UNIVERSITY OF HOUSTON
CULLEN COLLEGE OF ENGINEERING
Center for Integrated Bio and Nano Systems
SPEAKER SERIES

PRESENTS

When Ions Meet Electrons --- Modeling the Interfaces in Solid-State Batteries (a joint IBNS/TcSUH Seminar)

Dr. Yue Qi

Joan Wernig Sorensen Professor of Engineering
School of Engineering, Brown University

Friday, April 16, 2021 10:00 am
Room: Zoom*

https://uofh.zoom.us/j/845619943?pwd=QlZvYUV6M2dxNDkvNWxBd3F2YzdJZz09
Meeting ID: 845 619 943
Passcode: 016104

LECTURE 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.

One challenge for solid-state batteries is the high interfacial resistance, due to two main factors: physical contact and chemical effect. The chemical effect was captured by a density functional theory (DFT)-informed theoretical 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 the 1D Newman battery model. The model suggested how much pressure should be applied to recover the capacity drop due to contact area loss.

Another challenge for high energy density solid-state barriers using Li-metal electrodes is the soft Li dendrite growth inside the hard solid electrolytes. A DFT-informed phase-field method was developed and successfully explained the experimentally observed dendrite intergranular growth and revealed that the trapped electrons at grain boundaries and surfaces may be the main reason to reduce Li-ion and nucleate metallic Li. A new dendrite resistant criterion is therefore proposed.

These modeling advancements will be integrated into a new framework to guide the development of all-solid-state Li-ion batteries.

SPEAKER BIOSKETCH

Dr. Yue Qi is the Joan Wernig Sorensen Professor of Engineering at Brown University. She received her Ph.D. degree in Materials Science with a minor in Computer 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 served on the faculty in the Chemical Engineering and Materials Science Department at Michigan State University until 2020. Professor Qi and her "Materials Simulation for Clean Energy" Lab develops multi-scale simulation methods to design materials that are critically important for an energy-efficient and sustainable future. She has received several awards for her research, including the co-recipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work for her Ph.D. work; three GM Campbell awards for fundamental research on various topics while working in GM; and the 2017 Minerals, Metals & Materials Society (TMS) Brimacombe Medalist Award for her contributions in multidisciplinary computational materials science. She is also passionate about increasing diversity in Engineering and served as the inaugural Associate Dean for Inclusion and Diversity in the College of Engineering at MSU between 2018-2020.

Please contact Dr. Yan Yao (yyao4@central.uh.edu) or Dr. Jiming Bao (jbao@uh.edu) if you want to meet with the speaker.

SPONSORED BY

UNIVERSITY of HOUSTON

TEXAS CENTER FOR SUPERCONDUCTIVITY

UNIVERSITY of HOUSTON

CULLEN COLLEGE of ENGINEERING