Mesoscale Priority Research Direction

Ionomer and Solvent Structure\Interactions in Electrodes

Opportunity

Efficient electrode performance in energy conversion and storage devices requires optimized structures to manage mass and ion transport effectively and to optimize electrochemical reaction efficiency and rate. This requires that the structure, interactions, and material properties be fully understood under a variety of conditions. For example, in PEM fuel cells, it has been demonstrated that ionomer water content varies with substrate and film thickness, which can alter reaction dynamics, and excess liquid water can block reactant access to the catalytic sites.

Approach

Structural probes **e.g.** ***in situ*** **Neutron Imaging, X-Ray Computed Tomography (XCT), SAXS, SANS will** ***quantify*** **solvent structure and** ***identify*** **ionomeric constituent effects on transport in the electrodes.**

Experiments **will extend the understanding to designed structured electrodes.**

Multiscale modeling **will enable percolation of properties and concepts across the different length scales.**

Meso Challenge

Directed creation of complex meso porous structures with component surface characteristics that optimize properties including electronic and ionic conductivity and gas- and liquid-phase transport. Structures are functions of local conditions and perhaps even time/history.

Impact

Understanding, theory, and diagnostics which enhance the ability to design complex meso porous structures that optimize transport and understand synergistic interactions

Enhanced energy-conversion efficiency and stability of electrochemical systems

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