

Abstract Submitted  
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**First Principles Study of Electrochemical and Chemical Stability of the Solid Electrolyte-Electrode Interfaces in All-Solid-State Li-Ion Batteries**<sup>1</sup> YIZHOU ZHU, XINGFENG HE, YIFEI MO, Department of Materials Science and Engineering, Univ of Maryland-College Park — All-solid-state Li-ion battery is a promising next-generation energy-storage technology. Using novel ceramic solid electrolyte materials, all-solid-state battery has advantages of intrinsic safety and high energy density compared to current Li-ion batteries based on organic liquid electrolyte. However, the power density achieved in all-solid-state battery is still unsatisfactory. The high interfacial resistance at electrode-electrolyte interface is one of the major limiting factors. Here we demonstrated a computational approach based on first principles calculation to systematically investigate the chemical and electrochemical stability of solid electrolyte materials, and provide insightful understanding of the degradation and passivation mechanisms at the interface. Our calculation revealed that the intrinsic stability of solid electrolyte materials and solid electrolyte-electrode interfaces is limited and the formation of interphase layers are thermodynamically favorable. Our study demonstrated a computational scheme to evaluate the electrochemical and chemical stability of the solid interfaces. Our newly gained understanding provided principles for developing solid electrolyte materials with enhanced stability and for engineering interfaces in all-solid-state Li-ion batteries.

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Yizhou Zhu  
Univ of Maryland-College Park

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