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Lithium Ion Conduction Mechanisms in Some Solid Electrolytes

SANTOSH KC, San Jose State University — Solid electrolytes have been attracting a lot of attention because of its superior properties over liquid electrolytes like wider electrochemical stability and better safety. However, many of them suffer from relatively low ionic conductivity. Identifying a suitable solid electrolyte is challenging and necessary. Using first-principles method based on density functional theory, we investigate ion conduction mechanisms in several types of solid electrolytes such as orthorhombic, perovskite, garnet and anti-perovskite-type structures. The detailed Li ion defect formation and migration mechanisms are investigated which provide the quantitative information of ionic conductivity of electrolytes. Thus, such investigation will be helpful to understand the atomic level mechanisms of Li ion conduction mechanism and to optimize ionic conductivity of electrolytes in Li-ion battery.

Santosh KC
San Jose State University

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