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Computational Modelling Study on Stability of Li₂MnO₃ Cathode Material for Lithium-Ion Batteries.

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The demand for lithium-ion batteries has increased in the last decades due to their broad applicability as power storage systems. However, their energy density is too low for high-power applications such as electric vehicles and renewable energy storage grids. The most substantial electroactive component of a battery is the cathode and thus much research has been devoted to improving them. In this regard, lithium-rich layered oxide Li₂MnO₃ has been considered as a promising cathode material for lithium-ion batteries due to their high theoretical specific capacity of 459 mA h/g, environmental friendliness and a high operating voltage. Therefore, it is necessary to investigate its properties to gain a better understating of the system. In the current study, density functional theory calculations with Hubbard Hamiltonian (DFT+U) were employed to explore stability, structural and electronic properties of bulk Li₂MnO₃. The calculated lattice parameters were found to be in good agreement with the experimental data, validating the approach employed. Furthermore, the negative heats of formation suggest that the structure is thermodynamically stable. The density of states revealed the presence of a bandgap at the Fermi level, implying that pristine Li₂MnO₃ is semiconducting, this agrees with what was found in literature. The system was found to mechanically unstable due to negative C₂₅ and C₄₆ elastic constants. There were no soft modes observed in the phonon dispersion curves, suggesting vibrational stability. These findings gave an insight into the bulk properties and stability of Li₂MnO₃.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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