Mechano-Chemical Understanding of Solid Ion Conductors (MUSIC)
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Mission Statement*: to reveal, understand, model, and ultimately control the chemo-mechanical phenomena underlying the processing and electrochemical dynamics of ceramic ion conductors for clean energy systems.*

The recent emergence and discovery of new **ceramic ion conductors (CICs)** with fast ionic conductivity at near-ambient temperatures creates the opportunity to push the frontiers of electrochemical energy conversion and storage. The ability to replace traditional liquid or polymer electrolytes with ceramics has the disruptive potential to improve safety and enable next generation technologies including solid-state batteries with metal anodes, impermeable membranes to prevent crossover in redox flow batteries for long-duration energy storage (LDES), and intermediate temperature solid-oxide fuel cells and electrolyzers to propel the hydrogen economy. Enabling the next generation of electrochemical conversion and storage, however, requires fundamental research to understand and control the emergent **mechano-chemical** environments that arise when CIC materials are interfaced with other dissimilar materials. The overarching **scientific mission** of MUSIC is *to reveal, understand, and model, and ultimately control the chemo-mechanical phenomena underlying the processing and electrochemical dynamics of CICs for energy systems*.

This mission is supported by *specific hypotheses* that drive the research activities. To investigate and validate these hypotheses, MUSIC galvanizes a diverse team of internationally recognized leaders spanning the fields of electrochemistry, solid mechanics, ceramic synthesis and manufacturing, *in situ/operando* analysis, and multi-scale computational modeling. Within the MUSIC team, the convergence of the materials science, electrochemistry, solid mechanics, and manufacturing experts has the potential to solve critical problems that are central to CICs, yet would be challenging to solve by one discipline alone. Moreover, owing to growing industry, academic, and national lab workforce needs, MUSIC emphasizes career development through frequent and close interaction among early-career, mid-career researchers, and senior researchers, along with postdoctoral fellows, graduate, and undergraduate students.

MUSIC has been created to achieve the overarching scientific mission detailed above and to meet the growing need for a concerted effort to integrate the fields of mechanics, chemistry, and electrochemistry to understand electro-chemo-mechanical phenomena underlying the synthesis and use of CICs for clean energy. The Senior Personnel in MUSIC have world-leading expertise in the areas needed to advance CIC science. (Figure 1) Connecting experiments to theory,

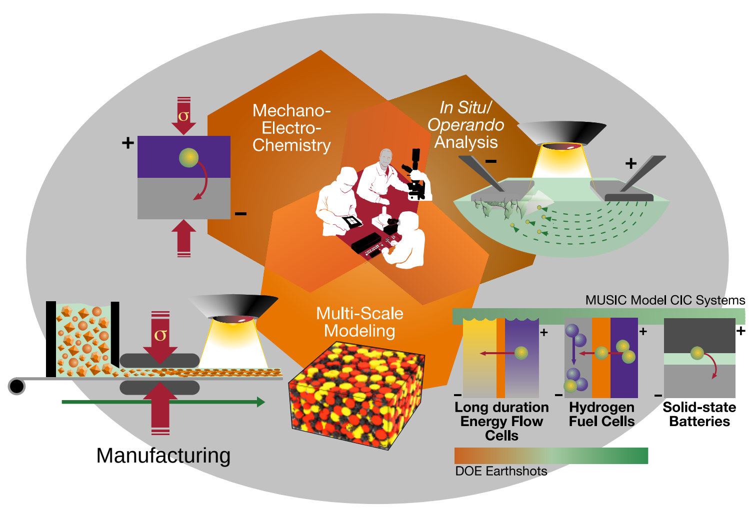

Figure 1. MUSIC will expand the field of mechano-electro-chemistry to accelerate progress toward DOE's Earthshots.

leaders in the fields of multi-scale modeling with experience in mechano-electro-chemistry are integral to MUSIC. Augmenting the ability to better understand complex phenomena under dynamic conditions and at buried interfaces, MUSIC also includes key researchers that are advancing the state-of-the-art of *in situ*/*operando* and multi-scale modeling over all relevant length and time scales. To bolster efforts to create a viable and independent energy industry, processing and manufacturing science pervades across all themes within MUSIC. Most importantly, MUSIC acknowledges the role that postdocs and students will play in enabling science within the center and in future decades. MUSIC emphasizes training and fostering the next generation of scientists through robust bylaws, activities, promotion of workforce development, and continuous focus on supporting diversity, equity, and inclusion (DEI) efforts at all levels of the center.

Science Goals

The overarching Scientific Goals that will guide MUSIC are as follows:

SG1. How do mechanical stresses influence stability and charge-transfer kinetics of interfaces in CIC-based electrochemical systems as they evolve dynamically in time?

SG2. How are stress, electrochemistry, microstructure, and morphology related in CIC systems?

SG3. How do chemo-mechanical phenomena impact degradation pathways and at their interfaces?

SG4. How do chemo-mechanical phenomena in CICs influence the design and manufacturing of high-performance and resilient interfaces?

Research Goals

To achieve this ambitious vision, the four-year Research Goals of the MUSIC EFRC are as follows:

RG1. Develop *in situ/operando* platforms to reveal material dynamics at solid-solid, solid-liquid, and solid-gas interfaces and interphases of CICs spanning the atomic, meso, and microscales

RG2. Model and experimentally validate the coupling of chemical potential, stress state, and electric field in CICs to predict their influence on interfacial electrochemical kinetics and ionic transport

RG3. Reveal emergent chemo-mechanical degradation pathways across various length/time scales

RG4. Apply knowledge of the coupled mechanical and chemical phenomena in CICs to enable new manufacturing processes to improve resiliency, safety, and enable atomically precise control.

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