Computer Modeling of Crystalline Electrolytes- Lithium Thiophosphates and Phosphates

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Recently, lithium thiophosphate materials suitable for usage as solid electrolytes in Li-ion battery applications have been developed. These materials possess room temperature ionic conductivities as high as 10^{-3} S/cm [1], 3 orders of magnitude greater than that of commercial solid electrolyte materials based on LiPON [2]. The most promising of these thiophosphates, a superionic conductor with stoichiometry $Li_7P_3S_{11}$ [1], is investigated in this work using first principles calculations. In addition to examining the stability and structure of this material, we analyze in detail the migration mechanisms for both $Li_7P_3S_{11}$ and for hypothetical LiPON-like phosphate and phosphonitride analogues. Our results [3] correlate well with experimental findings and offer an explanation for the high conductivity observed in $Li_7P_3S_{11}$.

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