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Li ion migration of lithium thiophosphate solid electrolyte materials¹ ROBERTO LONGO PAZOS, KA XIONG, WEICHAO WANG, KYEONGJAE CHO, Materials Science & Engineering Dept, The University of Texas at Dallas, Richardson, TX 75080 — $\text{Li}_2\text{S-P}_2\text{S}_5$ -based glasses are of great interest to be used as electrolytes in solid-state batteries. However, a detailed understanding on their structures and diffusion mechanisms is still missing. In this work, we investigate the atomic structures and ion diffusion mechanisms of various thiophosphate composites. These materials show intriguing structural similarities to their analogous Li phosphates. As a high ion conductivity battery material, interstitial and vacancy Li point defects should be reasonably stable within the host system. Besides, system with charged defect must be insulating to prevent electronic conduct which may low the ion conductivity. Our results show that interstitial Li has lower formation energy than Li vacancy, thus indicating that the ion conductivity may arise from the migration of interstitial Li. We propose possible solutions to optimize it. This study will help us to gain fundamental understanding on the Li ion diffusion process.

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