Mesoscale Priority Research Direction

Isotopic probes of ionic diffusion and solid surfaces

Opportunity

-The design of materials with particular diffusive transport properties for ions or gases can be greatly aided by measuring and understanding isotopic discrimination effects. Similarly, materials synthesis and purity is affected by the rates of atomic and molecular exchange at solid surfaces, which can be uniquely monitored by isotopic effects during growth.

Approach

-Technology improvements are allowing more elements to be measured, but better theory and simulation tools are also aiding in translating isotopic fractionation effects into information on material structure and bonding. There is a need for improved tools for doing isotopic microanalysis, and for molecular simulation tools that can capture longer timescale processes

Meso Challenge

- Transport of ions in complex materials such as electrolytes and polymers is a multiscale process and cannot be fully described by nearest neighbor interactions. X-ray, NMR and other probes cannot uniquely define speciation or bond strengths and exchange timescales that control transport and crystal growth.

Impact

- Improved understanding of molecular transport and exchange mechanisms and rates will aid in the rapid identification of new materials with tailored properties for energy storage, gas separations, solar energy conversion, and other energy applications

Ref: DePaolo, DJ, Geochimica Cosmochimica Acta, 2011; Nielsen et al., GCA, 2012

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