NEBRASKA CENTER FOR MATERIALS AND NANOSCIENCE
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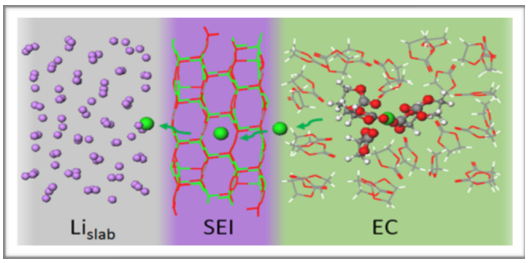
Modeling of the Interface and Interphases in Li-ion Batteries

One of the most significant challenges for current and future lithium ion batteries is the smart structure design at the nanoscale and the control of electron and ion transport at the electrode/electrolyte interface. This issue is further complicated by the existence of ultrathin solid electrolyte interphase (SEI) covering the electrode, forming a complex heterogeneous electrode/SEI/electrolyte interface. Based on joint multi-scale modeling and experimental results, we point out that the well-known two-layer structure of SEI also exhibits two different Li^+ ion transport mechanisms. The SEI has a porous (organic) outer layer permeable to both Li^+ and anions (dissolved in electrolyte), and a dense (inorganic) inner layer facilitate only Li^+ transport. This model suggests a strategy to deconvolute the structure-property relationships of the SEI by analyzing an idealized SEI composed of major components, such as Li_2CO_3, LiF, Li_2O, and their mixtures. After sorting out the Li^+ ion diffusion carriers and their diffusion pathways, we design methods to accelerate the Li^+ ion conductivity by doping and by using heterogonous structure designs. We can also predict the electron tunneling barriers and connect them with measurable first cycle irreversible capacity loss. Our challenge is to fully describe the electrochemical reactions at the electrode/SEI/electrolyte interface. This will be the subject of ongoing efforts.



Density functional tight binding (DFTB) method along with the newly developed parameters is used to understand lithium depletion and plating process, in the presence of a nanometer thick SEI layer. The work will lead to protective layer design on Li electrode for high energy batteries. ***Accounts of Chemical Research (2016).***

Professor Yue Qi is an associate professor in the Chemical Engineering and Materials Science Department at Michigan State University. She received her PhD in Materials Science from California Institute of Technology in 2001. She was a co-recipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work during her PhD study. After her PhD, she spent 12 years working at the Chemical Sciences and Materials Systems Lab, General Motors R&D Center. At GM, she developed multi-scale models starting from atomistic level to solve problems related to forming and machining of light weight alloys, and developing energy materials for batteries and fuel cells. She won three GM Campbell awards for fundamental research on various topics and TMS Young Leader Professional Development Award. She transitioned from industry to academia in 2013 and quickly built the "Materials Simulation for Clean Energy" Lab at MSU. Recently, she received the 2017 TMS Brimacombe Medalist Award.

Host:
Professor Jian Wang

Department of Mechanical & Materials Engineering

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Tuesday, March 7, 4:00 p.m. | 145 Jorgensen Hall