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COUPLED MULTI-SCALE AND MULTI-PHYSICS COMPUTATIONAL MODELS FOR ELECTROCHEMICAL SYSTEMS

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ABSTRACT

Electrochemical systems, such as batteries, electrolyzers, and fuel cells, interconvert chemical and electrical energy through redox reactions. These systems are pivotal to modern energy storage and conversion technologies. Besides experimental research that is essential to demonstrate the feasibility of these systems and enhance their performance computational modeling offers a complementary approach by performing a detailed analysis and prediction of system behavior under various conditions. Given that electrochemical systems involve multiple phenomena such as electrochemical kinetics, transport phenomena, and thermodynamics, coupled models are necessary to provide comprehensive insights into these systems. Coupled multi-scale computational models can facilitate our understanding of the interplay between intricate phenomena occurring at several length and time scales, ranging from kinetics behavior in the nanoscale (electrode-electrolyte interface) to the transport phenomena, i.e., mass, charge, momentum, and heat, in the mesoscale (pore scale) and the macroscale (cell or stack level). Moreover, these models can act as tools for assessing and optimizing the design of various components of electrochemical cells.

The session is meant as a venue to discuss the latest developments in computational modeling of electrochemical systems with special emphasis on the coupled phenomena contributing to their behavior. Interested participants are invited to submit their contributions to the modeling of various electrochemical technologies (e.g. redox flow batteries, CO_2/water electrolyzers, fuel cells, and lithium-ion batteries) on topics that include but are not limited to:

- Computational modeling of macro-scale transport phenomena in electrochemical reactors.
- Simulation of transport phenomena in porous electrodes and membranes/separators.
- Numerical modeling for assessment of the electrochemical performance in cells or stacks.
- Shape and topology optimization models for improving the design of components of electrochemical flow cells.
- Mathematical models of surface kinetics for understating the redox reactions on the surface of electrodes.
- Multi-scale modeling for bridging the gap from atomic simulations to cell models.