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Structural, mechanical, and electronic stability of Li7-xLa3Zr2-xNbxO12 (x = 0.25, 0.5) solid electrolyte

Lithium-ion batteries are extensively utilised in portable electronics and are increasingly employed in electric vehicles and stationary energy storage. To improve safety and energy density, solid-state electrolytes (SSEs) are being explored for their non-flammability and stability with lithium metal anodes. Among these, garnet-type Li₇La₃Zr₂O₁₂ (LLZO) is a leading candidate due to its high ionic conductivity (~1×10⁻⁴ S/cm) and chemical compatibility with lithium metal.
However, in its tetragonal phase, LLZO exhibits low room-temperature conductivity (~1×10⁻⁶ S/cm), limiting its practical use. Substitutional doping at the Zr site with niobium (Nb) offers a potential route to enhance both the structural and electrochemical performance of LLZO.
Therefore, in this study, first-principles calculations based on density functional theory (DFT) were performed using the projector augmented wave (PAW) method within the Vienna Ab initio Simulation Package (VASP), applying the PBE-GGA functional for exchange-correlation energy. The lattice parameters reveal that pristine LLZO adopts a tetragonal structure, whereas Nb-doped compositions Li_{6.75}La₃Zr_{1.75}Nb_{0.25} and Li_{6.5}La₃Zr_{1.5}Nb_{0.5}O₁₂ stabilize in monoclinic and orthorhombic phases, respectively. All structures satisfy mechanical stability criteria corresponding to their crystal symmetries. Moreover, the Pugh's ratio indicates enhanced ductility in the 12.5% Nb-doped system (x = 0.25), suggesting improved mechanical performance. The density of states analysis indicates insulating behavior, with band gaps decreasing from 4.345 eV (pristine) to 3.734 eV and 3.649 eV as Nb content increases. Despite this reduction, the high band gaps ensure low electronic conductivity, supporting the suitability of Nb-doped LLZO for solid-state electrolyte applications.
Keywords: Solid electrolyte, Nb-doped garnet-type, and Lithium-ion battery

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Primary author: Mr TIBANE, KHUMBULANI (University of Limpopo)

Co-authors: Dr MASEDI, Cliffton (University of Limpopo); NGOEPE, Phuti Esrom (University of LImpopo); LEDWABA, Raesibe (University of Limpopo)

Presenter: Mr TIBANE, KHUMBULANI (University of Limpopo)

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