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Analysis of structural and electronic properties of LiTi2(PO4)3 solid-state electrolyte material for application in lithium-ion batteries

Solid electrolytes (SEs) offer high energy densities, are compatible with high-voltage cathodes, and possess high thermal and electrochemical stability. Amongst other SEs, LiTi2(PO4)3 (LTP) with the NASICON-type structure has captured significant interest as a better SE owing to its excellent chemical stability, environmental friendliness, and economic viability. LiTi₂(PO₄)₃ (LTP) possesses the NASICON-type structure built from corner-sharing octahedra (LiO₆, TiO₆) and tetrahedra (PO₄) to form a chemically stable structural framework that facilitates Li+ transport. Unfortunately, the ionic conductivity (< 10-6 S/cm) of lithium ions was found to be less for practical use in LIBs. As such, the systematic introduction of sulphur will be carried out as a remedial approach for this challenge. However, prior to that, there is a need to understand the fundamental properties of LiTi₂(PO₄)₃ that will pave way as a benchmark for the contribution of sulphur towards the electrochemical enhancement of this solid electrolyte material. In this current study, the electronic and structural properties of undoped LTP are studied to form a strong foundation for the partial substitution of oxygen with sulphur. The Vienna ab initio Simulation Package was used to generate the ground state structure of LTP with a cutoff energy of 550 eV and Monkhorst-Pack K-points of 8x5x4. The lattice parameters we found to be a=b=8.618 Å and c=21.079 Å, which are comparable to the experimental values (a=b=8.534 Å and c=20.843 Å). Additionally, the electronic inactivity of the material was confirmed by band structure and density of states (DoS) calculations. The band structure and DoS showed a band gap of ~2.49 eV, comparable to the value of 2.38 eV determined by Chen L.J. et. al., indicating insulating properties of solid electrolyte materials, which is an essential parameter for application in LIBs. These findings and parameters set a good basis for the groundwork of investigating the effect of sulphur on the electrochemical properties of this structure.

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