Motion and Dynamics of Li in New Sulfide Electrolytes

권은지, 이상헌†
이화여자대학교
(sang@ewha.ac.kr†)

Solid-state electrolytes are considered as key materials for overcoming the limitations of the liquid-electrolyte-based Li-ion batteries in terms of energy capacity, cyclability, and safety. Among the many possible solid-state electrolyte materials, inorganic sulfides are of intensive research interest mainly because larger and more polarizable Sulphur anions tend to substantially enhance the mobility of cationic Li species. In particular, many Li-P-S electrolytes have been reported to have high room-temperature Li-ion conductivities, which are comparable to that of conventional liquid electrolytes. By performing a combined study of computation-based theoretical predictions, we investigate the motion and dynamics of a Li atom in recently reported unleaded inorganic solid materials for high performance inorganic transition metal sulfide electrolytes for high-energy-density electric Li batteries.