CORE-CM SEMINAR
Michigan State University

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Predicting Transport Properties of the Solid Electrolyte Interphases (SEI) in Li-ion batteries

Improving Li transport and preventing electron leakage through the solid electrolyte interphase (SEI) are critical to capacity drop and power loss of Li-ion batteries. A multi-scale modeling approach was developed to predict ionic and electronic transport properties in components of SEI, as a necessary step to understand the functionality of SEI before tailoring its properties. First, dominant Li diffusion carriers and ionic conductivity in idealized SEI components (Li_2CO_3 and LiF) were predicted with density functional theory (DFT) over a broad voltage range of the electrode materials. Meso-scale Li^+ ion diffusion equations were then formulated based on the diffusion mechanisms discovered by DFT and the boundary conditions of isotope exchange experiments in order to make direct comparison with TOF-SIMS measurements. A new mechanism of electron leakage via Li_i^0 interstitials diffusion through SEI was also proposed. The methods employed in this study can be generalized to other ionic conducting materials.

Thursday, March 31, 2016
12:00 NOON
Room 1400 – Biomedical & Physical Sciences