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When ions meet electrons – Modeling the interfaces in Solid-State Batteries

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Associate Dean for Inclusion and Diversity in the College of Engineering and at Michigan State University

Date: Tuesday, January 21 at 11:00am
Location: DLC 1B70

Abstract:

With the rapid development of fast Li-ion conductors, the major bottleneck for all-solid-state Li-ion batteries lies at the high interfacial resistance and Li dendrite growth. These problems require a fundamental understanding of the interfaces, where charge transfer reactions occur and electrochemistry, physics, and solid mechanics are coupled. This talk will focus on the new mechanistic understanding obtained by the recently developed multi-scale modeling approaches.

The high interfacial resistance is due to two main factors: physical contact and chemical effect. The chemical effect was captured by a new density functional theory (DFT) based model, which predicts the potential map inside a solid-state battery and determines the potential drop, electrostatic dipole, and space-charge layer at the electrode/solid-electrolyte interface. This new physics insight unified the seemingly contradictory experimental observations and led to new device design rules to promote interfacial ion transport in future solid-state batteries. The physical contact was described by combining contact mechanics and 1D Newman battery model. The model suggested how much pressure should be applied to recover the capacity drop due to contact area loss.

To simulate Li dendrite growth inside polycrystalline solid electrolytes, we coupled DFT calculations with the phase-field method. This model successfully explained the experimentally observed dendrite intergranular growth and revealed that the trapped electrons at grain boundaries and surfaces may produce isolated Li-metal nucleation, leading to a sudden increase of Li-dendrite penetration depth. Based on the model, we developed new dendrite resistant criteria by comparing the basic material properties for a number of solid electrolytes including LLZO, Li3PS4, LATP, and LiPON. These modeling advancements will be integrated into a new framework to guide the development of all-solid-state Li-ion batteries.

Bio:

Dr. Qi received her B.S. in Materials Science and Engineering and Computer Science from Tsinghua University and her Ph.D. in Materials Science from Caltech. She spent the next 12 years working at the General Motors R&D Center. At GM, she developed multi-scale models starting from the atomistic level to solve engineering problems related to lightweight alloys, fuel cells, and batteries. She transitioned from industry to academia in 2013 and built the "Materials Simulation for Clean Energy" Lab at MSU. She was a co-recipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work for her Ph.D. work; received three GM Campbell awards for fundamental research on various topics while working in GM; and won the 2017 Minerals, Metals & Materials Society (TMS) Brimacombe Medalist Award for her contributions in multidisciplinary computational materials science, from groundbreaking work on chemical-mechanical coupling to breakthroughs in understanding Li-ion battery failure.

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