First-Principles Molecular Dynamics Study of Interface Between Electrode and Electrolyte in All-Solid State Lithium-Ion Battery

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Objectives

All-solid state Li-ion batteries (ASS-LIBs) are expected to be the next generation battery, however, their large interfacial resistance hinders their widespread application. In order to elucidate the mechanism of high resistance at the interface, we investigated the possible origins of resistance are 1): the formation of a Li ion space-charge layer (SCL) at the interface and 2): the reaction between cathode and solid electrolyte by using first-principles calculations.

Outline of Results

We constructed the solid-solid interface of LiNiO\(_2\) and Li\(_3\)PS\(_4\) as one of the representative cathode and solid electrolyte materials, respectively. We calculated the Li-vacancy formation energies at the interface between cathode and solid electrolyte. The calculated energies of Li-vacancy formation at the interface suggested the existence of Li-depletion layer and the existence of high resistance region for Li transport at the interface. We also investigated oxide buffer layer (Li\(_4\)Ti\(_5\)O\(_{12}\)) ion for Li-depletion layer and the result of Li-vacancy formation energy at Li\(_4\)Ti\(_5\)O\(_{12}\) and Li\(_3\)PS\(_4\) layer suggested the suppression of the Li-depletion layer. On the reaction between the cathode and the electrolyte, we found the mixing of Ni in cathode and P in electrolyte is energetically preferable to the unmixed state at the LNiO/LPS interface.