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First-Principles Study of Anion-Doped $LiTi_2(PO_4)_3$ Solid Electrolytes.

Abstract:
Solid-state electrolytes face critical challenges in achieving sufficient ionic conductivity and structural stability for practical battery applications. NASICON-type $LiTi_2(PO_4)_3$ (LTP) offers a promising framework due to its 3D ion diffusion channels and thermal stability, but its bulk conductivity remains limited by restricted Li^+ migration pathways. Anion doping presents a strategic solution by modifying the host structure's chemical environment while preserving its NASICON framework. This study employs density functional theory (DFT) calculations to investigate how anion substitution ($PO_4^{3-} \rightarrow X^{n-}$) alters LTP's bulk properties. The results demonstrate that larger anions induce structural expansion, reducing Li^+ migration barriers by 30–40% while maintaining mechanical integrity. The r²SCAN functional reveals enhanced bond strength and formation energy compared to GGA-PBE, with C_{11}/C_{22} stiffness values confirming structural robustness. Electronic structure analysis shows preserved semiconductor behaviour (bandgap Eg = 2.504 eV) after doping. These findings establish anion doping as a viable approach to improve LTP's bulk transport properties while retaining its intrinsic advantages. The study provides insights for advancing the development of high-performance solid electrolytes.

Keywords: solid electrolyte, NaSICON-type, anion doping.

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