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Investigating the properties of Li9Al3(PO4)2(P2O7)3 solid electrolyte material for lithium-ion batteries: A computational study

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The development of electric vehicles and smart devices has been the primary driver of the rapid growth of the global market for lithium-ion batteries (LIBs). However, they suffer from challenges of safety, narrow electrochemical windows, and long-life cycles, which are ascribed to the usage of liquid electrolytes. The Li9Al3(PO4)2(P2O7)3 material is among the potential replacements for hazardous liquid electrolytes due to their high ionic conductivity (of the order of ~10-3 S/cm) and acceptable chemical stability for next-generation LIBs. However, the electronic structure, electronic, and vibrational properties of this material are not yet fully understood. Hence, in this work, we investigate the electronic structure Li9Al3(PO4)2(P2O7)3 to understand the performance in LIBs, through band structure and density of states calculations (DOS) and vibrational through phonons with the Vienna Ab initio Simulation Package (VASP) code. The calculations were performed using the generalized gradient approximation (GGA) with the Projector-Augmented Wave (PAW) pseudopotentials and Perdew-Burke-Ernzernhof (PBE) exchange-correlation function. The DOS and band structure results of the Li9Al3(PO4)2(P2O7)3 structure are both showing the wide bandgap, and they show that this material is an insulator with an indirect band gap of 5.403 eV. The wide band gaps of the insulator will ensure chemical stability during battery operation. As such, the cyclic performance of LIBs utilizing these solid electrolytes will be enhanced

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