Short Communication

First Principles Investigation of NASICON-Structured $\text{LiTi}_2(\text{PO}_4)_3$ and $\text{Mg}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ Solid Electrolytes

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The structural and electronic properties of NASICON-Structured $\text{LiTi}_2(\text{PO}_4)_3$ and $\text{Mg}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ were studied by performing first-principles Density Functional Theory (DFT) calculations. Geometrical optimization was conducted before the primitive cell of these structures by using different exchange-correlation energy functional. The Local Density Approximation (LDA) and Generalized-Gradient Approximation functional with Perdew-Burke-Ernzerhof (GGA-PBE) were used to execute structural and electronic properties for both materials. Calculated structural parameters and electronic properties such as band gap, the electronic density of states, and the partial density of states were presented.

Keywords: first-principles investigation, density functional theory, NASICON-structured, structural properties, electronic properties

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