state architectures in 2012, tremendous efforts have been devoted to research fundamental properties of perovskites as well as to advance relevant photovoltaic technologies. In this talk, I will present efficient and durable perovskite solar cells enabled by ionic additives. Our approach allows perovskites solar cells to sustain aggressive ageing conditions that combine high-strength light and heat. Meanwhile, I will share new insight into critical degradation mechanisms in perovskite absorbers. This understanding could help to develop perovskite solar cells that can resist extreme environmental conditions. Integrating our modified perovskites into monolithic two-terminal perovskite-on-Si tandem solar cells has led to an efficiency value beyond the highest efficiencies recorded for single-junction c-Si solar cells. Our work represents a significant advancement that validates the approach of using perovskite-on-Si tandem solar cells to ultimately enhance the absolute performance of market-dominating Si photovoltaics.

**Poster Session 2A (live presentations) also available in on-demand session**

1:00 PM

**(EHS-P-003-2021) Semi-analytic finite element method applied to short fiber-reinforced piezoelectric composite**

L. E. Barraza de Leon<sup>1</sup>; H. Camacho Montes<sup>1</sup>; Y. Espinosa Almeyda<sup>2</sup>; J. A. Otero Hernández<sup>3</sup>; R. Rodríguez Ramons<sup>4</sup>; J. C. Lopez Realpozo<sup>4</sup>; F. J. Sabina Ciscar<sup>2</sup>

1. Universidad Autonoma de Ciudad Juarez, Physics and Mathematics, Mexico
2. Universidad Nacional Autonoma de Mexico, Matematica y Mecanica, Mexico
3. Instituto Tecnológico de Estudios Superiores de Monterrey, Física y Mecánica, Mexico
4. Universidad de La Habana, Mecánica, Cuba

In this work, a 3D Semi-Analytical Finite Element Method (SAFEM) is developed to calculate the effective properties of piezoelectric fiber-reinforced composites. Here, the calculations are realized in one-eighth of the unit cell to simplify the method. The prediction of the effective properties for periodic transversely isotropic piezoelectric composites made of piezoceramic unidirectional fibers (PZT) with square and hexagonal space arrangements in a soft non-piezoelectric matrix (polymer) is reported and analyzed as a way to validate the 3D approach. The limit case, when short fiber becomes infinite ones, allows us to compare with results reported in the literature, and good coincidence is obtained. For the analysis of effective properties as a function of fibers relative length, two cases are considered: i) constant volume fraction and ii) constant fiber radius. The constant volume fraction case is of special interest because according to the Voigt–Reuss–Hill approximation, the effective properties should remain constant. Then, in order to analyze this case, mechanical and electric fields are also shown. The obtained results show a physically congruent behavior. Good coincidences are obtained by comparing with analytical asymptotic homogenization and finite element methods.

**(MCARE-P-030-2021) Dipole engineering of BaTiO<sub>3</sub> ceramics using [Mn<sup>2+</sup>, W<sup>6+</sup>]**

W. D. Senn\*<sup>1</sup>; W. J. Hogan<sup>1</sup>; N. Betancur-Granados<sup>2</sup>; K. Ning<sup>1</sup>; J. I. Tobón<sup>3</sup>; O. J. Restrepo<sup>3</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA
2. Alfred University/Universidad Nacional de Colombia, USA
3. Universidad Nacional de Colombia, Materials and Minerals Department, Cambodia

Dielectric performance of a ferroelectric ceramic material can be modified or enhanced through dipole-pair substitutions. A coupled dipole-pair with a larger valence difference offers a larger dipole strength that should affect the local electric field and material electronic properties. In this work, [Mn<sup>2+</sup>, W<sup>6+</sup>] dipolar pair substituted BaTiO<sub>3</sub> ceramics Ba[(Mn<sup>2+</sup>, M<sup>6+</sup>)<sub>y</sub>Ti<sub>1-2y</sub>]O<sub>3</sub>, 0 ≤ y ≤ 0.01875 are fabricated and the electronic properties including resistivity, permittivity, activation energy, band gap, etc., are investigated. The enhanced electric resistivity and the relaxor-like dielectric behavior are reported, further confirming the functioning of the [Mn<sup>2+</sup>, W<sup>6+</sup>] dipole-pairs in BaTiO<sub>3</sub> ceramics. These novel ceramic material through dipole engineering offers new opportunities for electronic devices and systems.

**(MCARE-P-031-2021) Electric and Dielectric Behaviors of [In, Ta] Dipole Pair Substituted BaTiO<sub>3</sub> Ceramics**

E. Merkey\*<sup>1</sup>; I. Chedzoy<sup>1</sup>; N. Betancur-Granados<sup>2</sup>; K. Ning<sup>1</sup>; J. I. Tobón<sup>3</sup>; O. J. Restrepo<sup>3</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA
2. Alfred University/Universidad Nacional de Colombia, USA
3. Universidad Nacional de Colombia, Materials and Minerals Department, Cambodia

[In, Ta] dipole pair substituted BaTiO<sub>3</sub> ceramics have been fabricated with high purity precursor powders in order to study the dipole pair concentration dependent electric and dielectric behaviors. Dilute [In, Ta] dipole pairs are designed to locate at Ti atomic position in the unit cell and are investigated within the concentration 0 to 0.05. With the increase of the dipole pair concentration, the dielectric permittivity evolves from ferroelectric behavior to diffuse phase transition, and to relaxor-like behavior. Material characterizations including crystal structure, resistivity, activation energy and band gap are systematically investigated. New Simple Material Model (NSMM) and Clausius–Mossotti relation are combined to provide an in-depth understanding of the unique dielectric properties.

**(MCARE-P-033-2021) Capacitive Thermoelectric Device Based on Dipole Engineered Ceramics**

K. Ning\*<sup>1</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA

Thermoelectric devices enable conversion of thermal energy to electrical energy with far-reaching implications in waste heat harvest, energy crisis relief, and greenhouse gas reduction. Low efficiency of the existing thermoelectric devices is one main drawback currently limiting widespread and large scale commercialization and application. Dipole engineering allows the creation of novel dielectric performance that enables innovative capacitive based thermoelectric devices. Preliminary device setup and results from [Ga, Ta] dipole engineered BaTiO<sub>3</sub> ceramics resulted in a Seebeck coefficient of 40 mV/K which is significantly larger than those of conventional thermal electric. The device can approach and even theoretically exceed a thermal to energy conversion efficiency of greater than 50%. Higher performance dipole engineered materials are under investigation using design guidance from the new simple material model, including Clausius – Mossotti relation.

### **(MCARE-P-034-2021) A Novel Photoanode with Hierarchical Forest-Like TiO<sub>2</sub> Structure with Plasmonic Nanoparticles for Flexible Dye Sensitized Solar Cells**

B. Choudhury<sup>\*1</sup>; C. Lin<sup>1</sup>; S. Shawon<sup>1</sup>; M. Uddin<sup>1</sup>

1. University of Texas Rio Grande Valley, Chemistry, USA

Due to their unique photovoltaic properties, different morphologies of TiO<sub>2</sub> on flexible substrate have been studied extensively in the recent years for applications in dye sensitized solar cells (DSSCs). Nanostructured electrode with high surface area can facilitate rapid charge transport and thus improve the light-to-current conversion efficiency. Herein we present a novel photoanode with forest like TiO<sub>2</sub> hierarchical structure using a simple and facile hydrothermal route. In order to utilize the surface plasmon response (SPR) and hence increase the photon conversion efficiency a plasmonic nanoparticle has also been deposited using a very facile photoreduction method. The branched structure of the photoanode increase the dye loading and charge transport whereas the multiple roles to increase the light-to-current conversion efficiency of the device. The high-density small nanoparticles at the middle part of the forest like structure decrease the charge recombination whereas the large nanoparticles at the upper part increase light chattering and thus the photovoltaic efficiency of the cells. The incorporation of nanoparticles in the branched structure also improves the dye loading. The flexibility of the device has also been tested by performing bending test.

### **(MCARE-P-035-2021) A Fiber Shaped Dye Sensitized Solar Cell with a Liquid Polysulfide Electrolyte Showing High Open Circuit Voltage and Photon Conversion Efficiency**

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1. University of Texas Rio Grande Valley, Chemistry, USA

Fiber shaped dye sensitized solar cells are very promising technology due to their light weight and flexibility making them suitable to be used for military and textile application. With the proper use of TiO<sub>2</sub>, quantum dots, a bulk heterojunction polymer layer and a liquid electrolyte a high open circuit voltage of 0.75V has been achieved. The TiCl<sub>4</sub> annealing of the oxide layer resulted into a uniformly coated substrate that facilitated efficient transfer of the photogenerated excitons. The chemical bath deposition technique was used to deposit different layers. A plasma sputtering system was used to fabricate the counter electrode. The photoelectric performance was evaluated at different cell length and a 4.0 cm cell length gave the highest light-to-current conversion efficiency of 14.30%. When the cells were connected in series for a 2.5 cm length a high open circuit voltage of 1.5V has been achieved. Future study can be conducted in this field to understand the role of a liquid electrolyte and bulk heterojunction layer in obtaining high performance flexible solar cells.

### **(MCARE-P-036-2021) Colour tuneability in rare-earth doped sol-gel nano-glass-ceramics for anti-counterfeiting luminescent stamps: an encoded lightkey**

S. Torres-García<sup>\*1</sup>; J. Méndez-Ramos<sup>1</sup>; P. Acosta-Mora<sup>1</sup>; A. Yanes<sup>1</sup>; J. del-Castillo<sup>1</sup>; C. Hernández-Álvarez<sup>1</sup>; M. Medina-Alayón<sup>1</sup>; A. Menéndez-Velázquez<sup>2</sup>

1. Universidad de La Laguna, Spain  
2. Centro IDONIAL, Spain

Spectral conversion materials, such as up-converting nanoparticles, are emerging as a cornerstone for the next generation of luminescent inks in anti-counterfeiting applications. In particular, rare-earth doped luminescent materials present significant advantages compared to standard fluorescent dyes, such as invisibility in ambient light, excitation by low cost commercial NIR irradiation and a lack in background noise due to negligible auto-fluorescence from the surface. However, to further improve the security level more attention needs to be paid on the codification of overall emitted

luminescence, so it will be more difficult to mimic by ever increasing sophisticated counterfeiters. Here, we present results based on colour tuneability in rare-earth doped sol-gel nano-glass-ceramics which has been analyzed and quantified in terms of CIE standard chromaticity diagram. In particular, intensity ratios among UV and VIS up-conversion emission bands can be tailored by modifying doping concentration level, that is, an encoded lightkey. Additionally, suitable electronic transitions of doping rare-earth-ions enable the possibility of dual-mode up-conversion and down-conversion luminescence displaying distinct fluorescence under 980 nm and under UV lamp. This feature implies that a predetermined read condition becomes a security feature itself. Thus, these materials provide a proof-of-concept example for light-responsive encryption security patterns.

## **Poster Session 2B (live presentations) also available in on-demand session**

1:30 PM

### **(MCARE-P-037-2021) TESTEC: PET and NBR based Cost Effective and Self-sustainable Triboelectric Energy Case for Powering Smart Electronic Devices**

A. Flores<sup>\*1</sup>; A. Abdullah<sup>1</sup>; A. Chowdhury<sup>1</sup>

1. University of Texas Rio Grande Valley, Science Department, USA

Triboelectric Nanogenerators (TENG) as one of the recent inventions, have been promoting sustainable development by utilizing mechanical motion through contact triboelectrification and electrostatic induction. In this work, A triboelectricity based self-sustainable and cost-effective energy case utilizing Polyethylene Terephthalate (PET) and Nitrile Butadiene Rubber (NBR) has been developed. The Triboelectric Stepping and Tapping Energy Case (TESTEC) has been designed to be compatible with touch electronic devices. It harnesses mechanical energy through the human motion created by foot stepping and finger tapping. The maximum output voltages were recorded as 14.2V for the front part (tapping motion) and 50.8V for the back part (stepping motion). The TESTEC was further tested with conventional electronics devices like bridge rectifiers, resistors, capacitor and LEDs which showed the capability to be used with conventional electronic components. TESTEC shows a huge new prospect in powering touch electronics, reducing the conventional way of powering.

### **(MCARE-P-038-2021) Hybrid Triboelectric-Electromagnetic Nanogenerator for Energy Scavenging**

E. Islam<sup>3</sup>; A. Chowdhury<sup>1</sup>; F. Tasnim<sup>\*1</sup>; A. Abdullah<sup>2</sup>; M. Martinez<sup>2</sup>; C. Olivares<sup>3</sup>; K. Lozano<sup>2</sup>; M. Uddin<sup>1</sup>

1. University of Texas Rio Grande Valley, Chemistry, USA  
2. University of Texas Rio Grande Valley, Mechanical Engineering, USA  
3. University of Texas Rio Grande Valley, The Mathematics and Science Academy, USA

This research shows the hybridization of Triboelectric Nanogenerator (TENG) and Electromagnetic generator (EMG) as a floor-tile, which converts the biomechanical energy of human footsteps to electrical energy. The TENG consists of oppositely charged layers of conductive aluminum and high-polarized Kapton with the electron acceptor layer of MoS<sub>2</sub>. The EMG is composed of copper coils and neodymium magnets. To ensure efficient performance, the hybrid system is connected via a parallel circuit with a bridge rectifier. The output reaches 5 mA of short-circuit current, 1200 V of open-circuit voltage, and 6 W of power. This hybrid nanogenerator produces 25 times more open-circuit voltage and 20% more power in comparison to a commercially sold energy-harvester floor tile, Pavegen. The novelty of TENG-EMG hybrid relies on the potential to be used for large scale practical applications. The developed hybrid NG allows for cost-effective, green, and sustainable energy conversion.



### (MCARE-P-039-2021) Novel Dipole-Pair [Zn, W] Substituted BaTiO<sub>3</sub> Ceramics

T. L. Whaley<sup>\*1</sup>; N. T. Smith<sup>1</sup>; V. R. Pellegrin<sup>1</sup>; K. Ning<sup>1</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA

Continued technology transformations with regard to electronic devices like capacitors, resonators, sensors, etc., require material enhancements with regard to properties and temperature range of operation of those properties. Relaxor ferroelectric materials have long been successful at supporting a myriad of electronic device technologies. Previous approaches to exploring relaxors is mainly based on morphotropic phase boundary (MPB) and polymorphic phase boundary (PPB) materials. The classic relaxors of the well-known PMN-PT variety are advantageous in the dielectric performance but contain Pb which is harmful to the environment. In this work, we report dipole-pair [Zn, W] substituted BaTiO<sub>3</sub> ceramics that show a unique relaxor-like behavior yet differ from classic relaxors. A systematic study includes crystal structure, microstructure, electric, dielectric and optic properties. The role of the dipole-pair concentration dependent relative permittivity is discussed. Current developments based on dipole-pair substitution imply an alternative methodology to creating novel relaxor-like ferroelectric materials.

### (MCARE-P-040-2021) Electric and Dielectric Behavior of the [Y, Ta] Dipole Engineered BaTiO<sub>3</sub> Ceramics

V. R. Pellegrin<sup>\*1</sup>; W. J. Hogan<sup>1</sup>; W. D. Senn<sup>1</sup>; K. Ning<sup>1</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA

Ferroelectric ceramics that provide relaxor/relaxor-like dielectric characteristics are essential for enhancing electronic devices and systems as well as for possible transformations to smaller footprint multifunction and multimode electronic devices. In this work, a series of [Y, Ta] dipole-pair engineered BaTiO<sub>3</sub> (BaTi<sub>1-2x</sub>[Y, Ta]<sub>x</sub>O<sub>3</sub>, x = 0 to 0.05) ceramics have been fabricated in order to achieve and assess the promising relaxor-like properties. The [Y, Ta] dipole-pairs have been introduced into BaTiO<sub>3</sub> matrix through a two-step process, in which Ba<sub>2</sub>ScTaO<sub>6</sub> is the source of dipole-pairs. The dipole-pair concentration dependent properties of microstructure, crystal structure, resistivity, activation energy, and band gap have been investigated and are reported. The diffuseness of the dielectric relative permittivity induced from the [Y, Ta] dipole-pair has been assessed and the relaxor-like dielectric behavior has been analyzed. This work offers useful guidance for creating novel ferroelectric materials, especially relaxor-like dielectrics, using dilute dipole concentrations.

### (MCARE-P-041-2021) Surface modified ZnSnO<sub>3</sub> nanocubes for enhanced piezoelectric power generation and sensory application

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

1. The University of Texas Rio Grande Valley, Chemistry, USA

In recent years, research on acquiring energy from innovative sources has been accelerated to address the energy crisis and demand for sustaining wireless, portable electronic devices. Piezoelectric nanogenerators and their mechanisms are held in high regard, due to their cost-effective structure and mechanical proficiency to harvest renewable energy, thus the need for their mechanical and functional advancement is in high demand. In this work, we propose a nanogenerator that comprises aluminum (Al)-doped zinc stannate (ZnSnO<sub>3</sub>) nanocubes as the piezoelectric material for energy harvesting and sensory applications. Furthermore, ZnSnO<sub>3</sub> was doped with 1 wt% to 5 wt% of Al nanoparticles. We reported that 2 wt% of Al-doped ZnSnO<sub>3</sub> showed the highest electrical output in terms of open-circuit voltages and short circuit current. The Al-doped ZnSnO<sub>3</sub> powder was evenly dispersed into Poly Dimethyl

Siloxane (PDMS) solution to create a piezoelectric film, that was encapsulated with pure PDMS and was bilaterally surrounded by two copper electrodes connected with copper wire. The nanogenerator device achieved an open-circuit voltage at a range of 80 V to 190 V with a load frequency range of 60 BPM to 240 BPM. With the presented high output-to-size ration taken into consideration, it can indicate a promising future for the field of piezoelectric sensors.

### (MCARE-P-042-2021) Emission Characteristics of Compression Ignition (CI) Engines Running on Waste Cooking Oil Based Biodiesel-nano Additive Blends

S. K. Fasogbon<sup>\*1</sup>; A. J. Apata<sup>1</sup>

1. University of Ibadan, Mechanical Engineering, Nigeria

Researchers have used nanoadditives with biodiesels in order to improve CI engines emissions characteristics; and behaviours have been found to be fuels-nanoadditives combinations specific. This work therefore studied CI engines on the combination effects of blends of diesel, waste cooking oil based biodiesel: B0 to B100 at 10 % incremental step; and aluminium oxide nanoparticles additive with dosages of 5g/l and 10g/l on each fuel blends. Results showed that 5g/l of aluminium oxide reduced CO emissions by a mean decrease of 2.04%-14% for all fuel blends and caused mean decrease of 3.45% - 16% in NO<sub>x</sub>, 10g/l of aluminium oxide also reduced CO emissions by a mean decrease of 6.1% - 28.6% for all fuel blends and a mean decrease of 10.3% - 32% for NO<sub>x</sub> emissions. (B20+10g/l) showed a mean decrease in CO and NO<sub>x</sub> by 22.6% and 34.6% respectively compared to B0, blends containing 5g/l had a mean decrease of 2.04% - 14% in CO and 4.5% - 18 % in NO<sub>x</sub> emissions compared to B0 while blends containing 10g/l had a mean decrease of 5.1% - 15.2% in CO and 7.5% - 27.5% in NO<sub>x</sub> emissions compared to B0. The paper concludes that (B20+10g/l) is the best blend in terms of lower CO and NO<sub>x</sub> emissions; and Introduction of aluminium oxide nano-additive is generally friendly to Waste Cooking oil Based Biodiesel, as it lowers both NO<sub>x</sub> and CO for all blends.

### (MCARE-P-043-2021) Fabrication of a Highly Sensitive Touchless Triboelectric Motion Sensor for Motion Sensing and Movement Monitoring Operations

D. L. Zamora<sup>\*1</sup>; A. Abdullah<sup>1</sup>; A. Chowdhury<sup>1</sup>; A. Flores<sup>1</sup>

1. University of Texas Rio Grande Valley, Chemistry, USA

Triboelectricity has been a wide used mechanism for motion sensing now a days. Almost all the device based on triboelectricity requires contact between two surfaces. In this work, we have developed a touchless triboelectric motion sensor for human motion sensing and movement monitoring. The device was primarily fabricated using commercially available latex rubber and copper which makes it a very cost-effective device for sensory applications. The device was tested with specimens of different areas and height in motion. The maximum output of the device was noted as 12V at a specimen height of 5cm. Further different types of human motion was applied Infront of the device. The device precisely provided significant output signals for each movement of human body which makes the device a perspective medium for motion sensing and movement monitoring. Further applications of this concept may be used in a variety of fields, such as medical and athletics, to measure and record the range of movement of the human body or a specific limb.

### **EHS S3: Multi-functional Energy Conversion Materials and Devices for Energy Harvesting and/or Sensing I**

Session Chairs: Yang Bai, University of Oulu; Chris Bowen, University of Bath

**2:15 PM**

#### **(EHS-026-2021) Core@shell nanoarchitectures as building blocks for single and hybrid energy harvesters (Invited)**

X. Garcia-Casas<sup>1</sup>; J. Castillo-Seoane<sup>1</sup>; N. Filippin<sup>1</sup>; F. Aparicio<sup>1</sup>; A. Ghaffarnejad<sup>1</sup>; L. Contreras-Bernal<sup>1</sup>; J. Budagoski<sup>1</sup>; C. Lopez-Santos<sup>1</sup>; A. Barranco<sup>1</sup>; J. Sánchez-Valencia<sup>1</sup>; A. Borras<sup>\*1</sup>

1. Materials Science Institute of Seville / Spanish National Scientific Council CSIC, Nanotechnology on Surfaces and Plasma Laboratory, Spain

During the last years, we have exploited the pioneering combination of small-molecule single-crystalline nanowires applied as soft-template with the deposition of a la carte functional layers by vacuum and plasma-assisted deposition methods. This approach has fostered the development of multifunctional supported nanoarchitectures with applications ranging from photonics to wetting, including nanosensors and nanostructured solar cells. In this communication, we will share the fundamentals of this innovative approach and the particular impacts on the development of piezoelectric and hybrid piezo-triboelectric nanogenerators. Thus, we will address the one-wire / one-device concept by developing core-multishell piezoelectric nanogenerators including conducting and polycrystalline piezoelectric shells in supported nanowires and demonstrate the advantages of the application of plasma-assisted deposition and plasma nanoengineering to optimize the performance of hybrid piezo-triboelectric harvesters. Finally, we will present the first steps towards the fabrication of nanoscale multisource energy harvesters by the plasma/vacuum one reactor approach.

**2:45 PM**

#### **(EHS-027-2021) Removing the need for a domain boundary in efficient photoexcited charge carrier separation (Invited)**

S. Dunn<sup>\*1</sup>; Y. Wang<sup>2</sup>; M. Zhang<sup>2</sup>; J. Liu<sup>3</sup>; H. Zhang<sup>4</sup>; F. Li<sup>5</sup>; C. Tseng<sup>6</sup>; B. Yang<sup>7</sup>; G. Smith<sup>7</sup>; J. Zhai<sup>2</sup>; Z. Zhang<sup>6</sup>; H. Yan<sup>2</sup>

1. London South Bank University, Chemical and Energy Engineering, United Kingdom
2. QMUL, SEMS, United Kingdom
3. Tsinghua University, Beijing, China., School of Environment, China
4. China Academy of Engineering Physics, IRTAC, China
5. Tongji University, Functional Materials Research Laboratory, China
6. Uppsala University, Solid State Electronics, Sweden
7. University of Chester, Faculty of Science and Engineering, United Kingdom

Ferroelectric materials exhibit anomalous behaviour due to domains and domain walls related to the spontaneous polarization inherent in the crystal structure. Control of ferroelectric domains and domain walls has been used to enhance device performances in ultrasound, pyroelectric detectors, and photovoltaic systems. It is also known that ferroelectrics including domain walls can double photocatalytic rate and increase carrier lifetime from microsecond to millisecond. However, there remains a lack of understanding on the different contributions of the domain and domain walls to photocatalytic activities. Herein it is found, by comparing samples of nanostructured  $\text{Ba}_{x}\text{Sr}_{1-x}\text{TiO}_3$  with and without a polar domain, that the material with polar domains has a faster reaction rate ( $k = 0.18 \text{ min}^{-1}$ ) than the nonpolar one ( $k = 0.11 \text{ min}^{-1}$ ). It is further revealed that the observed enhanced photoactivity of perovskite ferroelectric materials stems from the inherent polarization of the domain instead of domain walls. In this talk I will explore some experimentally derived new understanding of the underlying physics of materials with a spontaneous dipole. This new insight opens a door to enhance the performance of light induced energy

harvesting systems. It also has relevance for the range of systems that use functional materials to scavenge energy through vibration or thermal fluctuations.

**3:15 PM**

#### **(EHS-028-2021) Analysis and Experimental Results of Metamaterial for Vibration Energy Harvesting (Invited)**

Z. Hadas<sup>\*1</sup>

1. Brno University of Technology, Faculty of Mechanical Engineering, Czechia

This contribution deals with an analysis and design of metamaterials with embedded piezoelectric elements for energy harvesting purpose. The metamaterial consists of individual patterns which could be periodically repeated to final mechanical structure. Additive technologies for manufacturing of such mechanical structure could provide artificial layout of building blocks which embedded piezoelectric elements. The presented metamaterial is based on an auxetic structure with negative Poisson ration. The mechanical structure is printed from stainless steel and this design exploits PZT plates to provide electrical responses. Mainly characterization of individual multi-domain structure properties is an essential part of this contribution. The electric outputs depend on mechanical load or vibrations and several experimental outputs will be presented for vibration and impact loads. This metamaterial would open a doorway for design of a new class of smart structures for various energy harvesting purposes which cannot be realized now.

**3:45 PM**

#### **(EHS-029-2021) Modified Zinc Oxide Nanorods in Functional Polymer for Piezoelectric Energy Harvesting and Motion Sensing**

M. Sadat<sup>\*1</sup>; H. Majumder<sup>1</sup>; A. Abdullah<sup>2</sup>; M. Uddin<sup>1</sup>

1. University of Texas Rio Grande Valley, Chemistry, USA
2. University of Texas Rio Grande Valley, USA

Flexible Piezoelectric devices have garnered a lot of attention for their potential as energy harvesters and transducers. Zinc Oxide particularly has been doped with different metals and has been incorporated in functional polymers in order to produce flexible piezoelectric devices. In our study, we have incorporated 5 wt% Neodymium modified Zinc Oxide nanorods in PVDF matrix along with Multiwalled Carbon Nanotubes (MWCNT) to produce a flexible piezoelectric film. Wet chemical co-precipitation method was used to synthesize the Nd doped Zinc Oxide nanorods. Silver paste was applied on both sides of the piezoelectric film to produce a compact and flexible device. A linear response was shown by the film for variable stress. Compared to other modified Zinc Oxide nanostructures, superior electric output was also found when the device was being tested at different loads. The device also showed sensitivity during different body motion sensing. This demonstration shows that the piezoelectric film has a potential for being a superior energy harvester and a biological sensor.

**4:00 PM**

#### **(EHS-030-2021) Emerging halide perovskites with ultralow thermal conductivity for thermoelectric applications**

L. Zheng<sup>\*1</sup>; A. Nozariasmarz<sup>1</sup>; K. Wang<sup>1</sup>; B. Poudel<sup>1</sup>; S. Priya<sup>1</sup>

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

Halide perovskites have drawn tremendous attentions as next-generation solar energy harvesting materials thanks to their superior optoelectronic properties. Recent researches reveal their ultralow thermal conductivity because of phonon scattering effect and dynamic cation off-centering. These findings make halide perovskites to be considered as "electron-crystal and phonon-glass" materials, which are promising candidates for thermoelectric applications. In this presentation, we will review the state-of-art thermoelectric halide perovskites and discuss their unique features in details. The tunable charge and heat transport properties and

adjustable lattice structures by doping and substitution of ions in halide perovskites, the potential of harvesting both light and heat in a single device, as well as their cost-effective processing, predict the fast blooming of this field.

**4:15 PM**

**(EHS-031-2021) Relaxor-ferroelectrics: An efficient material for waste-heat harvesting**

A. Sharma<sup>\*1</sup>; M. Behera<sup>1</sup>; S. Pradhan<sup>1</sup>; M. Bahoura<sup>1</sup>

1. Norfolk State University, Materials Science, USA

The need for efficient energy utilization is driving research to harvest waste-heat, which is ubiquitous, abundant, and free. Thermal energy harvesting for low power electronic devices using ferroelectric materials is one of the emerging areas of research because they possess spontaneous polarization and exhibit excellent pyroelectric coefficients. These materials are unique as they only sense time-dependent temperature change to generate electric power. We have grown lead-free  $\text{BaZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  (BZT)/ $\text{Ba}_{0.7}\text{Ca}_{0.3}\text{TiO}_3$  (BCT) multilayer heterostructures on  $\text{SrRuO}_3$  (SRO) buffered  $\text{SrTiO}_3$  (STO) single crystal substrates by optimized pulsed laser deposition (PLD) technique. The large angle x-ray scans showed only diffraction peaks from the substrate and pseudocubic reflections (100) from the multilayer heterostructures. This confirms that these films are phase pure, highly crystalline, and epitaxial in nature. We have developed a device with a capacitive structure of 200 nm thick BZT/BCT multilayer heterostructures sandwiched between platinum top and SRO bottom electrodes. The device demonstrates excellent pyroelectric current of ~600 nA in response to temperature fluctuation of 11 K using a laser diode of wavelength 850 nm with a repetition rate of 0.1 Hz and power 150 mW. Our findings suggest that the relaxor-ferroelectric thin film may be competitive with thermoelectric materials for low-grade thermal harvesting.

**4:30 PM**

**(EHS-032-2021) Low Grade Waste Heat Recovery Using Shape Memory Alloys**

N. Liu<sup>\*1</sup>; B. Poudel<sup>1</sup>; R. LaSalle<sup>1</sup>; S. Priya<sup>1</sup>

1. penn state university, Materials Science and Engineering, USA

To harness the waste heat with low energy density and low temperature (<100 °C) in the daily life has become a rising topic for heat engine application. Shape memory alloys (SMAs) has become a good candidate to convert the low-grade thermal waste to the mechanical energy/electrical energy. Such materials are predicted to outperform thermoelectric materials' conversion efficiency in temperatures below 100 degrees Celsius. SMAs undergo shape memory and superplastic characteristics accompanying with the transformation between martensite and austenite phases. The reversible phase transformation under the proper thermal/strain cycling is the necessity condition for generating high efficiency, low figure and thermal hysteresis. The drawbacks of commercially used Nitinol SMAs are the weak mechanical properties-fatigue resistance. Hence, developing novel SMAs candidates for heat engine application turn to be increasingly significant. In this presentation, we will discuss the SMAs based on Ti-Ni-Cu Ti-Ni-Cu-Pd systems performed a room temperature transformation, high thermal cycle, and low thermal hysteresis by tuning the composition.

**MCARE S5: Development and Synthesis of Novel Optical Materials - II**

Session Chair: Yuanbing Mao, Illinois Institute of Technology

**2:15 PM**

**(MCARE-073-2021) Influence of Growth and Processing Conditions on the Properties of Si-C-N:H Thin Film Structures (Invited)**

A. Abdelal<sup>1</sup>; Z. Khatami<sup>2</sup>; P. Mascher<sup>\*1</sup>

1. McMaster University, Engineering Physics, Canada
2. University of New Brunswick, Canada

Silicon carbonitrides ( $\text{SiC}_x\text{N}_y$ ) have attracted interest for the manufacturing of materials with robust mechanical properties and promising optical features, suitable for applications in high-performance optoelectronics and in harsh environments. This is a consequence of their unique properties inherited from the combined properties of binary substructures, silicon carbide (SiC), silicon nitride (SiN), and carbonitride (CN). In this presentation, we will show that the visible photoluminescence emission from  $\text{SiC}_x\text{N}_y$  films fabricated by plasma enhanced chemical vapour deposition (PECVD) is stronger than that of SiC and SiN materials and the optical properties (band gap, transmittance, index of refraction, and light emission) can be controlled by adjusting the growth parameters, the process conditions (including the type of carbon precursor) and the carbon content.

**2:45 PM**

**(MCARE-074-2021) Low-power upconverting nanoparticle microlasers (Invited)**

E. Chan<sup>\*1</sup>

1. Lawrence Berkeley National Laboratory, The Molecular Foundry, USA

Lanthanide-doped nanomaterials exhibit complex photophysical dynamics that give rise to photon upconversion, which can be leveraged for optoelectronics and imaging. I will discuss the high-throughput discovery and application of new classes of upconverting nanoparticles, including one class that utilizes an avalanche-like energy looping mechanism to non-linearly amplify the population of excited states. This unique mechanism, excited at 1064 nm, enables such "energy-looping nanoparticles" (ELNPs) to be imaged through millimeters of brain tissue. By coupling ELNPs to the whispering gallery modes of polystyrene microspheres, the resonators achieve sufficient gain to exhibit continuous-wave, anti-Stokes lasing that is stable for hours at room temperature. We demonstrate that microlasers with record low thresholds and high quality factors can be fabricated with high fidelity by controlling the number of layers, surface charge, and ligand coordination of the nanoparticles as they assemble onto cavity surfaces. These microlasers operate even in complex biological media such as serum and through tissue-mimicking phantoms. We further reduce the dimensions and thresholds of upconverting nanoparticle lasers by tuning their compositions, shells, and by coupling them to plasmonic arrays. These results suggest that upconverting microlasers may be applied to in vivo sensing and super-resolution imaging through tissue.

**3:15 PM**

**(MCARE-075-2021) Novel Properties of Metal Halide Perovskites: From Quantum Dots to Magic Sized Clusters and Molecular Clusters (Invited)**

J. Z. Zhang<sup>\*1</sup>

1. University of California Santa Cruz, Chemistry and Biochemistry, USA

Metal halide perovskites (MHPs) with  $\text{ABX}_3$  structure exhibit novel electronic, optical and magnetic properties that are promising for various applications. However, instability due to various factors presents a major challenge to their applications. The surface of the perovskites strongly affects stability. We have developed different

surface passivation strategies to stabilize perovskite quantum dots (PQDs) and bulk films using surface chemistry approaches based on molecular ligands. One important finding is that ammonium ions and carboxylate groups have synergistic effects in surface passivation, attributed to simultaneous passivation of both anionic and cationic defects. Recently, we have found a simple strategy to synthesize and stabilize perovskite magic sized clusters (PMSCs), including doped PMSCs, for the first time, that exhibit interesting optical properties important for emerging applications such as single photon emitters. In our effort to understand the growth mechanism of PMSCs, we discovered a new species that we call molecular cluster (MCs) that do not contain the A component of the perovskites. The MCs can be converted into more stable MCs. Our studies demonstrate that surface chemistry approaches are promising for stabilizing MHPs, leading to generation of PMSCs, QDs, and ultimately QD solids, which is significant for many emerging applications.

### **MCARE S15: Materials and Devices for Energy Production and Storage**

Session Chair: Kelsey Stoerzinger, Oregon State University

#### **2:15 PM**

#### **(MCARE-076-2021) Light-driven control of ultrafast H-atom abstraction reactions (Invited)**

C. W. Schlenker\*<sup>1</sup>

1. University of Washington, Chemistry, USA

We use ultrafast pump-push-probe spectroscopy and time-resolved PL to monitor excited-state H-atom transfer from hydroxylic compounds to an anisole-functionalized heptazine (TAHz). The heptazine moiety is structurally related to the monomer unit of the ubiquitous organic polymeric photocatalyst, carbon nitride. We show that TAHz can photochemically abstract an H-atom from water, in addition to generating H<sub>2</sub> in aqueous suspensions with photocatalytic activity matching that of carbon nitride. In our multi-pulse experiment, we use resonant pump pulse to photoexcite TAHz to a bright high-lying excited state, and after a relaxation period of roughly 6 ps, we use a NIR (1150 nm) pulse to “push” the chromophore to a higher-lying excited state. When phenol is present, the push induces a persistent decrease ( $\Delta\Delta OD$ ) in the initial excited-state absorption, indicating the push pulse engenders a divergence in the photochemical branching ratios. These results reveal new insight into the branching ratio among unreactive localized heptazine excited states and reactive intermolecular charge transfer states of H-bonded heptazine chromophores. More generally, this work provides new insight into molecular design strategies to control the excited-state photochemistry of important reactions such as H-atom abstraction from water.

#### **2:45 PM**

#### **(MCARE-077-2021) Energetic Cost for Being “Redox-Site-Rich” Nickel–Aluminum Layered Double Hydroxide Pseudocapacitive Materials (Invited)**

D. Wu\*<sup>1</sup>; X. Zhang<sup>1</sup>; C. Cockreham<sup>1</sup>

1. Washington State University, Alexandra Navrotsky Institute for Experimental Thermodynamics, USA

Pseudocapacitors have fast charge-discharge kinetics, high power density and long cycling stability. Intralayer compositional tuning of redox site concentration is effective to enhance the performance of pseudocapacitive materials, such as specific capacitance and energy density. Here, I present our recent study on the structure-energetics-performance relationships of nickel–aluminum layered double hydroxides (NiAl-LDHs) as a function of Ni/Al ratio. Specifically, Ni/Al ratio increase leads to van der Waals gap expansion, resulting in fast charge-discharge kinetics, decreased crystallinity and high cycling stability. Interestingly, taking advantage of a full spectrum of

calorimetric methodologies in our lab, and several powerful in situ structural and spectroscopic techniques, we find that Ni enrichment decreases the energetic stability of both as-made (hydrated) and dehydrated NiAl-LDHs, evidenced by the calorimetrically measured enthalpies of formation. Moreover, the highest specific capacity (2128 F/g at 1 A/g) at Ni/Al = 3 is the product of subtly balanced compositional, structural and thermodynamic factors. Especially, the enthalpies of hydration, which energetically stabilize Ni redox sites, solvate carbonate ions, and fill interlayer space, in other words, paying for the “energetic cost” of being “redox site rich”.

#### **3:15 PM**

#### **(MCARE-078-2021) Energy Storage in Permanently Porous Polymorphs of Metal Chalcogenides (Invited)**

C. K. Brozek\*<sup>1</sup>

1. University of Oregon, Chemistry and Biochemistry, USA

Energy storage at electrode surfaces requires that stored charges be balanced by mobile charge-balancing counterions. Capacitance decreases if these ions sit far from the stored charges or if the energy storage mechanism necessitates large applied potentials. High-surface area electrodes are therefore desirable for permitting charge-balancing ions to be intimately paired at the electrical double layer with the stored charges. Impressive capacitances have been achieved with a family of 2D sheet materials composed of mixed-metal chalcogenides. Owing to the redox activity of the metals and chalcogenides, high capacitances can be achieved so long as cations can access the high-surface area planar sheets. At high concentrations, however, these sheets aggregate and block the accessibility of ions, which shuts off capacitance. Here, we report permanently porous metal chalcogenide materials that ensures constant exposure of electrode surfaces to charge balancing ions for robust energy storage.

#### **3:45 PM**

#### **(MCARE-079-2021) Novel radical conjugated polymer with high electrical conductivity for thermoelectric applications (Invited)**

E. Orgiu\*<sup>1</sup>

1. Institut National de la Recherche Scientifique (INRS), EMT Centre, Canada

While the chemical doping of conjugated organic polymers has been demonstrated to result in 6-order of magnitude increases in electrical conductivity, a novel type of non-conjugated polymer has also been recently reported to feature a similarly high electrical conductivity of 28 S m<sup>-1</sup>. While this achievement clearly demonstrated the potential of polymers with radical pendent group for highly conductive films, a very limited inter-chain transport was highlighted by a 6 order of magnitude decrease at channel lengths over 600 nanometers. In the framework of the development of alternative polymers with high doping levels for thermoelectric applications, we explore a novel polymer that aims to take advantage of the high conductivity provided by the radical pendant groups combined with doping capabilities provided by the conjugated backbone to achieve high performances at larger channel lengths. The results from the electrical and morphological characterization are compared to those obtained from a similar albeit radical pendent group-free polymer to highlight the role of the radical units in the charge transport capabilities of the novel material. This novel concept paves the way for a new class of organic (semi)conducting polymers.

4:15 PM

**(MCARE-080-2021) Atomistic Engineering of the Energy Materials of the Future (Invited)**S. R. Spurgeon\*<sup>1</sup>

1. Pacific Northwest National Laboratory, Energy and Environment Directorate, USA

The development of advanced thin film synthesis techniques over the past several decades has sparked a renaissance in the design of nanomaterials for clean energy and quantum computing technologies. While it is now possible to produce oxides and semiconductors in almost limitless configurations, engineering of desirable functionality for device applications depends on precise control of atomistic structure and defects. Complex synthesis pathways can lead to significant deviations from idealized structures, which occur at length scales that are difficult to probe experimentally and theoretically. This task is further compounded by dynamic changes imparted by the electron and ion beam during imaging and processing. We have developed a materials design strategy based on state-of-the-art synthesis, modeling, and characterization, underpinned by aberration-corrected scanning transmission electron microscopy. I will describe our efforts to control nanoscale defect formation in oxides and semiconductors using insights from atomistic imaging and spectroscopy informed by theory simulations. Our results illustrate how the full range of information from modern electron microscopy can unlock promising new materials for energy conversion and storage.

4:45 PM

**(MCARE-081-2021) Solvent-Based Synthesis and Integration of Nanostructured Alloying Electrode Materials with Controlled Surface Chemistry and Morphology (Invited)**V. C. Holmberg\*<sup>1</sup>

1. University of Washington, Chemical Engineering, USA

Careful control over composition, morphology, and surface chemistry are critical in virtually every materials system, and it is vital that these attributes are preserved in any scalable production process. This talk will explore the important role that the above characteristics play in our group's research on the supercritical-fluid-based synthesis and integration of nanostructured, high-capacity alloying electrode materials for electrochemical energy storage in Li- and Na-ion battery systems. Clearly, careful control over interfacial chemistry and surface reactions are critical for the design of robust electrochemical systems. These nanostructured composite materials have short internal diffusion pathways, possess robust mechanical characteristics, and can be processed in either liquid dispersion or solid/powder form. We show that careful control over active material surface chemistry helps to facilitate robust solid-electrolyte interphase layer formation, demonstrate that nanowire-based alloying electrodes can maintain capacity retention in the complete absence of fluorinated additives, fluorinated electrolytes, and fluorinated binders, and show that electrode processing plays a critical role in the formation of a robust composite architecture and overall device performance.

5:15 PM

**(MCARE-082-2021) 3D Lithium-ion Battery Architectures – From Design to Fabrication (Invited)**C. L. Cobb\*<sup>1</sup>

1. University of Washington, Department of Mechanical Engineering, USA

Technology progressions in wearable devices, portable electronics and electric vehicles have motivated a shift in Lithium-ion (Li-ion) batteries to accommodate rapid charge, long life, high power and energy materials with more efficient packaging. An emerging trend to address this technology shift is the use of Additive Manufacturing (AM) techniques to rapidly fabricate 3D batteries with customized geometries on a micron to millimeter scale, changing the way we

fundamentally design and manufacture energy storage devices today. 3D battery architectures enhance ion transport in existing battery materials, thereby increasing gravimetric and volumetric energy and power densities relative to conventional Li-ion batteries. Typically, increases in power density are only possible through sacrifices in energy density. Our research has shown that electrode architectures can mitigate these common trade-offs. This talk will focus on promising concepts in high-performance 3D batteries, with a focus on computational design and AM for Li-ion chemistries.

Thursday, July 22, 2021

**EHS S3: Multi-functional Energy Conversion Materials and Devices for Energy Harvesting and/or Sensing II**

Session Chairs: Chris Bowen, University of Bath; Steven Dunn, LSBU

9:00 AM

**(EHS-033-2021) Organic and organic-inorganic hybrid ferroelectric materials for piezoelectric energy harvesting applications (Invited)**R. Boomi Shankar\*<sup>1</sup>

1. Indian Institute of Science Education and Research, Pune, Department of Chemistry and Centre for Energy Science, India

Materials showing Ferro- and piezoelectric properties are of immense attention due to their utility in technology devices and recently as electrical energy harvesters from mechanical forces. Our group is interested in the generation of ferroelectric organic and hybrid organic-inorganic molecular salts supported by phosphonium or ammonium cations and various anions and employ them to fabricate nanogenerators. In a preliminary study, we showed the ferroelectric behavior of a salt of diphenyl diisopropyl phosphonium cation with  $\text{PF}_6^-$  anion. Its composites with polydimethylsiloxane (PDMS) were employed as the elusive all-organic mechanical energy harvesting devices. The use of tetrahedral anions such as  $\text{BF}_4^-$ ,  $\text{ClO}_4^-$  and  $\text{IO}_4^-$  ions gave rise to a family of Ferro- and piezoelectric phosphonium salts with excellent energy harvesting properties. Subsequently, we prepared the hybrid salts with  $\text{A}_2\text{MX}_4$ ,  $\text{AMX}_3$ , and  $\text{A}_4(\text{ML}_6)$  compositions from phosphonium or ammonium cations and halogenometallate or pseudo-halogenometallate anions. Composites of these frameworks with commercial polymers such as PDMS and polyurethane were employed as piezoelectric energy harvesters with relatively high output performances.

9:30 AM

**(EHS-034-2021) Porous piezoelectric particulate composites, processing, characterisation and modelling (Invited)**H. Khanbareh\*<sup>1</sup>; S. E. van Kempen<sup>2</sup>; K. de Boom<sup>3</sup>

1. University of Bath, Mechanical Engineering, United Kingdom  
 2. RWTH Aachen, Germany  
 3. Delft University of Technology, Netherlands

Piezoelectric particulate composites consisting of piezoelectric ceramic particles in a polymer matrix are a versatile class of piezoelectric materials due to the large variation in achievable properties via tuning the composition of the ceramic particles, their shape, volume fraction and topological orientation and by selecting the appropriate polymer. This presentation summarises modelling and experimental studies of the quasi 1-3 composites in which the piezoelectric particles are aligned via a dielectrophoretic process prior to curing of the polymer matrix. Final properties are linked to those of constituent materials and their topological arrangement. Effect of porosity on the overall mechanical and functional properties of the composites is investigated. Composites of PZT-porous PU are

manufactured in random and structured particle configurations, and their mechanical and functional properties are investigated. The addition of a gaseous phase in the form of spherical well-distributed inclusions effectively reduces the permittivity of PU polymer, which improves the piezoelectric voltage coefficient and FoM of the porous PZT-PU composites significantly. The unique combination of dielectrophoretic structuring of PZT particles and the addition of porosity to the polymer resin results in the best performance of the particulate composite reported in the literature.

**10:00 AM**

### **(EHS-035-2021) MOF Derived Fiber Nanogenerator for Efficient Acoustoelectric Energy Conversion (Invited)**

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

1. Institute of Nano Science and Technology, QMaD, India

Real time application of piezoelectric nanogenerators (PNGs) under harsh environment remain a challenge due to lower output performance and poor durability. Thus, development of flexible, sensitive and stable PNGs became a topic of interest to capture different human motions including gesture monitoring to speech recognition. Herein, a scalable approach is adapted where two-dimensional (2D) metal organic framework (MOF) reinforced poly(vinylidene fluoride) (PVDF) composite nanofibers mat is prepared to fabricate flexible and sensitive composite piezoelectric nanogenerator (C-PNG). The incorporation of single crystalline 2D MOF ensures a large content of electroactive phases (98%) with a resultant high magnitude piezoelectric co-efficient of 41 pC/N in composite nanofibers mat due to the interfacial specific interaction with  $-\text{CH}_2/-\text{CF}_2$ -dipoles of PVDF. As an outcome, C-PNG generates high electrical output with a very fast response time under periodical pressure imparting stimuli. Benefitting from bending and twisting functionality, C-PNG is capable to scavenge biomechanical energy by mimicking complex musculoskeletal motions that broaden its application in wearable electronics and fabric integrated medical devices. In addition, C-PNG also demonstrates an efficient acoustic vibration to electric energy conversion capabilities with improved power output and acoustic sensitivity.

**10:30 AM**

### **(EHS-036-2021) Li and Ta modified KNN nanofibers for vibrational energy harvesting applications**

A. Ichang<sup>1\*</sup>; S. V. Vladimirov<sup>2</sup>; D. C. Lupascu<sup>2</sup>; K. Le<sup>1</sup>; M. Grosch<sup>1</sup>; A. K. Schmidt-Verma<sup>1</sup>; C. Bohr<sup>1</sup>; A. Verma<sup>1</sup>; T. Fischer<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Inorganic Chemistry, Germany  
2. Institute for Materials Science and Center for Nanointegration Duisburg-Essen, Germany

Renewable energy harvesting has taken a central role in tackling 21st-century energy challenges. Reliable, efficient, and robust energy harvesting systems are the need of the hour. We are surrounded by systems that run on different sources of energy, and without any exception, a portion of this energy goes unutilized as waste energy—for example, the vibrations and heat emitted from a car's engine. On a big scale, renewable energy is harvested by many different methods like solar, geothermal, wind turbines, etc. However, on a micro-scale, piezoelectric materials have been among the most promising methods to harness energy. Currently, in most piezoelectric applications, the Lead Zirconate Titanate (PZT) finds usage owing to its high piezoelectric constant. However, as lead is a highly toxic material, the search for an alternative biocompatible lead-free piezoelectric material has become a priority. In this work, we present a flexible nanogenerator based on biocompatible Potassium Sodium niobate (KNN) nanofibers for their suitability in scavenging the vibrational energies. Herein, we provide a strategy to enhance the piezoelectric voltage output of the nanogenerator by engineering not only the morphology of the material but also by tuning the composition of KNN with Li and Ta inclusion in the unit cell lattice.

**10:45 AM**

### **(EHS-037-2021) Opto-electric, opto-mechanical and opto-thermo-electric control of ferroelectric domains for multi-source energy harvesting and sensing**

Y. Bai\*<sup>1</sup>; G. Vats<sup>2</sup>; J. Seidel<sup>3</sup>; J. Juuti<sup>1</sup>

1. University of Oulu, Finland  
2. KU Leuven, Belgium  
3. UNSW Sydney, Australia

In recent years, narrow band gap photoferroelectrics that are both ferroelectric and visible light responsive, have been developed and attracted attentions in both insulating ferroelectrics/piezoelectrics and semiconductor research. The generation of photo-excited charge carriers upon absorbing visible light in ferroelectric materials offers an additional degree of freedom to manipulate polarizations, domains and domain walls thus realizing many potential combinations of functionalities when subject to optical, electrical, mechanical and thermal stimuli in a single piece of material. In this talk, a series of research of such functionality combinations for multi-source energy harvesting and sensing applications based on a narrow band gap photoferroelectric material, KNBNNO ((K,Na,Ba)(Nb,Ni)O<sub>3-δ</sub>), carried out in our group in the recent five years will be overviewed. Emphasis will be put on the discussions of how manipulation of domain wall motion with two or more of the above-mentioned energy inputs can increase the performance of an energy harvester or sensor. This talk will hope to inspire researchers to further advance this emerging energy harvesting concept either by developing materials with higher properties than those of KNBNNO or applying KNBNNO in energy harvesting/sensing circuits, devices and systems.

### **MCARE S5: Plasmonic / Photonic Manipulation of Conversion Processes I**

Session Chair: Eva Hemmer, University of Ottawa

**9:00 AM**

### **(MCARE-076-2021) A Multi-functional Highly Efficient Upconversion Luminescent Film (Invited)**

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

1. Kyung Hee University, Applied Chemistry, Republic of Korea

Upconversion luminescence arise by converting low energy photons into one higher energy photon. However, low luminescence conversion efficiency of upconversion nanoparticles hinders their broader and more practical application for photovoltaics, bioimaging, and displays. In this work, we demonstrate multi-functional upconversion nanoparticles integrated with photonic platforms, which consists of dielectric microbeads decorated with plasmonic metal nanoparticles on an insulator/metal substrate. With the proposed platform, the upconversion luminescence intensity is enhanced by three orders compared to the reference, and functionalities such as wearability, flexibility and transparency are obtained.

**9:30 AM**

### **(MCARE-077-2021) Omnidirectional, Broadband Light Absorber with High Aspect Ratio (AR) Nanoturf structures for Solar-Thermal Conversion**

J. Kim\*<sup>1</sup>; T. Kim<sup>1</sup>

1. Sungkyunkwan University, School of Chemical Engineering, Republic of Korea

Although much attention has been paid to the development of photothermal materials and designs that can convert solar irradiation into exploitable thermal energy, it remains some obstacles such as limited light absorbing band and narrow incident angle. This study proposes a black gold-coated hierarchical nanoturf (Au/h-nanoturf) membrane incorporated with randomly distributed high aspect ratio (AR) nanostructures and micro-through

holes. Thanks to structural advantages, this large area membrane exhibited good absorption of the broadband solar light spectrum. The h-nanoturf is further combined with a microcone array to enhance solar absorption extended to the near-infrared range as well as the omnidirectional incident direction of the light. The fundamental mechanism of the strong omnidirectional broadband absorption performance of the h-nanoturf was thoroughly analyzed with computational electrodynamic simulations. Consequently, we employed the Au/3D h-nanoturf with microscale hole ( $\mu$ -hole) membrane to fabricate an advanced solar-vapor generator.

9:45 AM

**(MCARE-078-2021) Addressing Plasmonic Catalysis with Designer Nanoparticles (Invited)**

P. Camargo\*<sup>1</sup>

1. University of Helsinki, Finland

The localized surface plasmon resonance (LSPR) excitation in plasmonic nanoparticles can accelerate and control molecular transformations. This field, named plasmonic catalysis, opens possibilities for the solar to chemical energy conversion, new/alternative reaction pathways not accessible via thermally activated catalytic processes, and to address traditionally challenging chemical transformations. As both catalytic and optical properties can be tuned by controlling physicochemical parameters at the nanoscale, design-controlled nanomaterials can unlock the potential of plasmonic catalysis in terms of fundamental understanding and optimization of performances. This talk will cover developments on the solution-phase synthesis of well-defined plasmonic and plasmonic-catalytic hybrid nanoparticles and their use to gain an understanding of structure-performance relationships in plasmonic catalysis. We will start by discussing how size, shape, morphology, and metal-support interactions in plasmonic nanoparticles influence their performances. Then, we highlight how hybrid materials containing both catalytic and plasmonic components enable one to extend the use of plasmonic catalysis to metals or oxides that are important in catalysis but do not support LSPR excitation in the visible or near-infrared range. Examples of control over reaction selectivity under visible light excitation will be discussed.

10:15 AM

**(MCARE-079-2021) Optical Field Coupling in ZnO Nanorods Decorated with Silver Nanoparticles**

M. Gilzad Kohan\*<sup>1</sup>; A. Camelini<sup>2</sup>; S. You<sup>1</sup>; A. Vomiero<sup>1</sup>; I. Concina<sup>1</sup>; M. Zavelani-Rossi<sup>2</sup>

1. lulea university of technology, engineering sciences and mathematics, Sweden  
2. Politecnico di Milano, Italy

The energy transfer from plasmonic metals to electron-accepting semiconductors features an undeniable pattern for enhancing the performance of the energy conversion systems and optoelectronic devices. Within this scheme, understanding the underlying mechanisms of plasmonic charge transfer from noble metals to semiconductors and vice versa, due to optical light field interactions is of paramount importance for designing optoelectronic devices. In this work we comprehensively studied the carrier redistribution mechanisms of a 1-dimensional metal-semiconductor Schottky architecture, holding the dual feature as a hot-electron plasmonic system and a simple metal/semiconductor junction. We obtained strongly enhanced external quantum efficiency of the plasmonic Ag decorated ZnO semiconductor in both band-edge region of ZnO and the corresponding absorption profile of the Ag NPs. Simultaneously, insertion of an insulating  $\text{Al}_2\text{O}_3$  spacer layer resulted in parallel distinction of the two main non-radiative carrier transfer mechanisms of plasmonic NPs, i.e. direct electron transfer and plasmonic induced resonance energy transfer. The multi-wavelength pump-probe spectroscopy indicated the very fast radiative transfer dynamics of the system in <500fs below 389nm. We demonstrate the

13% increase of photogenerated current in ZnO upon visible irradiation as a result of non-radiative hot-electron injection from Ag NPs.

**MCARE S5: Plasmonic / Photonic Manipulation of Conversion Processes II**

Session Chair: Eva Hemmer, University of Ottawa

10:45 AM

**(MCARE-080-2021) Near-infrared driven photocatalysis for extending spectral response of water-splitting semiconductor electrodes: Up-conversion, what else? (Invited)**

J. Méndez-Ramos\*<sup>1</sup>; P. Acosta-Mora<sup>1</sup>; J. del-Castillo<sup>1</sup>; A. Yanes<sup>1</sup>; S. Torres-García<sup>1</sup>; C. Hernández-Álvarez<sup>1</sup>; M. Medina-Alayón<sup>1</sup>; A. Menéndez-Velázquez<sup>3</sup>; N. Khaidukov<sup>2</sup>

1. Universidad de La Laguna, Departamento de Física, Spain  
2. Russian Academy of Sciences, Russian Federation  
3. Centro IDONIAL, Spain

Spectral conversion of light is an emerging route for enhancing the efficiency of solar energy harvesting schemes. We present evidence of NIR-to-UV-VIS photon conversion for degradation of organic dyes and hydrogen and oxygen evolution via water-splitting. In particular high intense UV-blue up-conversion emissions in rare-earth doped  $\text{K}_2\text{YbF}_7$  hydrothermal crystals and solvothermal  $\text{Sr}_2\text{YbF}_7:\text{Yb}^{3+}/\text{Sr}_2\text{YF}_7$  core-shell nanocrystals have been implemented to methylene blue photocatalytic degradation experiments. Up-conversion driven photocatalysis is proved, as a solely photonic effect, converting incident NIR radiation before reaching the contaminated solution. Reported emphasis on control checks is of extreme importance to avoid false narrative, experimental flaws or misinterpretation of up-conversion sensitized photocatalysis. In other words, up-conversion emission by itself can boost the photocatalytic reaction efficiency, without other adsorption or possible side effects due to NIR laser radiation, as a univocally photonic effect. Up-conversion, what else? These results would shine a light on the effective harvesting of the near-infrared part of sunlight for green hydrogen generation and environmental purification.

11:15 AM

**(MCARE-081-2021) Catalysts for Water splitting: 2D layered materials and transition metal phosphides (Invited)**

T. A. Shifa\*<sup>1</sup>; A. Vomiero<sup>1</sup>

1. Lulea University of Technology, Experimental physics, Sweden

The catalysis of water splitting reaction has been considered the most promising way to produce pure hydrogen economically and efficiently. In this regard, 2D layered materials and transition metal phosphides have got copious attention. The current research trend focuses on the efforts to maximize the exposure of active sites. Here, I present strategies to enhance the catalytic (electrocatalysis, photocatalysis) performance of these materials giving a particular emphasis for transition metal dichalcogenides (TMDs), transition metal phosphorus trichalcogenides (MPX<sub>3</sub>; X=S,Se) and nickel phosphides. I discuss the advantages of these materials for catalysis and the different routes available to tune their electronic states and active sites. Experimental results show that doping and hybrid material formation play a significant role in optimizing the free energy of hydrogen adsorption and desorption on the vertically oriented nanosheets of WS<sub>2</sub>, NiP<sub>2</sub>, and Ni<sub>5</sub>P<sub>4</sub>. Moreover, layered MPX<sub>3</sub> (M= Mn, Ni, Fe, Cu/In) nanosheets demonstrate a promising activity in sacrificial agent-free photocatalytic water splitting under simulated Sun light (AM 1.5G) illumination.

11:45 AM

## (MCARE-082-2021) Catalyst synthesis and characterization for electrochemical water splitting

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For electrolysis of water, the development of cheap and efficient catalysts is needed to efficiently catalyze oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) activities which are essential for the advancement of renewable energy technologies. In both OER and ORR cases, the catalysis process is limited by the requirement of the 4-e transfer process which is considered as sluggish kinetics. In this regard, we develop Ag<sub>2</sub>S and MoS<sub>2</sub> composite anchored on reduced graphene oxide (RGO), silver nanoparticles decorated on MoS<sub>2</sub> nanosheets, and a core-shell structure of NiMoO<sub>4</sub>@Co<sub>3</sub>O<sub>4</sub> which are used as HER, OER, and ORR electrocatalyst. Due to the presence of silver, the Ag-doped MoS<sub>2</sub> catalyst shows more than 1.5 times an increase in the roughness-normalized rate of OER. In other work, we propose a core-shell structure of hydrated NiMoO<sub>4</sub> nanorods conformally covered by Co<sub>3</sub>O<sub>4</sub> nanoparticles via Atomic layer depositions, resulting in a promising catalyst. In-situ Raman analysis and Synchrotron-based photoemission spectroscopy confirm that the catalyst reconstructs and transformed irreversibly to NiOOH, which can be considered as the centers of the active site maintaining the highest activity towards OER. In general, the results can significantly boost the practical water splitting process using a very cheap and efficient catalyst which can minimize the needs of precious noble metal.

## MCARE S6: Materials, Components and Devices for Self-powered Electronics II

Session Chair: Miso Kim, Sungkyunkwan University

9:00 AM

### (MCARE-083-2021) Enhancement of energy conversion efficiency achieved of magneto- mechano-electric generators by optimization of interfacial layer

S. Kim<sup>\*1</sup>; A. Thakre<sup>1</sup>; D. Patil<sup>1</sup>; G. Hwang<sup>2</sup>; J. Ryu<sup>1</sup>

1. Yeungnam university, Materials science and engineering, Republic of Korea
2. Pukyong National university, Republic of Korea

Among various energy harvesters to satisfy demand of power requirement under low magnetic field, a cantilever structured magneto-mechano-electric (MME) energy harvester comprising interfacially coupled magneto-electric (ME) composites via epoxy adhesive having a permanent magnetic proof mass is promising candidate. In MME energy harvester, the mechano-electric coupling at interface is major factor to achieve enhanced performance which depends on interfacial adhesive layer. However, researchers have attempted to enhanced the output power of ME composites by improving interfacial adhesive layer not in the MME energy harvester. Here, we investigated the effects of four types of adhesive interfacial layers on the output power and reliability such

as environmental and fatigue resistances of MME harvesters. We confirmed the thickness and Young's modulus of adhesive interfacial layer were important parameters that influence the conversion efficiency in MME harvester. By optimizing the adhesive interfacial layer thickness of 18.8  $\mu\text{m}$  and elastic modulus of 3.1 GPa, we achieved significant enhancement ( $\sim 300\%$ ) with a maximum output power density of 0.92 mW/cm<sup>2</sup> under a 10 Oe magnetic field. Moreover, we demonstrated a robust endurance of continuous 10<sup>8</sup> fatigue cycles (20 days) and excellent temperature stability in the range of -30 to 70 °C.

9:15 AM

### (MCARE-085-2021) Improved Energy Harvesting Performance of Magneto-Mechano-Electric Generator with Permeability Variation of Magnetic Flux Concentrator

H. Choi<sup>\*1</sup>; A. Thakre<sup>1</sup>; J. Ryu<sup>1</sup>

1. Yeungnam University, Gyeongsan, Korea (the Republic of), School of Materials Science and Engineering, Republic of Korea

The magneto-mechano-electric (MME) generator harvests electrical energy from the stray magnetic field formed around electrical power transmission cables. An MME generator comprises a magnetostrictive material coupled with a piezoelectric material and Nd proof mass magnets. In the presence of an AC magnetic field, the magnetostrictive material undergoes physical deformations which generates strain. Further, this strain is transferred to the piezoelectric layer in form of stress which converts the stress into an electric potential. To enhance the output power of the MME generator, it is necessary to concentrate magnetic noise flux around the MME generator structure. In our previous report, the magnetic field concentrator (MFC) was proposed as an excellent way to concentrate the magnetic field. In this study, three magnetic materials were employed (Nickel, STS430, high purity Iron) as MFCs which possess different magnetic permeability. The electrical output performance of the MME generator coupled with MFC were investigated via FEA modeling and confirmed experimentally. The MFC having highest permeability shows the highest output performance at a magnetic field of 1 Oe. In addition, the generated output power of the MME generator at low magnetic field (generated around hair dryer cable) was demonstrated to drive the electronic clock.

9:30 AM

### (MCARE-086-2021) Study of energy harvesting performance of magneto-mechano-electric generator with aspect ratio variation of piezoelectric constituents

A. Kumar<sup>\*1</sup>; S. Park<sup>1</sup>; D. Patil<sup>1</sup>; G. Hwang<sup>2</sup>; J. Ryu<sup>1</sup>

1. Yeungnam University, School of Materials Science & Engineering, Republic of Korea
2. Pukyong National University, Department of Materials Science and Engineering, Republic of Korea

In recent years, the cantilever-structured energy generators such as the piezoelectric energy harvester (PEH) and magneto-mechano-electric (MME) generator are being used to harvest the energy from the mechanical vibrations and weak stray magnetic, respectively. The MME generator is a newer concept than PEH and its needs geometric optimization for optimum power generation. In this work, the effect of aspect ratio (length (L)/width (W)) of piezoelectric single crystal fiber plates on the energy harvesting performance of the MME generator comprised of magneto-electric composites is investigated. PMN-PZT single crystal fiber (SCF) plates with different aspect ratios (0.59, 0.78, 1, 1.25, and 1.6), a magnetostrictive Ni plate and NdFeB permanent magnet proof mass were used to fabricate the MME generator. The MME harvester with a PMN-PZT SCF aspect ratio of 1.6 shows a  $\sim 440\%$  increment in the RMS voltage and power and  $\sim 300\%$  enhancement in the power density measured at an R<sub>L</sub> of 100 k $\Omega$  and a magnetic field of 10 Oe. The MME structure shows completely different results where the



piezoelectric element with longer lengths ( $L_{\text{piezo}} > W_{\text{piezo}}$ ; larger aspect ratio) shows the optimized output (for PEH;  $L < W$ ) due to the additional in-plane (longitudinal) magnetostrictive vibrations confirmed by the finite element analysis.

**9:45 AM**

**(MCARE-087-2021) Enhancement of output power of magneto-mechano-electric generator by optimizing the magnet proof mass position with magnetic flux concentrator**

D. Patil<sup>\*1</sup>; J. Ryu<sup>1</sup>

1. Yeungnam University, Materials Science and Engineering, Republic of Korea

Recently we demonstrated a noble method to enhance the output power of the given Magneto-mechano-electric (MME) generator by concentrating its magnetic noise flux by using a magnetic flux concentrator (MFC) fabricated from a high-permeability magnetic material. The output power of the MME generator was significantly enhanced by optimizing the MFC structure in terms of its shape, aspect ratio, magnetic permeability, and a number of layers both through finite element analysis and experimentally. However, the position of magnet proof mass which play important role in enhancing the output power of MME generator was not optimized. In the present work, we optimized the position of magnet-proof mass with respect to the MFC in order to further enhance the output power of MME generator. By positioning the magnets at the tip of the MME generator (2mm from the MFC) we could enhance the output power up to 5.4 mW, which is 340% larger than that without MFC (1.17 mW) under a weak magnetic field of 10 Oe. Furthermore, we demonstrated a realistic practical application by scavenging the power from the magnetic fields around the electric dryer (220 V, 60 Hz, 1.9 kW) to turn on 60 white blue LEDs.

**10:00 AM**

**(MCARE-090-2021) Biomaterial-Based Energy Harvesting Sensors for Structural Health Monitoring**

F. Okosun<sup>\*1</sup>; S. Guerin<sup>2</sup>; V. Pkrashi<sup>1</sup>

1. University College Dublin, Mechanical Engineering, Ireland
2. University of Limerick, Bernal Institute, Ireland

Biological piezoelectric materials offer an inexpensive, non-toxic and renewable high-performance alternative to current commercial piezoelectrics which require the use of lead-based perovskites, rare earth metals and fossil fuels. Despite a large increase in the number of organic piezoelectrics being discovered, they are yet to be tested and validated for real-world applications. Here, we present the development and laboratory validation of a flexible amino acid-based energy harvesting sensor that is capable of real-time detection of pipe leakage, which is a global challenge for sustainable water access. The polycrystalline film device exploits the proportional relationship between leak-induced strain and piezoelectric voltage in detecting and monitoring leaks in water distribution pipelines. Peak output voltage in the region of 2 V is recorded for the time signal at higher flow rates and larger leak sizes, due to the longitudinal piezoelectric response of the low-dielectric organic film. The sensor can identify leaks as small as 2 mm and can monitor a worsening pipe leak condition over time. The very simple crystal growth and deposition is suitable for large-scale batch processing of these sensors, and the results demonstrate the effectiveness of simple biomolecule-based energy harvesters for pipe leak detection and monitoring and possibly other Structural Health Monitoring (SHM) applications.

**10:15 AM**

**(MCARE-091-2021) Electronic Structure of Nano-crystalline Soft Magnetic Materials for Energy Storage and Conversion**

M. Choi<sup>\*1</sup>; Y. Hong<sup>1</sup>; H. Won<sup>1</sup>; W. Lee<sup>2</sup>; S. Kim<sup>3</sup>

1. The University of Alabama, Electrical and Computer Engineering, USA
2. Samsung Electro-Mechanics, RF Product Development Group, Republic of Korea
3. Mississippi State University, Department of Physics & Astronomy and Center for Computational Sciences, USA

Soft magnetic materials are used to store energy and convert or generate electricity for electrical devices. Nanocrystalline (NC) magnetic alloy outperforms over the conventional soft magnetic materials in permeability, saturation magnetostriction, and magnetization. Therefore, the nanocrystalline magnetic materials enable electrical components to be smaller, lighter, energy-saving, and cost-effective. NC NANOMET (Fe-Si-P-B-Cu) shows a low core loss and high magnetic flux density ( $B_s$ ) and is a structure of Fe-based crystallite (CR) embedded amorphous matrix (AM). In this paper, we embed CR (Fe-Co) into the AM (Fe-B-P-Cu) to consider the magnetic interactions between CR and AM. First, the ab initio molecular dynamics (AIMD) is performed to prepare the AM. Then, we embed the CR (Fe-Co) into the AM (Fe-B-P-Cu). Lastly, we perform first-principle calculations (VASP package) on Fe-Co embedded Fe-B-P-Cu system to calculate its electronic structure. As a result, the total magnetic moment ( $\mu_B$ ) increases from 244 for 1 CR (128 atoms) to 265 for 2 CRs (136 atoms). These  $\mu_B$  convert to  $B_s$  of 1.9 T for 1 CR and 1.91 T for 2 CRs. However, the anisotropy constant (K) dramatically decreases from 5.2 kJ/m<sup>3</sup> for 1 CR to 142 J/m<sup>3</sup> for 5 CRs. We will present our calculation methodology and results in details. This work was supported in part by the NSF IIP under grant No. 1650564.

**10:45 AM**

**(MCARE-092-2021) Novel Ferroelectric Ceramics through [Ga, Ta] Dipole Engineering**

K. Ning<sup>\*1</sup>; H. Shulman<sup>1</sup>; S. M. Pilgrim<sup>1</sup>; W. A. Schulze<sup>1</sup>; S. Tidrow<sup>1</sup>

1. Alfred University, New York State College of Ceramics, School of Engineering, USA

Dipole engineering is a promising method for creating novel ferroelectric materials that may offer opportunities for next generation electronic devices. BaTiO<sub>3</sub> based ceramics have been manufactured by incorporating [Ga, Ta] dipolar-pairs, and are systematically studied through reporting microstructure, electric, dielectric and optical properties as a function of dipole-pair concentration. A unique diffuse phase transition dielectric behavior possessing both ferroelectric- and relaxor-like attributes is reported. The Clausius – Mossotti relation, the new simple material model (NSMM), and the dipole strength provide in-depth understandings for the unusual properties of these materials.

**11:00 AM**

**(MCARE-093-2021) Design of High Power Magnetolectric Transducers for Wireless Power Transmission**

R. Sriramadas<sup>1</sup>; S. S. Hosur<sup>\*1</sup>; S. K. Karan<sup>1</sup>; M. Kiani<sup>1</sup>; S. Priya<sup>1</sup>

1. Pennsylvania State University, USA

The wireless transmission of power using magnetolectric (ME) composites offers greater power densities at small scales compared with conventional inductively coupled coil-based power transfer devices. The compact ME transducers are ideal for implantable medical device applications. The performance of the ME transducer can be described by a lumped element model, however, most of the existing lumped models have the least consideration for the dependence of the piezomagnetic constant and the device quality factor on the magnetic field bias. In the present work, a complete continuum model of the ME transducer including the effect of the

biasing magnetic field, quality factor, and external load resistance is proposed. Moreover, the conditions at which the peak power is achieved in terms of piezoelectric and piezomagnetic coupling factors are derived. The explicit dependence of the piezomagnetic coupling and Young's modulus of the magnetostrictive material on the biasing magnetic field is corroborated by evaluating six different ME transducers, experimentally. Furthermore, the optimum thickness ratios for peak ME voltage and power coefficients are independently derived and validated by evaluating the experimental devices. The proposed model of the ME composite provides a generalized approach for designing high-power ME transducers for applications in wearable and biomedical implants.

### **MCARE S9: Critical Materials for Energy**

Session Chair: Nobuhito Imanaka, Osaka University

#### **9:00 AM**

##### **(MCARE-094-2021) Recovery and recasting of used perfluorosulfonic membrane in vanadium flow battery by ion exchange resin**

W. Chen<sup>1</sup>; Y. Chen<sup>\*1</sup>; C. Lee<sup>1</sup>; S. Mesaki<sup>1</sup>; Y. Chen<sup>1</sup>

1. National Cheng-Kung University, Resource engineering, Taiwan

This study provides a method for recovery and recasting of used perfluorosulfonic Nafion<sup>®</sup> membrane in vanadium flow battery by dissolving and removing the impurity through ion exchange resin. The used membrane containing vanadium which penetrated from the electrolyte can be regenerated by removing the vanadium ion. In this experiment, the used Nafion 117 membrane was dissolving in 50% ethanol at 240°C for 6 hours. Then, five types of ion exchange resin were used to absorb the vanadium in the membrane solution. In this process, the most effective resin will be determined, and the L/S ratio and reactant time were controlled to obtain the best absorption efficiency. After that, the membrane solution was evaporated and replaced by DMSO. The prepared Nafion/DMSO solution was cast to obtain the recast Nafion membrane. The morphology of recast membrane was evaluated by water uptake, sheet resistance and ion exchange capacity. With the optimal condition, the resin could eliminate 98.0% vanadium of used membrane, and the morphology showed the recast membrane could be reuse in vanadium flow battery.

#### **9:15 AM**

##### **(MCARE-095-2021) Synthesis of copper, indium, and gallium oxides from waste thin-film solar panels**

F. Liu<sup>\*1</sup>; T. Cheng<sup>1</sup>; Y. J. Chen<sup>2</sup>; C. Lai<sup>1</sup>; W. Chen<sup>2</sup>; Y. Chueh<sup>1</sup>

1. National Tsing Hua University, Department of Materials Science and Engineering, Taiwan
2. National Cheng Kung University, Department of Resources Engineering, Taiwan

It is a potential challenge to treat the waste solar panels including valuable metals, since the waste copper, indium, and gallium selenide (CIGS) base thin-film solar panels have been increasing year by year. A synthesis process of copper, indium, and gallium oxides from the waste panels has been studied. To obtain the CIGS materials, the waste panels were separated due to thermal strain difference of the component materials. The CIGS materials were annealed first and then leached by sulfuric acid to extract the valuable metals individually. Di-(2-ethylhexyl) phosphoric acid (D2EHPA) was used as an extractant to separate copper, indium, and gallium. After a stripping process, the copper, indium, and gallium aqueous-phase solutions were obtained. Chemical precipitation was conducted to recover copper, indium, and gallium in the solutions into hydroxides. Copper, indium, and gallium oxides were the final products from the hydroxides via calcination. With the optimal conditions, the recovery of indium, gallium and copper could be up to 90%.

#### **9:30 AM**

##### **(MCARE-096-2021) Investigation on ferro/anti-ferro coupling and magnetic moment by substitution of RE (RE=Pr,Tb,Dy) for Nd in Nd<sub>2</sub>Fe<sub>14</sub>B crystal**

D. Kim<sup>\*1</sup>; S. Kim<sup>1</sup>; V. Galkin<sup>1</sup>; R. Kuchi<sup>1</sup>

1. Korea Institute of Materials Science, Republic of Korea

A novel route to prepare Nd-Fe-B magnetic powder was designed and investigated in this work. Precursors were synthesized from aqueous solutions with chloride salts and boric acid such as Neodymium chloride, Iron chloride and the like. Magnetic particles of Nd<sub>12</sub>RE<sub>3</sub>Fe<sub>77.5</sub>B<sub>7.5</sub> (RE = Pr, Tb, Dy) were prepared by co-precipitation, followed by reduction-diffusion (R-D) process. The particles were formed with the mean size of 2.0 μm and the morphology was round in shape. After substitution of RE during R-D, the magnetic moment was increased after substitution of Pr into Nd-Fe-B, but decreased after substitution of Tb and Dy. It was revealed by the calculation of electron spin density with simulation technique that Pr was ferromagnetic, but Tb and Dy were anti-ferromagnetic to Nd and Fe in the Nd-RE-Fe-B crystal lattice. The magneto-crystalline anisotropy energy was increased from 0.2284 MJ/m<sup>3</sup> to 0.3910 and 0.3924 MJ/m<sup>3</sup> after the substitution of Tb and Dy for Nd in Nd-Fe-B, respectively. However, the magneto-crystalline anisotropy energy decreased to 0.2050 MJ/m<sup>3</sup> after the substitution of Pr for Nd.

#### **9:45 AM**

##### **(MCARE-097-2021) Separation of valuable metal from waste tin anode slime by solvent extraction after oxidation leaching**

W. Chen<sup>1</sup>; S. Mesaki<sup>\*1</sup>; C. Lee<sup>1</sup>; Y. Chen<sup>1</sup>; Y. Chen<sup>1</sup>

1. National Cheng-Kung University, Resource Engineering, Taiwan

Tin anode slime, a by-product of electrolytic refining, is mainly containing tin, copper, bismuth and antimony. After oxidation leaching with hydrochloric acid by previous study, the leaching solution contained 700ppm of Bi, 1600ppm of Cu, 3600ppm of Sn and 900ppm of Sb. To recover those valuable metal, this study used solvent extraction processes with TBP (tri-n-butyl phosphate) and LIX<sup>®</sup> 984N for separation. The optimum condition of first extraction process was 4M of HCl concentration, 0.5M of TBP concentration, 3 of O/A ratio and 5 minutes of stirring time. Under this condition, more than 95% of tin and 90 % of antimony was loaded into organic phase and stripped respectively with different concentration of H<sub>2</sub>SO<sub>4</sub>. However, copper and bismuth were still in the aqueous phase. Next, copper was extracted by LIX<sup>®</sup> 984N and stripped with 3M H<sub>2</sub>SO<sub>4</sub>. The extraction efficiency of copper was higher than 95%, and bismuth was unextracted. These solvent extraction processes could provide a useful method for recovery of valuable metal from tin anode slime.

#### **10:00 AM**

##### **(MCARE-098-2021) Optimization of bulk crystal growth method for improved performance and yield of CdTe for solar and detector applications**

S. Swain<sup>\*1</sup>; S. Kakkireni<sup>1</sup>; J. McCloy<sup>1</sup>

1. Washington State University, USA

Cadmium telluride and its alloys are important materials for energy conversion and detection in the fields of infrared sensing, photovoltaics and gamma ray detection. Some of the major material challenges responsible for limiting performance and high cost in CdTe based technologies are achieving controlled and stable doping, reducing extended defects associated with non-stoichiometry, limited single crystal yield. Our study focused on addressing these challenges via innovations in bulk material synthesis will be presented. Single crystals of CdTe and its alloy with Zn or Se, were grown by melt growth methods using low pressure and high pressure Bridgman technique. P-type doping in CdTe was investigated using (phosphorus) P, Arsenic (As) and antimony (Sb) dopants for

photo-voltaic applications. It is shown that hole density exceeding  $10^{17} \text{ cm}^{-3}$  can be achieved with group V doping and dopant solubility can be enhanced by applying external melt convection during growth. Similar growth method applied to gamma ray detector grade crystal growth yields low density of extended defects/precipitates and high performing devices. Strategies to produce these materials by fast, low cost and industrially scalable methods will be discussed. These techniques can be potentially applied to other bulk optoelectronic materials where doping and phase control are critical.

### **MCARE S8: Advanced Materials for Fuel Cells and High Temperature Electrolysis**

Session Chair: Yongchai Kwon, Seoul National University of Science and Technology

**10:50 AM**

#### **(MCARE-099-2021) Tuning 3-Dimensional Nanoarchitectures for More Efficient Energy Conversion via High-resolution Printing (Invited)**

Y. Jung<sup>\*1</sup>

1. KAIST, Dept. of Materials Science and Engineering, Republic of Korea

This talk introduces our novel solvent-assisted nanotransfer printing (S-nTP) strategy that can controllably generate extremely fine (down to sub-10 nm) functional 3D nanostructures with excellent transfer yield (~100%). As an example, we demonstrate that 3D metal nanostructures can be used as highly active electrocatalysts for polymer electrolyte membrane fuel cells and water electrolysis due to increased materials transport in the well-ordered 3D geometry. We show that woodpile (WP)-structured Ir, consisting of 3D-printed, highly-ordered Ir nanowire building blocks, improve OER mass activity markedly. The WP structure secures the electrochemically active surface area (ECSA) through enhanced utilization efficiency of the extended surface area of 3D WP catalysts. On the other hand, high-yield conversion from  $\text{CO}_2$  to carbon compounds is essential for the sustainable production of fuel feedstock and for balancing nature's carbon cycle to resolve the greenhouse effects caused by  $\text{CO}_2$  emission. We present that S-nTP can produce various novel 3D structures, which can realize electro-reduction of  $\text{CO}_2$  to CO with high efficiency and selectivity at low overpotentials based on the control of local pH gradient.

**11:20 AM**

#### **(MCARE-100-2021) Improvement of Durability of the Cathode under Start-up/Shut-down process with IrRuOx/C catalyst in Polymer Electrolyte Membrane Fuel Cell**

M. Min<sup>2</sup>; E. You<sup>3</sup>; S. Lee<sup>3</sup>; C. Pak<sup>\*1</sup>

1. Gwangju Institute of Science and Technology, Graduate Program of Energy Technology, Republic of Korea
2. Samsung SDI, Fuel Cell Group, Republic of Korea
3. Hyundai Mobis Co., Fuel Cell Engineering Group, Republic of Korea

The polymer electrolyte membrane fuel cell (PEMFC) is an attractive alternative power train for fuel cell electric vehicles (FCEVs) because of its higher energy density, higher conversion efficiency and lower emission of environmental pollutants than other conventional energy sources. Despite the developments of PEMFC systems, there are still three major challenges such as cost, performance, and durability for expanding the FCEV market. In this study, the cathode durability is improved using the 2.5 wt.% oxygen evolution reaction (OER) catalyst to the cathode catalyst layer of a membrane electrode assembly (MEA) by c.a. 88% under start-up/shut down (SU/SD) process, which frequently occurs during the FCEV operation. The OER catalysts such as IrRuOx, which prompt the water oxidation prior to the carbon corrosion reaction at high voltage, were

synthesized using a sub-substrate method, and their electrochemical and physicochemical properties were analyzed with several analysis methods. The Ir<sub>1</sub>Ru<sub>1</sub>Ox/C was the best catalyst in terms of activity and stability. After 4,000 SU/SD cycles in the MEA, the electrochemical surface areas of the Pt in the OER-added and reference MEAs reduced by 15% and 57%, respectively, which implies that durability of the MEA is improved without significantly compromising the performance.

**11:35 AM**

#### **(MCARE-101-2021) Synthesis of high dispersed FeNC single atom oxygen reduction reaction catalyst using solution plasma process**

H. Son<sup>\*1</sup>

1. Pusan National University, Republic of Korea

In order to commercialize fuel cells, it is necessary to develop transition metal catalysts that can replace expensive platinum used as oxygen reduction reaction (ORR) catalyst. Among promising candidates, iron single atom catalysts are mostly attractive because of their usable shape and functionalities. Moreover, iron-based catalysts are highly desired of comparable catalytic performance to platinum. However, the agglomeration of iron atoms on supporting carbon material is one of major challenges to limit its catalytic properties. In our studies, iron is highly distributed on mesoporous carbon through solution plasma processing which can synthesize materials to have uniform size and dispersion using one-step method. It is key point that Iron single atom on nitrogen doped carbon can derive excellent ORR catalytic property. The morphology of synthesized iron single atom catalysts was characterized by using XRD and TEM (including element mapping) which employed carbon crystalline structure and morphology. And the best ORR catalytic material (6mmol FeNC-800) shows 0.94V (vs. RHE) of onset potential and 0.84V (vs. RHE) of half wave potential in alkaline media. The features demonstrate possibility of iron single atom catalyst to be alternative to Pt/C catalysts.

**11:50 AM**

#### **(MCARE-103-2021) A Novel Vanadia Doped YSZ Ceramic for Solid Oxide Cell Applications**

J. Drazin<sup>\*1</sup>; D. McLarty<sup>1</sup>

1. WSU, MME, USA

A vanadia doped yttria stabilized nanoceramic (VYSZ) has been synthesized, processed, and sintered in monolithic and functional geometries. The new nanoceramics can be co-sintered with the industrially relevant electrolyte YSZ. The VYSZ nanoceramics are thermally and mechanically stable in reducing environments up to 1250C. Initial conductivity measurements show significantly increased total conductivity (>30x) compared to YSZ ceramics indicating electronic transmittance. The co-sinterability with YSZ and electrical conductivity of VYSZ make it a promising new electrode material on the fuel side of a solid oxide cell. Here we report the electrical conductivity of VYSZ in reducing environments with some solid oxide fuel cell button cell results. A vanadia doped yttria stabilized nanoceramic (VYSZ) has been synthesized, processed, and sintered in monolithic and functional geometries. The new nanoceramics can be co-sintered with the industrially relevant electrolyte YSZ. The VYSZ nanoceramics are thermally and mechanically stable in reducing environments up to 1250C. Initial conductivity measurements show significantly increased total conductivity (>30x) compared to YSZ ceramics indicating electronic transmittance. The co-sinterability with YSZ and electrical conductivity of VYSZ make it a promising new electrode material on the fuel side of a solid oxide cell.

## **MCARE S10: Lifecycle Impacts of Clean Energy**

### **Materials**

Session Chair: Gabrielle Gaustad, NYS College of Ceramics, Alfred University

#### **10:20 AM**

### **(MCARE-104-2021) Processes for separating photovoltaic modules (crystalline-Si and CIGS) layer by layer**

W. Chen<sup>1</sup>; Y. Chen<sup>\*1</sup>; Y. Chen<sup>1</sup>; F. Liu<sup>2</sup>; C. Lee<sup>1</sup>; S. Mesaki<sup>1</sup>

1. National Cheng-Kung University, Resource Engineering, Taiwan
2. National Tsing Hua University, Material Science, Taiwan

As the rate of photovoltaic modules installation and recycling increasing, the technology of recovering modules becomes a big issue on Earth. According to the research, the accumulation of waste modules will reach to 8600 tons in 2030. Moreover, Crystalline-silicon (c-Si) Photovoltaic modules account for more than 90% of the waste; CIGS modules account for 2% of the waste. To decline the waste storage, several countries such as Japan and Europe have developed the commercial process to separate the complete plate of the c-Si modules. However, it's common to discover the broken c-Si waste in the real case of the waste PV modules and the waste of CIGS modules shouldn't be avoided. In this assay, after auto frame dismantling, layers of CIGS and molybdenum were separated by liquid nitrogen. The modules' tempered glass was removed and collected through the process of organic solvent soaking, and the recovering rate of tempered glass was up to 99%. The organic solvent soaking process also separated c-Si PV cells from the EVA resin. To collect the CIGS powder from the Ethylene Vinyl Acetate Copolymer (EVA) resins 0.1M hydrochloric acid was employed to wash down and collect the powder attaching on the resin. Finally, the resin was pyrolyzed at high temperatures. This assay provides several physical and chemical processes to separate and collect high purity of silicon, CIGS powder, glass, and Mo.

## **MCARE 14: Chemical and Biological Sensors**

Session Chairs: Praveen Sekhar, Washington State University, Vancouver; Sanjay Mathur, University of Cologne

#### **9:00 AM**

### **(MCARE-106-2021) Reactive Oxygen Species Scavenging and Improvement Effect of Inflammatory Disease Treatment by Functionalized Nanoparticles**

S. Hong<sup>\*1</sup>; J. An<sup>2</sup>; H. Hong<sup>3</sup>; O. Kim<sup>3</sup>; S. Yoon<sup>2</sup>; S. Kim<sup>3</sup>; K. Yoon<sup>1</sup>

1. Hannam University, Chemistry, Republic of Korea
2. Konyang University, Internal Medicine, Republic of Korea
3. Catholic University, Surgery, Republic of Korea

Various types of nanomaterials are recently under research for diagnostic and therapeutic applications in the biomedical area while our information for their potential effects and fate in living cells is still limited. Also the interaction of nanoparticles with cellular functions, such as repression/activation of genes and activation of specific cell organelle. Here we demonstrate for the ceria-zirconia nanoparticles (CZNPs) that localize intracellular organelle could effectively reduce reactive oxygen species (ROS) as a result of the improvement effect of inflammatory disease. In this process, CZNPs are faster change from Ce<sup>4+</sup> to Ce<sup>3+</sup> than those indicated by other ROS scavenging nanoparticles. This research has significant consequences for understanding the nanotherapeutics for the treatment of diseases.

#### **9:15 AM**

### **(MCARE-107-2021) 2D metal-organic framework derived co-loading of Co<sub>3</sub>O<sub>4</sub> and PdO nanocatalysts on In<sub>2</sub>O<sub>3</sub> hollow spheres for high performance breath acetone sensors**

Y. Jo<sup>\*1</sup>; K. Lim<sup>1</sup>; J. Yoon<sup>1</sup>; J. Lee<sup>1</sup>

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Nanolayers of Pd-intercalated leaf-like cobalt zeolitic-imidazolate frameworks (Co-ZIF-L), the two-dimensional (2D) metal-organic frameworks, were uniformly coated on the surface of the In<sub>2</sub>O<sub>3</sub> spheres within 10 nm thickness by controlling the growth and self-assembly of 2D Co-ZIF-L on In<sub>2</sub>O<sub>3</sub>, and converted into Co<sub>3</sub>O<sub>4</sub> nanoclusters (size: < 10 nm) encapsulating PdO nanoparticles (size: ~ 4 nm) by subsequent heat-treatment. The Co<sub>3</sub>O<sub>4</sub>/PdO catalyst co-loaded In<sub>2</sub>O<sub>3</sub> sensors showed ultra-high responses to 5 ppm of acetone (145.9) as well as high selectivity over the interference gases at 225 °C, even in 80% relative humidity conditions, thereby suggesting as promising ketogenic diet and diabetes monitoring sensor. This sensing performance can be explained by the electronic sensitization due to the formation of p-n heterojunction between Co<sub>3</sub>O<sub>4</sub> and In<sub>2</sub>O<sub>3</sub>, and the chemical sensitization due to the synergistic catalytic effect of Co<sub>3</sub>O<sub>4</sub> and PdO.

#### **9:30 AM**

### **(MCARE-108-2021) Dual-mode gas sensors using Nb-doped NiO hollow spheres for highly selective and sensitive detection of xylene and toluene**

T. Kim<sup>1</sup>; Y. Jo<sup>\*1</sup>; S. Jeong<sup>1</sup>; Y. Moon<sup>1</sup>; J. Lee<sup>1</sup>

1. Korea university, Republic of Korea

Pure and Nb-doped NiO hollow spheres were prepared by facile one-pot ultrasonic spray pyrolysis followed by heat treatment at 500 °C for 2 h and their gas-sensing characteristics were investigated. The high-concentration Nb-doped NiO sensor ([Nb]/[Ni] = 0.1) exhibited ultrahigh responses to p-xylene and toluene with extremely high selectivity to various interference gases such as ethanol, formaldehyde, carbon monoxide, and benzene. In addition, the sensor showed excellent dual sensing characteristics detecting p-xylene at 350 °C and toluene at 400 °C. The unprecedentedly high gas responses to p-xylene and toluene were attributed to improved gas reforming reaction due to the Nb-doping-induced change in the catalytic activity and the high gas accessible morphology as well as the electronic sensitization by Nb doping. Moreover, the dual sensing characteristics of p-xylene and toluene could be achieved by controlling the reforming of analyte gases and the oxidative filtering of interference gases depending on the film thickness and operating temperature. The Nb-doped NiO hollow spheres can be used to design a single sensor with dual functionality to detect p-xylene and toluene in an ultrasensitive and highly selective manner, which can pave a new path for discriminate sensing of aromatic indoor air pollutants.

#### **9:45 AM**

### **(MCARE-109-2021) Bilayer Gas Sensors Composed of Metal Oxide Sensing Layer and Au Nanoparticle Catalytic Overlayer: Highly Tunable Gas Sensing Characteristics**

Y. Moon<sup>\*1</sup>; S. Jeong<sup>1</sup>; Y. Kang<sup>1</sup>; J. Lee<sup>1</sup>

1. Korea University, Materials Science and Engineering, Republic of Korea

Metal oxide gas sensors are widely used for their distinctive advantages, including high/rapid gas response, reversibility, and cost-effectiveness. However, low selectivity and limited kind of detectable gases remain challenging issues. Herein, we propose a novel bilayer sensor design with an oxide sensing layer and Au nanoparticle catalytic overlayer to provide high controllability for gas sensing characteristics. The Au nanoparticle overlayer significantly enhances the methylbenzene response of a SnO<sub>2</sub> thick film sensor by reforming gases into more reactive species and suppresses

the responses to reactive interference gases through oxidative filtering. Gas sensing characteristics can be tuned by controlling the morphology, amount, and number density of Au nanoparticles through the variation in the Au coating thickness and thermal annealing conditions. Moreover, the general validity of Au nanoparticle catalytic overlayer can be confirmed again from the increase of selectivity to methylbenzene by coating of Au nanoparticles onto ZnO and Co<sub>3</sub>O<sub>4</sub> thick film. Finally, the separation of gas sensing and catalytic reactions into independent processes can not only provide excellent controllability over sensing characteristics but also avoid abrupt changes in sensor resistance in air by catalyst loading.

#### 10:00 AM

##### (MCARE-110-2021) Gas-Sensing Nanoreactors using Au@SnO<sub>2</sub> and SnO<sub>2</sub>@Au Hollow Spheres: Tunable Gas Selectivity

S. Park\*<sup>1</sup>; S. Jeong<sup>1</sup>; J. Yoon<sup>2</sup>; J. Lee<sup>1</sup>

1. Korea University, Department of Materials Science and Engineering, Republic of Korea
2. Jeonbuk National University, Department of Information Materials Engineering, Republic of Korea

Catalyst-loaded hollow spheres have been attracting attention as a gas-sensing platform due to the improved surface reaction by the hollow structure and loaded catalyst. Herein, we report a new strategy to prepare gas sensing nano-reactors by using catalyst-loaded hollow spheres enabling highly selective detection of xylene. We prepared SnO<sub>2</sub> hollow spheres with Au nanoclusters on the inner (Au@SnO<sub>2</sub>) or outer shell surface (SnO<sub>2</sub>@Au) and compared their gas sensing characteristics. Au@SnO<sub>2</sub> sensor showed unprecedented xylene selectivity and ultra-high xylene response enough to be used for indoor air quality monitoring, whereas SnO<sub>2</sub>@Au sensor exhibited typical ethanol-sensitive sensing behaviors as frequently reported in the literature. Additionally, we optimized the xylene response and selectivity by preparing Au@SnO<sub>2</sub> with different shell thickness and porosity via layer-by-layer technique. The mechanism underlying the unprecedented xylene sensing performance is discussed in relation to the location and configuration of Au nanoclusters and morphological characteristics of SnO<sub>2</sub> hollow spheres including shell thickness and pore size distribution. The novel nano-reactor concept provides a general pathway to design highly selective gas sensors, especially for less-reactive gases.

#### 10:15 AM

##### (MCARE-111-2021) VOC-sensing properties of semiconductor-type gas sensors: Effects of CuO loading onto porous SnO<sub>2</sub>

S. Torai\*<sup>1</sup>; T. Ueda<sup>1</sup>; K. Kamada<sup>1</sup>; T. Hyodo<sup>1</sup>; Y. Shimizu<sup>1</sup>

1. Nagasaki University, Graduate School of Engineering, Japan

Exhaled breath of the patients contains a higher concentration of specific volatile organic compounds (VOCs) than those of healthy people. Especially, the patients suffering from lung cancer and diabetes release a high concentration of acetone and toluene, respectively. Therefore, the highly sensitive and selective detection of these gases enables diagnoses of these diseases non-invasively. In this study, spherical porous (pr-)SnO<sub>2</sub>-based particles were prepared by ultrasonic spray pyrolysis employing home-made PMMA microspheres (typical particle size: 70 nm in diameter), and their VOC-sensing properties were examined. Thick film sensors were fabricated by screen printing employing spherical SnO<sub>2</sub>-based particles obtained (dense SnO<sub>2</sub>, pr-SnO<sub>2</sub>, and x wt% CuO-loaded pr-SnO<sub>2</sub> ((pr-xCuO/SnO<sub>2</sub>), x: 0.5, 1.0 and 2.0), and their sensing properties to 20-100 ppm acetone and toluene were measured at 300-500°C in air. The introduction of well-developed porous structures into the spherical SnO<sub>2</sub> particles was quite effective in enhancing the VOC-sensing properties. In addition, the loading of CuO onto the spherical pr-SnO<sub>2</sub> particles improved their VOC responses in the temperature range of 300-450°C. Among all the sensors tested in this study, the pr-2.0CuO/SnO<sub>2</sub> sensor showed the largest responses to acetone and toluene at 350°C and 300°C, respectively.

\*Denotes Presenter

#### 10:45 AM

##### (MCARE-112-2021) Toluene-sensing properties of yttria-stabilized zirconia-based gas sensors attached with thin CeO<sub>2</sub>-added Au sensing electrodes

S. Kamura\*<sup>1</sup>; T. Ueda<sup>1</sup>; K. Kamada<sup>1</sup>; T. Hyodo<sup>1</sup>; Y. Shimizu<sup>1</sup>

1. Nagasaki University, Graduate School of Engineering, Japan

It is well known that the concentration of toluene in exhaled breath of the patients suffering from lung cancer is much higher than that of healthy people, and thus highly sensitive toluene sensors were needed to diagnose non-invasively. We have so far demonstrated that yttria-stabilized zirconia (YSZ)-based gas sensors attached with a CeO<sub>2</sub>-added Au sensing electrode (SE) and a Pt counter electrode show relatively large toluene responses. In this study, thin-film CeO<sub>2</sub>-added Au SEs were fabricated by a spin-coating method, and the impacts of the amount of CeO<sub>2</sub> added into the Au SEs and the operating temperature on their sensing properties to toluene were examined. The precursor solution for n wt% CeO<sub>2</sub> added Au (n: 24, 32, 50) SEs were prepared by the addition of Ce(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O and polyvinyl alcohol into a HAuCl<sub>4</sub> aqueous solution. The solution was dropped on a YSZ substrate, and it was spun at 3000 rpm for 30 s. After drying, this process was repeated 15 times to increase the film thickness to ca. 100 nm. The electromotive force between the two electrodes (E, mV) of the sensors (Au(nCeO<sub>2</sub>)) was measured in dry air as well as in 2.5-50 ppm toluene balanced with dry air at 450-500°C. The E values of all the sensors negatively shifted upon exposure to toluene, and the Au(24CeO<sub>2</sub>) sensor showed the largest toluene response at 450°C, among the sensors tested.

#### 11:00 AM

##### (MCARE-113-2021) Rational design of oxide chemiresistors for exclusive detection of plant hormone ethylene: Tailoring gas selectivity by nanoscale catalytic overlayer

S. Jeong\*<sup>1</sup>; Y. Moon<sup>1</sup>; T. Kim<sup>1</sup>; S. Park<sup>1</sup>; K. Kim<sup>1</sup>; Y. Kang<sup>1</sup>; J. Lee<sup>1</sup>

1. Korea University, Materials Science and Engineering, Republic of Korea

Ethylene (C<sub>2</sub>H<sub>4</sub>) is a hormone gas for stimulating the development and growth processes of plants. Thus, a precise monitoring and control of the sub-ppm-level ethylene is important for a wide range of agricultural applications and smart farming. However, the ethylene of non-polarity is chemically stable and thus less reactive to oxide semiconductor gas sensors. In this study, a novel bilayer sensor design consisting of nanoscale catalytic Cr<sub>2</sub>O<sub>3</sub> overlayer and metal oxide semiconductors (SnO<sub>2</sub>) is suggested to detect ethylene in a highly selective and sensitive manner. The gas response of the proposed sensor to 2.5 ppm ethylene was 16.8 at 350 °C, which was 2–15 times higher than those to food-related interfering gases (TMA, DMA, and NH<sub>3</sub>), ubiquitous C<sub>2</sub>H<sub>5</sub>OH, and indoor pollutants (HCHO and CO). The extremely high response and selectivity to ethylene were attributed to the catalytic oxidation of reactive interfering gases into less- or non-reactive species (CO<sub>2</sub> or H<sub>2</sub>O) prior to gas-sensing reaction. Moreover, the potential of the present sensor to assess fruit freshness was demonstrated by investigating the ripening of various fruits: a banana, an apple mango, a peach, a kiwifruit, and a blueberry. We believe that the proposed sensor will open various pathways for a wide range of agricultural applications.

#### 11:15 AM

##### (MCARE-114-2021) Hybrid structures of F-MWCNT/ZnO Nanocomposites for Ammonium Sensing Applications

N. K. S K<sup>1</sup>; A. K. Aliyana\*<sup>1</sup>; A. Baburaj<sup>1</sup>; M. Adetunji<sup>2</sup>; R. E. Fernandez<sup>2</sup>

1. Mangalore University, Electronics, India
2. Norfolk State University, USA

There is significant interest in real-time monitoring the levels of various ionic species in water. We report the fabrication of Functionalized Multi-Walled Carbon Nanotube (F-MWCNT) with Zinc Oxide (ZnO) nanocomposite active layers and their sensitivity to Ammonium ions (NH<sub>4</sub><sup>+</sup>). A thin layer of F-MWCNT/ZnO

nanocomposites was developed over the screen-printed interdigitated electrodes (IDEs). The subsequent hybrid structure was found to have proportional impedance characteristic changes with respect to  $\text{NH}_4^+$  levels. The performance of the sensor was investigated in the 1- 10 kHz range and showed a sensitivity of  $53.35 \Omega / \text{mM}$  in the linear range of  $\text{NH}_4^+$  concentration levels of 1-20 mM.

**11:30 AM**

### **(MCARE-115-2021) Direct Integration of Surface Decorated Metal Oxide Nanowire Networks and Porous Nanofiber Meshes for Selective Gas Detection**

D. Graf<sup>\*1</sup>; I. Gessner<sup>1</sup>; S. Mathur<sup>1</sup>

1. Institute of Inorganic chemistry, Chemistry, Germany

The high surface-to-volume ratio as well as the typically high crystallinity and directional charge carrier transport of metal oxide NWs are beneficial for the use in chemo-resistive gas sensors. Semiconducting n-type  $\text{SnO}_2$  nanowire networks have been site-selective deposited on gas sensor platforms by chemical vapor deposition approach based on a catalyst-mediated vapor-liquid-solid (VLS) growth mechanism. Compared to classical screen-printed  $\text{SnO}_2$  sensors showed the direct integrated nanowire network superior sensing performance in terms of sensitivity and response time. The selective detection of target gas molecules in complex gaseous composition or high humidity is quite challenging. We improved the lack of selectivity toward gaseous species through surface decoration with metal oxides ( $\text{VO}_2$ ) and noble metals (Rh) nanoparticles by a second CVD step. For this approach, we developed tailored volatile molecular precursors based on bidentate heteroarylalkenolate and enaminate ligands. An enhanced gas detection capability under high humidity was achieved by deploying hydrophilic zeolite microcrystals embedded in nanofiber meshes on top of the sensing material.

**11:45 AM**

### **(MCARE-116-2021) Electrochemical Ammonia Sensor on a Flexible Substrate**

P. Sekhar<sup>\*1</sup>; D. Graf<sup>2</sup>; O. Ojerle<sup>2</sup>; S. Mathur<sup>2</sup>

1. Washington State University, Vancouver, Dept. of Engineering and Computer Science, USA  
2. University of Cologne, Germany

An electrochemical sensor for the detection of extremely low concentration of ammonia (1 part per billion, ppb) was fabricated by integrating vanadium monoxide ( $\text{VO}_x$ ;  $x = 0.8-1.2$ ) nanowires on the platinum electrodes. The nanowire-based sensor responds at room temperature non-linearly to a staircase sequence of ammonia from 1 ppb to 100 ppb. The rise and fall time of the nanowire sensor was found to be 10 s and 9 s, respectively. While the immobilization of VO nanowires increased the electrochemical surface area, the defect rich and ionic nature of the VO surface ( $\text{V}^{2+}\text{O}^{2-}$ ) facilitated the chemical interaction and adsorption of polar ammonia molecules as evident in the room temperature response of the VO@Pt amperometric electrochemical sensor. The availability of metal centered d-electrons and the semiconductor nature of vanadium monoxide lowered the interfacial resistance of the nanowire-modified sensor enabling the lower detection limit of ammonia. The sensor seems to respond to  $\text{CH}_4$ ,  $\text{H}_2\text{S}$  and  $\text{C}_3\text{H}_6$  as well although the  $\text{NH}_3$  response is nearly six-fold compared to these common interfering compounds. The results pave the way for a low-cost alternative paper-based sensor to monitor ammonia emissions primarily from confined animal feeding operations (CAFOs).

## **EHS S2: Integrated Energy Harvesting and Storage Systems for Wearables and IoT**

Session Chair: Yang Bai, University of Oulu

**11:15 AM**

### **(EHS-038-2021) Towards the realization of greener electroactive transducers (Invited)**

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

1. University of Catania, DIEEI, Italy

In next future, the diffusion of transducers will be required in strategic fields. These systems will be required to embed a number of functions including, electric power generation and storage, signal sensing and processing capabilities. Also, their miniaturization and biocompatibility, will be of interest. New technologies and materials will complement silicon-based solutions. Polymeric materials are suitable for energy scavenging, for the realization of organic electronic devices, and for obtaining reversible energy transduction. More specifically, Ionic Electroactive Polymers (IEAPs) are nanocomposited materials, with electromechanical transduction capabilities, which have been already demonstrated to be suitable for the realization of post-silicon smart systems, since they have sensing, power harvesting and acting capabilities. Unfortunately, many of the proposed polymer-based transducing systems are not green and research is ongoing to find greener polymer-based transducers. The presentation will focus on the evolution of solution proposed in about twenty years of research activity in this field at the University of Catania. IPMCs, based on Nafion, will be described as a first solution. All-polymeric Ionic Polymer-Polymer Composites (IP<sup>2</sup>Cs) solutions will be, described, as an intermediate solution. Finally, transducers based on Bacterial Cellulose, as a greener polymer will be discussed.

**11:45 AM**

### **(EHS-039-2021) Inductor-less adaptive impedance matching with ultra-low power consumption for piezoelectric energy harvesting**

H. Jung<sup>\*1</sup>; K. Lu<sup>1</sup>

1. Pyro-E, LLC, USA

In the low power application (less than 1 mW) of energy harvesting systems, Intermittent and random energy source requires high performance of power management circuit to extract the harvested energy. maximum power point tracking (MPPT) is the most popular method to transfer maximum power to the load or battery, but controllers for MPPT are needed to operate high switching frequencies, which results in high power loss of power management circuit. This paper proposed the inductor-less adaptive impedance matching with ultralow power consumption designed specifically for piezoelectric energy harvesting. The proposed topology of circuit that is inductor-less switching enables MPPT with ultra-low switching frequency ( $< 3\text{kHz}$ ) for ultra-low power consumption. MPPT adaptively tune the impedance to track the condition of maximum power. Controller in proposed circuit is implemented using low power microcontroller. experimental results show that average current consumption of microcontroller with proposed topology is 30  $\mu\text{W}$ , which can operates with ultra-low power generation ( $< 100 \mu\text{W}$ ) from piezoelectric energy harvesting system.

## **MCARE S4: Advanced Materials for Perovskite and Next Generation Solar Cells**

Session Chair: Guozhong Cao, University of Washington

**12:20 PM**

### **(MCARE-117-2021) Electrospun Hybrid Perovskite Fibers – Flexible Networks of One-Dimensional Semiconductors for Light Harvesting Applications**

C. Bohr\*<sup>1</sup>; M. Pfeiffer<sup>1</sup>; S. Öz<sup>1</sup>; F. von Toperczer<sup>1</sup>; A. Lepcha<sup>1</sup>; T. Fischer<sup>1</sup>; M. Schütz<sup>1</sup>; K. Lindfors<sup>1</sup>; S. Mathur<sup>1</sup>

1. University of Cologne, Germany

The interest in perovskite solar cells is growing rapidly due to their versatile applicability for energy harvesting systems. In a short period of time, devices already reached efficiencies up to 25%, making them comparable to established thin-film solar cells like Cu(In,Ga)Se<sub>2</sub> or CdTe. The quantity of publications dealing with planar and rigid solar cells is growing tremendously; however, fibrous solar cells have not been in focus yet. Since the 1D structure provides a greater flexibility in comparison to planar systems, applications ranging from e-textiles/wearables to lightweight applications are feasible. Here, the single step fabrication of phase-pure organic-inorganic lead halide perovskite fibers by inert electrospinning technique is presented. Morphological, as well as optical/photonic properties have been studied and demonstrate first comprehensive data on electrospun organic-inorganic hybrid materials. Substitution of the absorbing layer in planar heterojunction solar cells with perovskite fibers resulted in a photoelectric response under simulated sunlight conditions. These flexible 1D hybrid perovskite fibers are potential elements for flexible optoelectronics and mark a starting point towards competitive fibrous solar cells.

## **MCARE S5: Lanthanides, Dyes and Quantum Confined Nanomaterials for Photovoltaic Applications**

Session Chair: Eva Hemmer, University of Ottawa

**1:00 PM**

### **(MCARE-118-2021) Improving the performance of luminescent solar concentrators: Squeezing the sun (Invited)**

A. Menéndez-Velázquez\*<sup>1</sup>; J. Méndez-Ramos<sup>2</sup>; A. García-Delgado<sup>1</sup>; M. Morales-Sabugal<sup>1</sup>; P. Acosta-Mora<sup>2</sup>; J. del-Castillo<sup>2</sup>; S. Torres-García<sup>2</sup>; C. Hernández-Álvarez<sup>2</sup>; M. Medina-Alayón<sup>2</sup>; A. Yanes<sup>2</sup>

1. IDONIAL Technology Center, Photoactive Materials Research Unit, Spain  
2. Universidad de La Laguna, Departamento de Física, Spain

The interest in photovoltaic solar energy has grown exponentially in this century. However, the high cost is still a limiting factor for massive uses. Luminescent solar concentrators provide a promising solution for cheaper photovoltaic (PV) energy. A luminescent solar concentrator (LSC) consists of a piece of glass or plastic plate coated with luminescent centers that absorb sunlight and emit it at a longer wavelength. A substantial part of the longer-wavelength light is trapped by total internal reflection and guided to the edges of the LSC plate, where it is absorbed by small area photovoltaic cells. LSCs provide an exciting new approach to harvest solar energy in buildings and mobile electronics. Efforts to translate this technology to the market have been limited due to the performance. Several strategies, such as spectral conversion of light and vertical alignment of dyes have been proposed to increase the performance of LSCs. Up/down conversion of light is a route for improving energy harvesting over the whole solar spectrum. Via such processes it could be possible to exceed the Shockley-Queisser limit for a single-junction PV device.

Vertical alignment of dyes can increase the fraction of light reaching the edges instead of being lost through the faces of the LSC.

**1:30 PM**

### **(MCARE-119-2021) Tuning the optoelectronic properties in composite systems for solar energy harvesting (Invited)**

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

1. Division of Materials Science, Department of Engineering Sciences and Mathematics, Sweden

The processes of light absorption, exciton generation, charge separation and collection are critical to solar energy harvesting applications. All these processes are regulated by the optoelectronic properties of complex systems, in which the electronic band structure can be finely tuned by adjusting chemical composition, size and morphology of each component. One of the most interesting systems is composed of semiconducting nanocrystals exhibiting quantum confined effects (the so-called quantum dots, QDs), which act as light absorbing materials and generate excitons as a consequence of photon absorption. The QDs are typically coupled to a wide-bandgap semiconductor (SnO<sub>2</sub>, ZnO, TiO<sub>2</sub>), which acts as electron transport material. In this case, the optoelectronic properties are determined by the dynamics of hole/electron dissociation and recombination, and the structure of the interface between the QD and the semiconductor regulates such dynamics. Another option is core-shell QDs, in which the relative band alignment can be tuned by tailoring the interface between the core and the shell. We will illustrate a series of examples, in which exciton dynamics in composite systems influences the functionality of the final device, including solar cells, photoelectrochemical hydrogen production and luminescent solar concentrators.

**2:00 PM**

### **(MCARE-120-2021) New organic-inorganic hybrids towards broad band photocatalysis (Invited)**

S. J. Ribeiro\*<sup>1</sup>

1. São Paulo State University- UNESP, Institute of Chemistry, Brazil

Photocatalysis is being explored by using different light sources. Sunlight through an optical fiber bundle coupled with a solar concentrator is treated together with silver vanadate nanobelts. Low-cost blue LEDs or sunlight is being used together with bismuth vanadate. The fast recombination of photogenerated electrons and holes and poor electron transport properties remain as the bottlenecks in the way of efficient utilization of BV for such applications. Aiming to address these issues, we prepared Ag/Ag<sub>2</sub>O-loaded BV particles using a facile chemical deposition method. The as-prepared BV/Ag/Ag<sub>2</sub>O Z-scheme photocatalysts show light absorption in an extended region of the visible spectrum as compared to pure BV. TiO<sub>2</sub> together with upconversion particles (UCPs) were used aiming to develop near-infrared (NIR)-driven TiO<sub>2</sub>-based photocatalysts. The UCPs@TiO<sub>2</sub> core@shell composite photocatalysts showed good photocatalytic activity under both ultraviolet (UV) and NIR light. Finally, new organic-inorganic aerogel hybrids that have been prepared based on bacterial cellulose (BC) aerogels and inorganic photocatalysts like TiO<sub>2</sub>, BiVO<sub>4</sub> and MoS<sub>2</sub>. These innovative materials gather the BC aerogel properties like mechanical stability, flexibility, and microporous structure together with the unique photocatalytic and surface properties, and mesoporous structure of the inorganic counterpart.

2:30 PM

## (MCARE-121-2021) Metal Organic Frameworks for Photocatalysis and Photoelectrocatalysis (Invited)

N. Wu<sup>\*1</sup>

1. University of Massachusetts Amherst, USA

This talk presents our effort to engineer metal organic frameworks (MOFs) for photocatalysis and photoelectrocatalysis. The metal centers in MOFs have been explored to improve the catalytic activity toward the oxygen evolution reaction. Also, ligands have been functionalized to tailor the catalytic activity toward specific chemical reactions. In addition, MOF have been coupled to the inorganic material to form a heterojunction to compensate the shortcomings of each other. The engineered MOFs have been used for solar water splitting.

## MCARE S11: Materials for Super Ultra-low Energy and Emission Vehicles

Session Chair: Kwan-Young Lee, Korea University

2:00 PM

## (MCARE-122-2021) Designing Catalysts for Meeting the DOE 150 °C Challenge for Exhaust Emissions (Invited)

A. K. Datye<sup>\*1</sup>

1. University of New Mexico, Chemical & Biological Engineering, USA

As more efficient combustion engines are developed for transportation, it is expected that less heat will be wasted in the exhaust, leading to lower exhaust temperatures. Hence the US DOE has set a goal of achieving 90% conversion of target pollutants by 150 °C. To meet exhaust emission standards, it is necessary to develop catalysts that are active at lower temperatures than the current generation of catalysts (which become active at ~200 °C). But these catalysts must also meet the stringent protocols for thermal durability that all exhaust emission catalysts must meet. The DOE targets cannot be achieved simply by increasing the loading of noble metals. One way to achieve higher reactivity at low temperatures is by control of the crystal-lite size of the platinum group metal (PGM) nanoparticles. Smaller particles and sub-nanometer clusters show higher reactivity, and in the limit, we can envision single atom catalysts, which provide the highest atom efficiency to reduce noble metal usage, since every atom is involved in the catalytic cycle. The challenge is to make these single atom and sub-nm structures durable so they can survive high temperature aging protocols and demonstrate performance under realistic conditions. This presentation will highlight our approach to enhance the reactivity and thermal durability of emissions control catalysts using single atom catalysts (SACs).

2:30 PM

## (MCARE-123-2021) Role of Ag/CeO<sub>2</sub>-MnO<sub>x</sub> catalysts in NO<sub>x</sub>-assisted soot oxidation

E. Lee<sup>\*1</sup>; M. Kim<sup>1</sup>; J. Lee<sup>1</sup>; K. Lee<sup>1</sup>

1. Korea University, Republic of Korea

As the regulation for particulate matter (PM) emission are greatly strengthened, it is necessary to remove PM at low temperature. In order to remove PM, oxygen or nitrogen oxide acts as oxidizing agent. Nitrogen oxide, especially NO<sub>2</sub>, plays an important role for low temperature oxidation. For this purpose, it is necessary to develop a catalyst which is good for reactive oxygen supply and NO oxidation. According to previous studies, CeO<sub>2</sub> with high oxygen storage capacity is mainly used for PM oxidation. In addition, noble metals were added to increase the supply of reactive oxygen. Especially, silver has the advantage of exhibiting excellent supply of reactive oxygen compared to other noble metals. In NO oxidation, several types of catalyst used, including noble metal, transition metal etc. Among them, MnO<sub>x</sub> is known to exhibit high activity when used with CeO<sub>2</sub>. In this study, for the NO<sub>x</sub>-assisted soot

oxidation, ceria-manganese mixed oxide was synthesized to improve NO oxidation & NO<sub>x</sub> storage capacity and silver was introduced to promote the ability to supply reactive oxygen. Ag/CeO<sub>2</sub>-MnO<sub>x</sub> catalysts showed the increased NO<sub>x</sub>-assisted soot oxidation performance, and the optimum ratio of CeO<sub>2</sub> & MnO<sub>x</sub> was investigated. Also, several analyses were carried out to explain properties of the prepared catalysts. It was confirmed that Ag/CeO<sub>2</sub>-MnO<sub>x</sub> catalyst is suitable as PM oxidation containing NO.

2:45 PM

## (MCARE-124-2021) Morphology engineering of Cu-doped CeO<sub>2</sub> for increased support reducibility and Pd dispersion to achieve a highly efficient water-gas shift reaction

M. Jang<sup>\*1</sup>; S. Yoon<sup>2</sup>; D. Shin<sup>1</sup>; K. Lee<sup>3</sup>; K. An<sup>3</sup>; J. Han<sup>1</sup>

1. POSTECH, Department of chemical engineering, Republic of Korea

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Water-gas shift reaction (WGS) is important for chemical processes that use hydrogen resources. It has been widely used in fertilizer and petroleum refining industry. Nowadays, the WGS is also aimed at preventing carbon monoxide (CO) poisoning which deactivates fuel cells. To prevent deactivation, the WGS process is performed to oxidize the contained CO before the hydrogen is supplied to the fuel cell anode. Supported metal catalysts are mainly used for the WGS. It is an advantage to express various effects through combination of oxide support and metal particle. The active supports have excellent redox property and contribute to the interfacial interaction by geometric and electronic properties when metal is loaded. Furthermore, the activities of these catalysts can be improved by support tuning. In this study, we prepared supported metal catalysts that controlled the dispersion and reducibility of catalyst by metal-doping and morphology modification. And the synthesized catalyst was confirmed to have higher activity than un-modified catalysts. Various analyses were conducted to prove that the enhanced activity was related to dispersion and reducibility. Furthermore, we designed the catalyst using two strategies simultaneously to improve the activity described above.

3:00 PM

## (MCARE-125-2021) One-Dimensional Modelling of a Three-Way Catalytic Converter

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The gradually stricter regulations against automobile exhaust emissions have increased the necessity for research on three-way catalytic converter (TWC), which eliminates carbon monoxide, hydrocarbon and nitrogen oxides. Recently, the automotive industry has invested significant manpower and resources to develop low-emitting vehicles. A high-fidelity model of catalytic converter system is able to reduce the cost of catalyst development. In this study, a first-principle model for a three-way catalytic converter based on material and energy balance equations is suggested. Particle swarm optimization, which is a global optimization algorithm, is used to calibrate more than 70 kinetic parameters related to 37 reactions including oxygen storage, CO oxidation, HC oxidation, and NO<sub>x</sub> reduction. This work reduces search dimension by utilizing the experimental data obtained from several reactions only. The experimental data used to estimate kinetic parameters reflect various conditions from rich condition ( $\lambda = 0.96$ ) to lean condition ( $\lambda = 1.05$ ). The suggested one-dimensional model is validated by actual driving data from Hyundai Motor Company.



**3:15 PM****(MCARE-126-2021) Low temperature challenge in diesel emission abatement: NH<sub>3</sub> selective catalytic reduction of NO and passive NOx adsorbers (Invited)**J. Szanyi\*<sup>1</sup>

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The continuously decreasing exhaust emission temperature with the introduction of advanced diesel engines requires the development of new catalytic processes and adsorbers for the elimination of NO<sub>x</sub> at ultralow temperatures. Selective catalytic reduction (SCR) of NO with NH<sub>3</sub> is a viable low temperature catalytic process that can provide very high NO<sub>x</sub> removal efficiency and N<sub>2</sub> formation selectivity at the relatively low catalyst temperature of ~200 C. Small pore zeolites, in particular with the CHA structure, ion exchanged with Cu show remarkable activity and selectivity in NO<sub>x</sub> reduction and excellent high temperature hydrothermal stability. However, this technology is not suitable to eliminate NO<sub>x</sub> at temperatures below 150 C due to 1. their low catalytic activity at these temperatures and 2. the high (~180 C) decomposition temperature of urea that supplies the reductant NH<sub>3</sub> for the process. In order to eliminate NO<sub>x</sub> from the exhaust stream passive NO<sub>x</sub> adsorbers (PNA) have been developed based on the same small pore zeolite materials as the SCR catalysts (i.e.), but this time containing Pd instead of Cu. Atomically dispersed Pd in CHA has shown very high NO<sub>x</sub> adsorption capacity and NO release temperature in the range where the SCR catalysts are activities.

**3:45 PM****(MCARE-127-2021) Development of Adsorbents for Lean NOx Trap and Passive NOx Adsorber**H. Kim<sup>1</sup>; Y. Choi<sup>1</sup>; K. Lee\*<sup>1</sup>

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For increase of fuel efficiency and decrease of CO<sub>2</sub> emissions in automobiles, the lean-burn technology has been developed and widely used for engine. However, using lean-burn engine for automobile with excess oxygen increases NO<sub>x</sub> emissions and also reduces the NO<sub>x</sub> removal efficiency of conventional three-way catalysts. NO<sub>x</sub> gases react to form photochemical smog, acid rain, and particulate matter pollution, therefore effective technologies for NO<sub>x</sub> removal are required for vehicles. To develop vehicles having both low energy consumption and low pollutant emission, lean NO<sub>x</sub> trap (LNT) or passive NO<sub>x</sub> adsorber (PNA) with improved adsorption performance for NO<sub>x</sub> gas at low temperature should be developed. In this study, we developed NO<sub>x</sub> adsorbents based on BaO/γ-Al<sub>2</sub>O<sub>3</sub> and hydrotalcite for LNT and PNA application and evaluated their NO<sub>x</sub> adsorption/desorption performance. The physical and chemical properties of the developed NO<sub>x</sub> adsorbents were analyzed using X-ray diffraction, nitrogen adsorption analysis, X-ray photoelectron spectroscopy, temperature programmed desorption, and in-situ Fourier transform infrared spectroscopy.

**4:00 PM****(MCARE-128-2021) Hydrocarbon removal in cold start period using Cu-impregnated MFI zeolite**J. Shim\*<sup>1</sup>; J. Choi<sup>1</sup>

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Representative Hydrocarbon (HC) traps adsorb HCs at low-temperature section and release it over the active temperature range of the three-way catalyst. In this study, we designed an HC trap that can oxidize hydrocarbons at low temperatures, and to achieve this, we added Cu<sup>+</sup> ions to MFI zeolite using the wet impregnation method. To explain the effect of the zeolite support, Na-form and H-form MFIs zeolite were used as supports. Interestingly,

in Na-form MFIs, CuO particles prefer to be formed on the outer surface. On the other hand, in H-form MFIs, Small CuO particles were formed on the outer surface and Cu<sup>+</sup> ions were impregnated inside the zeolite. Accordingly, the Cu-impregnated H-form MFI showed much improved efficiency comparative to representative HCs. We also found a clear correlation between the CST performances and physiochemical properties of Cu-impregnated MFI zeolites. To the best of our knowledge, we show for the first time that the chemical properties of Cu<sup>+</sup> ions and Lewis acid sites can be modified with appropriate physical properties to explain the HC removal abilities of fresh and hydrothermally treated Cu-impregnated MFI zeolites. Finally, the small CuO particles of Cu-impregnated H-form MFI exhibit effective oxidation capacity at low temperatures, thus creating an active HC trap performance.

**4:15 PM****(MCARE-129-2021) Relationship between mobility and activity of Cu ion species in the Cu-SSZ-13 for selective catalytic reduction**H. Lee\*<sup>1</sup>; I. Song<sup>1</sup>; s. Jeon<sup>1</sup>; D. Kim<sup>1</sup>

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Cu ion exchanged SSZ-13 is a state of the art NH<sub>3</sub>-SCR catalyst successfully commercialized in the industrial field, especially an after-treatment system of automobile due to its excellent reactivity and hydrothermal stability. Recently, nature of Cu ion which is known as an active site of the catalyst is a main topic of research to understand the Cu-SSZ-13 catalyst for the NH<sub>3</sub>-SCR. Here, we investigate higher NH<sub>3</sub>-SCR reactivity of 1Al-Cu species than the 2Al-Cu in the Cu-SSZ-13, which are two kinds of Cu ion species in the SSZ-13 with different properties. We modified the Cu-SSZ-13 by using hydrothermal treatment to control the ratio of 1Al-Cu and 2Al-Cu. The ratios of 1Al-Cu and 2Al-Cu were measured by comparing the EPR spectra of hydrated and dehydrated Cu-SSZ-13. There was also no structural degradation, as evidenced by the BET, <sup>29</sup>Si-NMR and XRD results. As the ratio of the 1Al-Cu which has a higher mobility than the 2Al-Cu increased, low temperature activity of catalysts enhanced under dry SCR condition, demonstrating a higher activity of the 1Al-Cu. The kinetic studies led us to reveal that the superior activity of 1Al-Cu appeared only under the reaction condition limited by diffusion of Cu ion. This result indicates that the higher low temperature activity of the catalysts was derived from higher mobility of the 1Al-Cu ion species.

**4:30 PM****(MCARE-130-2021) Improvement of surface properties of various metal substituted hexaaluminate catalyst for removing saturated hydrocarbons from automobile**S. Park<sup>1</sup>; K. Sin<sup>2</sup>; K. Lee<sup>3</sup>; S. Cho\*<sup>2</sup>

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2. Chonnam National University, Chemical Engineering, Republic of Korea  
3. Korea University, Chemical and Biological Engineering, Republic of Korea

Automotive after-treatment technology has been greatly developed to effectively remove various pollutants generated by the use of diverse fuels. Nevertheless, some saturated hydrocarbons, including methane, are not easily removed, so it is necessary to improve their abatement technology in order to respond with increasingly strengthened environmental regulations. Although hydrocarbons can be removed using precious metal loaded alumina catalysts, these catalysts have a dramatic deactivation due to sintering of active metals under high temperature hydrothermal conditions. In this study, we used hexaaluminate as a support to prepare a catalyst with improved hydrothermal stability. Hexaaluminate synthesized by using an organic surfactant and alumina sol has a stable surface area of 138 m<sup>2</sup>/g even after high thermal treatment at 1100 °C. Nevertheless, the hexaaluminate catalyst did not effectively inhibit

the sintering of the active metal due to the lack of interaction with the metal. Therefore, we have improved the surface properties of hexaaluminate by substituting various metals for the hexaaluminate frameworks. The strong interaction induced between the modified hexaaluminate and the precious metal is expected to improve the dispersion of the active metal and suppress sintering during hydrothermal treatment.

### **MCARE S13: Theory and Experiment Meeting in Energy Materials Research**

Session Chair: Heechae Choi, University of Cologne

**1:00 PM**

#### **(MCARE-131-2021) Electric Field Assisted Sintering of Gadolinium-doped Ceria (GDC) (Invited)**

T. Mishra\*<sup>1</sup>; O. Guillon<sup>1</sup>; M. Bram<sup>1</sup>

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Ceria based materials have good chemical stability, ionic conductivity and catalytic properties in redox processes. These unique properties make them attractive for applications in electro-chemical devices as electrolytes, diffusion barrier layers in solid oxide cells and/or oxygen ion conducting membranes. Gadolinium Doped Ceria (GDC) is one of the promising representative of this class of materials. Sintering of GDC is usually done in air at high temperatures, in the range of 1400° C to 1600° C, and dwelling time of several hours to achieve almost theoretical density. A promising approach to achieve high densification rate at lowered temperatures is electric field assisted sintering. In this work, the prospective of densifying  $Ce_{0.9}Gd_{0.1}O_{1.95-\delta}$  (i.e. GDC10, gadolinium-doped ceria, with Gd 10 mol %) by electric field assisted sintering technologies, primarily by, (i) Field Assisted Sintering Technology/Spark Plasma Sintering (FAST/SPS) and (ii) Flash sintering has been studied. The interaction between Electro-Chemo-Thermo and related mass transport and grain growth in GDC was studied. Furthermore, optimization of the sintering parameters for GDC10 powders and tailoring the microstructure by controlling the material synthesis and processing conditions were investigated.

**1:30 PM**

#### **(MCARE-132-2021) Theoretical approach to the photochemical reactions on semiconductor surfaces**

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Since the electrochemical/photochemical reactions involve charge transfer between matters, solid description on the energetics of charge transfer is necessary. In general, (photo)catalytic reaction activities of materials are predicted or analyzed using normal density functional theory calculations, which can give theoretical overpotentials based on the computed adsorption free energies. However, in reality wide gap semiconductor materials can have varying Fermi level. Therefore, adsorption energy of charge acceptor or charge donor on a semiconductor surface must be expressed as a function Fermi level. In this talk, I will present recent theory-guided experimental works which demonstrate the Fermi level dependency of anion adsorption energies on n-type semiconductors and the theoretical framework which can accurately predict  $H_2O_2$  formation kinetics on wide band gap semiconductors.

**1:45 PM**

#### **(MCARE-133-2021) Design and optimization of $CuSb_{1-x}Bi_xS_2$ alloy as a promising photovoltaic material: Theoretical and experimental study**

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Here we report the miscibility gap of  $CuSb_{1-x}Bi_xS_2$  (CABS), a promising photo energy conversion material for band gap engineered solar cells, and evaluate its applicability via a combination of theoretical predictions and experimental verifications. Our density functional theory calculation found that the optimal composition of CABS using Gibbs free energy. Also, in order to examine the phase stability of alloyed  $CA_{1-x}B_xS$  ( $x=0.46, 0.79$ ) phase, we demonstrated the stable regions of  $CA_{1-x}B_xS$  ( $x=0.46, 0.79$ ) under various Sb and Bi chemical potential. It revealed that the CABS random alloy system has optimal band gap values in the range of 1.1–1.5 eV when synthesized at room temperature. The CABS system, synthesized by mechanochemical methods, exhibited optical band gap values in very good agreement with theoretical predictions, as well as lowered kinetic energy barriers for enhanced nucleation.

**2:00 PM**

#### **(MCARE-134-2021) Fermi-level dependent catalytic activity of semiconductor**

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Adsorption energy of adsorbates is the key indicator of the catalytic reactivity of a material. Especially in catalytic reactions involving charge transfers, the intermediate adsorbates play the roles of electron acceptor or donor. Therefore, the efficiency of catalysis should be expressed as a function of electron chemical potential, Fermi level. In semiconducting catalysts, the Fermi levels are manipulatable with doping and/or defect equilibria, which can be determined by synthesis and processing conditions. Density functional theory (DFT) calculations have been a useful method to predict and analyze the reactivities of catalytic materials. However, Fermi level dependency of catalytic materials of semiconductors has been mostly neglected in adsorption energy calculations even when the catalysis reactants are charge acceptors or donors. In this study, we modified a theoretical method by considering the Fermi level contribution to the adsorption energies of adsorbates on semiconductor catalyst surfaces. Using this method, we provided advanced analyses on the catalytic activity of  $CeO_2$  methane ( $CH_4$ ) oxidation, which has been known to depend on synthesis conditions.

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