Mesoscale Priority Research Direction

Non-equilibrium Multi-body Transport Phenomena in Functional Materials

Opportunity

Non-equilibrium transport & exchange mechanisms play vital role in hierarchical systems (biology, functional materials, information technology). Non-equilibrium transport phenomena are only poorly understood in “real” (i.e. non-model) systems. Multi-body hierarchical transport phenomena are widely neglected (heat, mass, charges, defects, photons, entropy, i.e. information); prime examples: photosynthesis, conductivity in complex electrolytes. Better understanding of non-equilibrium transport phenomena in *real* hierarchical systems may advance knowledge for a deterministic design of smart functional materials for energy conversion & storage, quantum solar energy conversion and high-temperature superconductors.

Meso Challenge

Time & length scale of transport phenomena mainly determined by interface morphology between constituting phases and the structure and dynamics of matrix (defects, pore size, percolation, degree of order/disorder).Understanding hierarchical transport phenomena under non-equilibrium condition and on the meso time and length scale require advanced computational and analytical methods which exploit new capabilities in CPU resources and real-time *selective* analytical techniques.How does multi-body transport phenomena impact structure and dynamics in functional materials on the meso-scale?

Approach

Extend analytical methods for interacting multi-body transport phenomena to “real” system, e.g. Debye-Hueckel systems → complex electrolytes (LiClO4/THF).

Development of new computational techniques that build on national high-performance computing capabilities to investigate non-equilibrium multi-body transport phenomena and their hierarchical interactions.

in-situ & time-resolved investigations of the structure and dynamics of functional materials under process conditions through non-destructive imaging, scattering & spectroscopic techniques that allow for chemical selectivity (e.g. AXS, Neutron Scattering/Imaging/Spectroscopy, XPCS etc.).

Impact

Fundamental understanding of non-equilibrium multi-body transport phenomena will allow us to establish deterministic design principles for functional materials, where “function” depends on the transport of mass, charges, heat, electromagnetic radiation and information.

Design principles are not limited to natural sciences and engineering, but may also be applicable to fundamental principles in social & economic sciences and information technology (e.g. data processing and storage).

U.S. DEPARTMENT OF ENERGY | Office of Science

Contact: Volker Urban, urbanvs@ornl.gov, Oak Ridge National Laboratory