

Poster Abstracts

<p>Chaitali Morey, University Of South Carolina</p>	<p>Computational Analysis of Solid Oxide Iron Air Battery with Catalyzed Iron-bed Energy Storage Material <i>Chaitali Morey, Qiming Tang, Xinfang Jin, Kevin Huang</i></p> <p>Long-term energy storage (LDES), lasting for durations of 10 hours or more, is widely recognized as a crucial technology for advancing the integration of renewable energy into the commercial utility sector. However, the current storage technologies cannot achieve LDES's duration requirement at a competitive cost. Therefore, a newly emerged solid oxide iron air battery (SOIAB) with energy-dense solid Fe as an energy storage material is a competitive LDES-suitable technology compared to conventional storage technologies. Our recent results have shown that SOIAB delivers 12.5-hours of storage per cycle with high energy storage capacity and round-trip efficiency. This work focuses on the description of a high-fidelity 2D axis symmetrical multiphysics model to simulate the performance of a solid oxide iron air battery. The model battery system consists of an anode-supported solid oxide cell and energy storage unit (ESU) of iron bed with Ir as a catalyst. The Multiphysics model comprehends charge transfer, mass transport, and chemical redox kinetic cycle occurring across all components of the battery and is validated with experimental results. The motivation for combining the Ir catalyst in ESU is to boost the sluggish FeOx reduction kinetics related to the charging process. Compared to baseline Fe₂O₃/ZrO₂, with Ir catalyst Fe₂O₃/ZrO₂ shows excellent energy density, long stability cycle, and high round trip efficiency. The work will also show the performance of improved reduction kinetic rate of SOIAB with Fe₂O₃/ZrO₂-IrO₂ over the baseline Fe₂O₃/ZrO₂.</p>
<p>Siddhartha Sarkar, Clemson University</p>	<p>Ultra-fast laser sintering of iron-alumina material system <i>Siddhartha Sarkar</i></p> <p>The Fe-Al₂O₃ metal-ceramic system has recently demanded interest for structural components and functional coatings. Historically, several processing techniques have been used to fabricate this metal-ceramic pair such as physical vapor deposition, chemical vapor deposition, thermal spray, arc melting as well as furnace sintering. Each technique has its own disadvantages, with some of the major issues being the lack of a chemical bond between the metal and ceramic, porosity within the microstructure as well as oxidation. Most importantly, due to the instability and non-wetting behavior of the metal-ceramic interface, it is difficult to obtain and control viable microstructures. On the other hand, laser sintering promises extremely fast heating and cooling rates and facilitates non-equilibrium microstructures comprising of both metal and ceramic phases. This study reports the novel use of a CO₂-laser sintering approach under an inert environment to process different volume ratios of the iron-alumina composition. Slurries of Fe-Al₂O₃ in volume ratios 20:80, 40:60 and 50:50 respectively are prepared and cast onto a glass substrate, up to a thickness of 300 μm. Consequently, by varying the scan speed and laser power, optimum laser parameters are developed to both melt and sinter the iron and alumina respectively. The resultant microstructures are well-mixed, uniform and dense. SEM, TEM and EDS results showed a clean bonding between iron and alumina, with no intermediate phases. Characteristic peaks of hercynite (FeAl₂O₄ spinel) were observed while collecting XRD data. STEM-EDS results showed the presence of the spinel phase in between the alumina grains, thereby facilitating the wetting behavior between iron and alumina. These results show a new path towards processing of metal-ceramic pairs which have stable, dense, crack-free and non-equilibrium microstructures.</p>

<p>Roya Rajabi, University Of South Carolina</p>	<p>Fabrication and modification of polymer electrolyte for zinc ion batteries <i>Roya Rajabi, Shichen Sun, Kevin Huang</i></p> <p>Polymer electrolytes have emerged as a promising solution to address the limitations associated with aqueous electrolytes in energy storage systems, particularly regarding issues such as water splitting, evaporation, and leakage, which have hindered progress in this field. Furthermore, their inherent flexibility holds significant potential for applications in wearable electronics. Despite increasing interest in polymer electrolyte-based zinc ion batteries (ZIBs), their development is still in its early stages due to numerous challenges. In this study, we explored the potential of carboxyl methyl chitosan with acrylamidmonomer (CSAM) compared to polyacrylamide monomer hydrogel electrolytes. Notably, the CSAM hydrogel contains zinc salt without the need for pre-soaking in a zinc salt solution. Additionally, both CSAM and polyacrylamide hydrogels were compared with a p-PBI membrane known for its robust mechanical and thermal properties. Two different zinc salts, namely Zn(ClO₄)₂ and Zn(OTf)₂, were utilized in the investigation. Results indicated that the mechanical strength provided by the p-PBI membrane alone is insufficient to ensure high battery performance. While the p-PBI membrane exhibited prolonged durability compared to glass fiber separators, it also led to increased resistance, overpotential, and degradation in full-cell batteries. Conversely, the presence of carboxyl groups in CSAM and polyacrylamide electrolytes facilitated ion movement, resulting in enhanced ionic conductivity and resistance against dendrite formation. Mixing these hydrogels with a high-performance zinc salt such as zinc triflate (Zn(OTf)₂) yielded impressive stability, with the symmetric cell demonstrating over 4000 hours of uniform and stable voltage profile.</p>
<p>Ziba Rahmati, University Of South Carolina</p>	<p>Exploring a solid-state Li-ion battery with perovskite electrolyte and soft polymer interlayer <i>Ziba Rahmati, Dr. Kevin Huang</i></p> <p>Solid state batteries (SSBs) represent a next-generation electrochemical device for safe and high-energy-density energy storage. Solid state electrolyte (SSE) is a key component in SSBs. Among all types of SSEs (sulfides, halides, oxides, and polymers), oxide-based SSEs exhibit a good balance between conductivity and stability. However, one critical issue is the high interfacial resistance with solid electrodes. For perovskite SSEs, an additional issue is the reducibility upon contact with Li metal, lowering Faradaic efficiency. Here in this study, we explore a multi-functional structure with a flexible solid polymer electrolyte (SPE) as an interlayer between electrodes and a ceramic perovskite electrolyte Li₆/16Sr₇/16Ta₃/4Hf₁/4O₃ (LSTH). The polymethylmethacrylate (PMMA)-polyethylene glycol diacrylate (PEGDA) SPE with a room-temperature ionic conductivity of 2.20×10^{-3} S cm⁻¹ minimizes the interfacial resistance while protecting LSTH from catastrophic Li-reduction, preventing concentration polarization and suppressing Li dendrite attack. We show that application of this structure enables the cyclability of Li/Li half-cells, which is otherwise unattainable with pure LSTH, and achievement of 129.8 mAh g⁻¹ specific discharge capacity at 0.1 C of a full cell with LiFePO₄ cathode and Li anode.</p>

<p>Habib Rostaghi Chalaki University Of South Carolina</p>	<p>Nanoscale Freestanding La_{0.8}Sr_{0.2}CoO₃ Thin Films Through Water-Soluble Sacrificial Oxide Layers <i>Habib Rostaghi Chalaki, Mohammad El Loubani, Maxwell Robert Stewart, and Dongkyu Lee*</i></p> <p>Transition metal oxides (TMOs) possess a variety of fascinating properties, ranging from superconductivity and ferroelectricity to electrochemical and piezoelectric phenomena due to the intricate interplay of charge, orbital, spin, and structural properties within TMOs. Particularly, ABO₃ perovskites are widely used in many energy applications. With the rapid development of two-dimensional (2D) thin films, it is highly anticipated that exemplary functionalities will be achieved from epitaxial oxide thin films. However, the application of epitaxial thin films in energy devices faces limitations, especially the substrate impact on the properties. A breakthrough involves weakening epitaxial crystals and integrating water-soluble sacrificial layers, enabling the detachment of ultrathin oxide crystals from substrates, and forming freestanding thin films. Despite various methodologies, the wet etching method using water-soluble sacrificial oxide layers is considered the most promising approach for producing high-quality freestanding perovskite oxide single crystals. However, achieving freestanding perovskite thin layers remains challenging due to a lack of understanding of the sacrificial layers and transfer step. In this project, we demonstrate the synthesis of freestanding La_{0.8}Sr_{0.2}CoO₃ (LSC) nanomembranes, which are widely used in electrochemical energy applications. Membranes are fabricated by employing water-soluble (Sr,Ca)₃Al₂O₆ sacrificial layers epitaxially grown on SrTiO₃ (001) substrates by pulsed laser deposition. Once LSC thin films with the sacrificial layer are synthesized, all samples are coated with a polymer support layer that enables the transfer of the sample onto other substrates. Subsequently, wet etching in DI water is employed to dissolve the sacrificial oxide. Electrochemical impedance spectroscopy and electrical conductivity relaxation are employed to determine the electrochemical properties of the samples. This study demonstrates the potential to transfer perovskite films with tailored properties onto desired substrates."</p>
<p>Mohammad El Loubani, University Of South Carolina</p>	<p>Effect of Metal Particles Formed by Metal Exsolution on the Thermoelectric Properties of Epitaxial ABO₃ Thin Films <i>Mohammad El Loubani, Benjamin Richardson, Habib Rostaghi Chalaki, and Dongkyu Lee</i></p> <p>Transition metal oxides (TMOs) exhibit significant potential for use in high-temperature thermoelectric (TE) applications. To develop oxide TE materials with a large power factor (PF), enhancing both electrical conductivity (σ) and thermopower (S) is indispensable. However, due to the trade-off relationship between S and σ, the maximum achievable PF has a limit. To overcome this trade-off relationship, metal exsolution recently emerged and shows promise to improve both S and σ. However, the effect of metal exsolution with different particle sizes and densities on S and σ is still largely unexplored. This study demonstrates an unusually large PF enhancement through the exsolution of Ni nanoparticles in epitaxial La_{0.7}Ca_{0.2}Ni_{0.25}Ti_{0.75}O₃ (LCNTO) thin films. Metal exsolution leads to a decrease in the carrier concentration while increasing the carrier mobility due to energy filtering effects. Consequently, the exsolution of metal particles results in a significant enhancement in S in accordance with the highly increased σ compared to the as-grown film. Overall, the TE power factor of LCNTO is dramatically enhanced by up to 8 orders of magnitude owing to the presence of exsolved metal particles. This study highlights a novel approach for tailoring the interconnected physical and chemical properties of oxides, thereby leading to the significant enhancement of TE conversion efficiency.</p>

<p>Ting Shen, Clemson University</p>	<p>High Entropy Oxide Lithium Ion Battery Anodes <i>Ting Shen, Xiaoxiao Jia, Chaofeng Liu, Guozhong Cao*, Rajendra K. Bordia*</i></p> <p>High entropy oxides (HEOs), known for their extensive compositional diversity, while maintaining a single phase, and tunable electrochemical properties, are emerging as promising anode material for lithium ion batteries (LIBs). The challenge of sluggish kinetics during prolonged cycling, has hampered their widespread adoption. In this study, we address this limitation by introducing oxygen vacancies into a rocksalt HEO oxide ((MgCoNiCuZn)O) via calcination under Ar atmosphere, with a goal to enhance ion and electron mobility. This modification significantly improves conductivity and Li ion diffusion kinetics compared to the original HEO material. As a result, the modified anode achieves an impressive specific capacity of 598 mAh/g at 0.1 A/g, maintaining 99% capacity after 85 cycles at 0.2 A/g. Even after 1900 cycles at 3 A/g, the material shows a capacity of 249 mAh/g. The results demonstrate that the introduction of engineered defects into HEOs can markedly improve the lithium storage efficiency, charge transfer, and diffusion kinetics, thereby improving the electrochemical performance. Our approach provides a scalable strategy and valuable insights for developing defect engineered HEO LIB anodes."</p>
<p>Miranda Stone, Clemson University</p>	<p>Pushing Compositional Limits of Optical Fibers Fabricated Using the Molten Core Method <i>Miranda P. Stone, Thomas W. Hawkins, John Ballato</i></p> <p>One of the many goals for continued advancement of specialty optical fibers is pushing the compositional limits of the fiber core to suit specific applications. While many forms of fabrication exist, this research focuses on the Molten Core Method (MCM). This method allows for a greater range of compositional flexibility to be achieved than the more traditional chemical vapor deposition methods, while being a much more straightforward fabrication process than those used for photonic crystal fibers and other such complex core geometries. As a result, the MCM can be used to push the compositional limits of optical fibers with relatively few fabrication steps. However, pushing limits to the extremes is not a simple process and can yield some unexpected and interesting results. This paper provides an overview of results to date and offers new insights into future opportunities, glass systems, and properties critical to next generation fibers.</p>
<p>Komalakrushna Hadagalli, Clemson University</p>	<p>Structural, morphological, and mechanical properties of hydroxyapatite scaffolds with unidirectional pores <i>Komalakrushna Hadagalli, Bikramjit Basu, Rajendra K. Sordia</i></p> <p>Hydroxyapatite (HA) is one of the widely investigated calcium phosphate compounds in the field of tissue engineering due to its similarity in structure and chemical composition to human bone. Porous HA with unique pore architecture is frequently used as a biocompatible ceramic to support cell fate for bone tissue engineering applications. In this study, we have investigated engineered porosity bone scaffold bioceramics via freeze cast with tunable porosity and pore architecture. This simple process, where a material suspension is simply directionally frozen and then sublimated, provides materials with unique porous architectures, where the porosity is almost a direct replica of the frozen solvent crystals. It leads to hierarchical porosity with interconnected micro- and aligned macro-pores. The porous scaffolds were sintered at 1250, 1350 and 1450 °C, for 2 h to control the micro and macro porosity. The microstructure of interconnected lamellar pore channels examined by SEM and phase purity by XRD. As the HA content was increased from 10 to 30 vol.%, the porosity decreased from 80 to 49%. The scaffolds with 30 vol% of HA (1450°C) content possessed unidirectional pore channels with a porosity of around 49 % and showed compressive strength of up to 16.3 MPa and compressive modulus of 1.2 GPa. In vitro and in vivo investigations are underway to determine the potential of these engineered porosity scaffolds."</p>

<p>Deeksha Kodangal, Clemson University</p>	<p>Densification and microstructure evolution of alumina samples processed via Direct Ink Writing <i>Deeksha M. Kodangal and Rajendra K. Sordia</i></p> <p>Additive manufacturing of ceramics has gained widespread attention enabling the fabrication of ceramics with complex geometries. Direct Ink Writing (DIW) also called Robocasting, is an extrusion-based technique that uses a slurry with non-Newtonian viscosity and has been able to print at room temperature. The slurry must possess shear-thinning behavior to flow through small diameter nozzles and must show a dilatant behavior upon releasing from the nozzle. The characteristics of the initial powder and the additive manufacturing (AM) technique used in the early stages lead to the formation of a unique green structure. This structure exhibits inherent anisotropy at macro- and micro-scale, distinguishing it from conventionally processed green bodies. In this study, we have investigated the differences in the densification kinetics and microstructure evolution of samples made via slip-cast and robocast processing techniques. A slurry with optimized solid content of 55 vol% Alumina was prepared in distilled water. The slurry was printed using a robocaster from Robocasting LLC. A 50 vol% Alumina slurry was prepared in distilled water and samples were prepared via slip casting to compare those with the robocast samples. Both the samples were sintered in air at 1000, 1100, 1200, 1300 and 1400 °C for 2 hours. A density measurement and microstructure analysis using SEM were performed for all the samples and compared for both the techniques. The kinetics of densification as a function of temperature and time using a dilatometer are underway to develop a kinetic model for the densification of AM produced green components.</p>
<p>Dillip Kumar Panda, Clemson University</p>	<p>Hierarchically structured silicon oxycarbide/reduced graphene oxide composite anodes for lithium-ion batteries with enhanced electrochemical performance <i>Dillip K. Panda, Nawraj Sapkota, Gangadhar Jella, Sujith R, Apparao M. Rao, Rajendra K. Bordia</i></p> <p>Silicon oxycarbides (SiOCs) have attracted attention due to their outstanding theoretical capacities and structural stability owing to their application in lithium-ion batteries (LIBs). The low electronic conductivity of SiOCs, however, has adversely affected their overall performance, therefore limiting their practical use in Li-Ion batteries. To address this, we engineered high-performance anodes by creating a hierarchical interconnected configuration of silicon oxycarbide integrated within a chemically modified reduced graphene oxide matrix, utilizing the surface modification capabilities of reduced graphene oxide for SiOC. In particular, the SiOC/rGO anodes exhibit a high initial reversibility.</p> <p>The capacity of this battery is approximately 1000 mA h/g at 0.37 A/g (0.1 C for graphite), exceeding that of conventional SiOC batteries. In addition, the composite anodes exhibit a considerable capacity of 700 mAh/g at 0.744 A/g (2 C for graphite) even after 800 cycles, highlighting excellent long-term cycling stability and high capacity at high rate. In addition to improved electronic conductivity, shortened ion diffusion length, and reduced charge-transfer resistance, composite structures provide enhanced electrochemical performance. SiOC/rGO composite anodes present a promising development for the commercialization of lithium-ion batteries due to their high rate of cycling and long cycle life. A range of spectroscopic, microscopic, and electrochemical techniques have been utilized in this study to characterize the materials and to understand how the batteries perform.</p> <p>Keywords: SiOC, reduced graphene oxide, composite, battery, Acknowledgement: This work was supported in part by the National Science Foundation EPSCoR Program under NSF Award# OIA-165740"</p>

<p>Anasheh Khecho, University Of North Carolina At Charlotte</p>	<p>Direct Ink Writing of SiC-Fe304-Polymer Nanocomposites for Magnetic Humidity Sensors <i>Anasheh Khecho, Erina Baynojir Joyee</i></p> <p>3D printing is a transformative manufacturing technology that has achieved notable advancements in the fabrication of complex polymer-ceramic nanocomposite structures that exhibit enhanced properties for various applications. Fabrication of sensor-based devices has significantly benefited from the development of 3D printing techniques. A wide array of sensors has been successfully fabricated via 3D printing methods with polymer-ceramic nanocomposite. Within the complex framework of additive manufacturing, (AM), extrusion-based techniques such as the Direct Ink Writing (DIW) method, significantly contribute to broadening the range of 3D-printable materials with unconventional structures, particularly for sensors. The extensive range of compatible materials makes this method considerably ideal for fabricating composite structures. In this study, a novel 3D-printable ink based on SiC-polymer nanocomposites is investigated for DIW process. The inks are composed of SiC and magnetite (Fe₃O₄) particles dispersed within a polyvinyl alcohol (PVA) matrix. Magnetite particles were added to reinforce the humidity sensing and create a multimodal magnetic-humidity sensing of the nanocomposite. As the rheology plays a vital role in the DIW process and printing resolution of the printed sample, the printability including extrudability and viscoelasticity of the inks was thoroughly evaluated for proper flow through the nozzle and rapid shape recovery of the ink after deposition."</p>
<p>Oriyomi Opetubo, Clemson University</p>	<p>Oxygen vacancy formation Energies in MgO-based HEOs from OFT and Experiments <i>Oriyomi Opetubo</i></p> <p>High-entropy oxides (HEO) consist of equi or near equimolar concentrations of multiple cations randomly distributed on the crystal lattice, which is in contrast to conventional oxides that contain one principal cation, and one or two dopants in small concentrations. The random distribution of cations in HEOs causes a wide diversity of nearest-neighbor environments around oxygen atoms creating a range of bond lengths and electronic structures, which consequence is a range of oxygen vacancy formation energies. We investigate oxygen vacancy formation energies in Mg(CuCoNiZn)O-based HEO using density functional theory (OFT). We find that vacancy formation energy trends are controlled by nearest-neighbour environments and cation valence charge. Our results show that oxygen vacancy formation energy decreases as the total Bader charge of nearest-neighbour cations decreases, as Cu²⁺ plays a major role in lowering oxygen vacancy formation energy. Our predictions agree with the experimental observations by our collaborators, which also indicate that the presence of Cu²⁺ lowers the oxygen vacancy formation energy.</p> <p>Experimentally, a series of binary, ternary, quaternary and quinary HEOs are synthesized using a simple and scalable polymeric steric entrapment method. By annealing in an inert environment, oxygen vacancies are analyzed by XPS and TGA. This understanding contributes to oxygen vacancy transport useful in microstructure evolution, and electrochemical applications.</p>

<p>Kangkang Zhang, University of South Carolina</p>	<p>H₂O-enhanced CO₂ transport through a proton conducting ceramic-molten carbonate dual-phase membrane" <i>Kangkang Zhang, Kevin Huang</i></p> <p>High-temperature membranes for CO₂ transport and separation has attracted significant interest from academia and industries due to their potential to mitigate the emissions of CO₂ and ultimately global warming/climate change. In this study, we report a dual-phase CO₂ membrane fabricated from a porous proton conducting BaZr_{0.8}Y_{0.2}O_{3-δ} (BZY) matrix and eutectic mixture of Li₂CO₃-Na₂CO₃ (denoted as MC). The membrane exhibits a high CO₂ permeation flux density in the range of 550-750 oC in both dry and wet conditions. Through microstructural optimization, a CO₂ flux density as high as 0.34 mL·cm⁻²·min⁻¹ at 650 oC and 0.53 mL·cm⁻²·min⁻¹ at 750 oC have been achieved with an 0.8 mm thick BZY-MC membrane containing 52% porosity and 50%CO₂-N₂ feed gas. The high flux is attributed to synergistic effects of microstructure, MC loading and high bulk conductivity of BZY. In addition, we also demonstrate the positive effect of H₂O in the permeate side on CO₂ flux density and proposed a reasonable mechanism to explain the H₂O-enhanced CO₂ flux density. With 3% H₂O-added into the sweeping gas, the membrane exhibits 30% CO₂ flux density enhancement and good stability over 250 h at 650 oC.</p>
<p>Danyi Sun, University of South Carolina</p>	<p>Harvest Lithium Metal from Seawater via Electrodialysis with Li₆/16Sr₇/16Ta₃/4Hf₁/4O₃ (LSTH) Solid State Lithium Ion conductor <i>Danyi Sun, Nan Wu, Yeting Wen, Shichen Sun, Changyong Qin, Ralph White, Kevin Huang</i></p> <p>As the world transitions from gasoline-powered vehicles to those utilizing lithium-ion batteries (LIB), the demand for lithium, a crucial component in lithium-ion battery (LIB) based EVs, has surged from 38 thousand tons in 2016 to 180 thousand tons in 2023. However, the identified lithium reserves on land until 2022, is only 98 million tons. Besides, the conventional lithium extraction processes, mining and brine evaporation, are inefficient and environmentally unfriendly. The cumulative lithium content in seawater reaches an astonishing 230,000 metric tons, vastly surpassing the 96 metric tons of lithium reserves on land.</p> <p>Extracting lithium from seawater faces challenges due to its extremely low concentration and the high concentration of competing ions. Electrodialysis, an advanced separation process, is crucial to meet this threshold, offering advantages such as high selectivity, short processing times (a few hours), and high cyclability. The efficiency of electrodialysis depends on the lithium-selective membrane, a critical component governing lithium separation. In comparison, the inorganic LIB electrolyte could provide 100% lithium selectivity due to their lithium ion conductor nature. The perovskite-type lithium-ion conductor, LSTH, stands out as the sole solid-state electrolyte stable in both water and strong acid environments, making it an optimal candidate for electrodialysis applications."</p>