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Insights into the Structural, Thermodynamic, Electronic, and Mechanical Properties of CaMn2O4 Polymorphs via Density Functional Theory Analysis

Calcium, the fifth most abundant element in the Earth's crust, has emerged as a promising alternative to lithium for next-generation rechargeable ion batteries due to its natural abundance, low cost, and favourable redox potential. However, identifying a suitable cathode material capable of accommodating the reversible insertion and extraction of Ca^{2+} ions without undergoing significant structural or volume changes remains a major challenge. In this context, the density functional theory (DFT) serves as a powerful tool for the screening and evaluation of potential cathode materials. This study employs DFT calculations to investigate the structural, electronic, and mechanical properties of various polymorphs of CaMn2O4 as potential cathode materials for rechargeable Ca-ion battery chemistries. The simulations were performed using the CASTEP code within the Materials Studio 2020 environment, utilizing the Perdew–Burke–Ernzerhof (PBE) form of the generalized gradient approximation (GGA) for exchange-correlation interactions. The calculated structural parameters align well with existing experimental data, validating the computational methodology. Electronic density of states (DOS) analysis reveals that all CaMn2O4 polymorphs exhibit semiconducting behaviour. Mechanical property assessments, including elastic constants and moduli, indicate that the materials are mechanically stable. Further elasticity analysis suggests the onset of permanent deformation at strain levels above 0.6. This study provides valuable insights into the theoretical potential of CaMn2O4 as a cathode material for calcium-ion batteries.

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