Department of Materials Science and Engineering Seminar Series 2025

Revealing the effects of Extended Defects on Electronic Conductivity and Mechanical Stability in Solid State Electrolytes

Weihang Xie

Date and time: 4th July 2025(Friday) 11:00AM - 1:00PM

Venue: EA-06-04

Abstract

Advanced energy storage devices with higher energy and power densities are facing increasing demand, and all-solid-state batteries using solid electrolytes have become potential solutions to this demand. As bulk solid electrolytes are theoretically stiff enough to prevent the metal ingress from negative electrodes during charge/discharge cycles, surface and grain boundary, which are extended defects that are ubiquitous in polycrystalline solid electrolytes, have suspected roles in facilitating metal ingress in solid electrolytes of all-solid-state batteries. This PhD work revolves around the study of the effect of grain boundaries and surfaces on the electronic and mechanical properties of polycrystalline solid electrolyte. To meet the challenge, we developed Pygrain, a Python package to effectively generate surface and grain boundary models that satisfy all defined criteria with minimum supervision from humans. We found that the energy required to mechanically "separate" grain boundaries can be significantly lower than in the bulk region of materials, which can trigger preferential cracking of solid electrolyte particles in the grain boundary regions. Extended defects of solid electrolytes introduce new electronic "interfacial" states within bandgaps of solid electrolytes. These interfacial states alter and possibly increase locally the availability of free electrons and holes in solid electrolytes.

Biography

Weihang Xie received his Bachelor of Science in Materials Science and Engineering from Beihang University, China in 2020 and earned his M.Sc in Materials Science from Carnegie Mellon University in 2021. He is currently a Ph.D. candidate in the Department of Materials Science and Engineering at NUS. His research focus on understanding the role of extended defect in solid electrolyte using computational simulations.

Please join us!

HOST: Prof Zhu Di