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Density functional Theory study of $NaMnO_2F$ as a Cathode Material for Sodium-Ion Batteries

Sodium-ion batteries (SIBs) represent a cost-effective and sustainable alternative to lithium-ion batteries, especially in the context of large-scale energy storage applications. This study utilized first-principles calculations grounded in density functional theory (DFT) with a spin-polarized generalized gradient approximation (GGA + U), applying a U value of 4.0 eV for all transition metals. This study examines the structural, electronic, mechanical, and thermodynamic properties of pristine $NaMnO_2$ and its fluorinated variant, $NaMnO_2F$, as potential cathode materials for sodium-ion batteries (SIBs). Our results indicate that the Mn d-orbitals and F-2p orbitals are predominant in the conduction and valence bands of the density of states (DOS). Fluorination significantly decreased the band gap and induced half-metallic behavior, resulting in enhanced electronic conductivity and improved electrochemical performance. The partial density of states (PDOS) revealed shifts in the energies of Mn-3d and F-2p orbitals, which contributed to an increase in states near the Fermi level. This indicates that fluorination improves charge carrier mobility and lowers the activation energy for conduction. The structural properties calculation indicates that fluorination results in local distortion, lattice parameter stretching, and a minor increase in volume. Mechanical stability was validated through elastic constants that meet Born stability criteria; however, both materials demonstrated brittle behaviour. Thermodynamic analyses indicate that specific heat and entropy increase with temperature, whereas Helmholtz free energy decreases, suggesting favourable thermal behaviour. Our results indicate that fluorination significantly improves the structural, electronic, and thermodynamic properties of $NaMnO_2$, positioning $NaMnO_2F$ as a highly promising cathode material for next-generation sodium-ion batteries. Oxyfluoride compositions are particularly appropriate for strained electrode configurations and thin-film battery applications. The computational insights establish a basis for the advancement of fluorine-containing intercalation frameworks in practical sodium-ion battery systems.

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