The 86th GREEN Seminar

From Atoms to Devices --- Multiscale Modeling the Interfaces in Solid-State Batteries

Chair: Dr. Yoshitaka Tateyama (GREEN)

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With the rapid development of fast Li-ion conductors, the major bottleneck for solid-state batteries (SSBs) lies in the high interfacial resistance and Li dendrite growth. These problems require a fundamental understanding of the interfaces between the electrodes and the solid electrolytes (SEs), 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 as follows.

(1) High interfacial resistance due to physical contact & chemical effect by DFT-informed theoretical model, and combination of contact mechanics and the 1D Newman battery model.

(2) Li dendrite growth inside the hard SEs by DFT-informed phase-field method.

These modeling advancements will be integrated into a new framework to guide the development of SSBs.

Venue: Auditorium, 1F, NanoGREEN/WPI-MANA Bldg., Namiki-site / Zoom (Hybrid)

Date: Wednesday, 15 March 2023

Time: 13:30-14:30

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