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Structural, Mechanical and Electronic Properties of Lithium Nickel Oxide Bulk(LiNiO2) and Surface Stability

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Lithium-ion batteries have gained a lot of interest as a result of the increased demand for renewable energy sources, with LiNiO2 (monoclinic) being an ideal choice to be used as the cathode material. This is due to its high specific capacity (275 mAhg−1) and energy density (629 Whkg-1). However, LiNiO2 has low cycling stability and voltage fading, which restricts its usefulness. In this work we discuss the bulk structural properties using the First-Principle density functional theory and the low Miler index surfaces of LiNiO2 calculations were modelled using METADISE code. It was found that the lattice parameters are in good agreement with the reported results, with less than 1.5% difference and it have heats of formation of -624.37 kJ/mol which shows that our system is thermodynamically stable. Calculated elastic constants show that the structure is mechanically stable due to the agreement with the monoclinic stability criteria. Furthermore, the phonon dispersion curves show imaginary vibrations along the gamma region, indicating that the structures instability. LiNiO2 depicts an indirect bandgap of 0.00eV around the fermi-level suggesting that the structure has magnetic metal characteristic. Finally, we were able examine the following Miller index surfaces (i.e. (110), (100), (100), (010), (001), (111), and (101)), and found the most stable facet to be (101).

Keywords: Lithium-ion batteries, LiNiO2, Density functional theory(DFT),

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