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Computational investigation of Structural, Electronic, and Mechanical Properties of Spinel LiMn₂O₄

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Over the last decade, energy storage became one of the greatest challenges mainly because of natural depleting recourses and enhanced technology. Several investigations have been made in the quest of alternative energy sources, which are renewable, rechargeable and sustainable to current technologies. Lithium-ion batteries appeared as a promising energy source in low-carbon electricity and electric vehicles. However, one of the major difficulties for improving the performance of lithium-ion batteries required to meet the increasing demand for energy storage devices is the development of efficient and stable cathode materials. In particular, lithium manganese oxide spinel has attracted the most attention as potential cathode material because of its three-dimensional crystal structure that allows a reversible Li⁺ diffusion. In this study, we employ the Density Functional Theory (DFT) to investigate the stability of the LiMn2O4 spinel bulk through structural, electronic and mechanical properties. The pristine bulk structure was found to be a magnetic semiconductor with a direct band gap of 0.041 eV. The Density of States (DOS) indicated that the structure is metallic, which is in agreement with the reported literature. The phonon dispersion curves show that the spinel bulk structure is stable, since there is no imaginary frequencies. Our findings give insight on the electronic properties and spinel stability of the bulk structure.

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MSc

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