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**First-principles study of lithium ion diffusion in crystalline $\beta$-$Li_3PS_4$ for solid state electrolytes** MYUNG-SOO LIM, Division of Advanced Materials Science, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced materials Science, POSTECH — The safety and stability are major issues to resolve in developing high-capacity lithium secondary batteries, particularly for application to electric vehicles. Solid-state lithium-ion electrolytes have been studied as a substitute of liquid electrolytes in order to enhance the stability and increase the energy density. However, low ion-mobility and poor material integrity are limiting the use of the solid electrolytes. We study the lithium-ion diffusion in crystalline $\beta$-$Li_3PS_4$ using first-principles methods and the nudged elastic band method. Considering diffusion paths through both interstitials and vacancy exchanges, we calculate the migration energies of lithium ions. Our results suggest that lithium ion diffusion is likely to occur through the zigzag-shaped paths along the $b$-direction that comprises of two lithium ion sites with fractional occupancy factors. We discuss the implication of our calculations for understanding the lithium ion diffusion in solid electrolytes.

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