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First-Principles Study of $NaMnPO_4F$ as a Cathode for Sodium-Ion Batteries

Polyanionic phosphate-based materials have gained significant interest as cathode materials for sodium-ion batteries (SIBs) owing to their intrinsic thermal stability, structural integrity, and elevated operating voltage. This study employed first-principles density functional theory (DFT) computations with the generalized gradient approximation (GGA + U) in Materials Studio, applying an effective U value of 4.5 eV to all transition metals. The investigation concentrated on the structural, electrical, mechanical, and sodium-ion transport features of fluorine-doped $NaMnPO_4F$ as a prospective high-voltage cathode material. Our results indicate that the electronic band structure and density of states (DOS) influenced by fluorine exhibit a diminished band gap and an increase in electronic conductivity. The partial density of states (PDOS) exhibited substantial alterations in the contributions of the Mn-3d and F-2p orbitals, accompanied by a marked increase in the density of states proximate to the Fermi level. These modifications signify increased charge carrier mobility and reduced activation energy for electronic conduction, crucial for improved electrochemical performance. The computation of structural characteristics indicates that the insertion of fluorine caused little lattice distortion and an increase in lattice parameters, due to the local strain and polyhedral modifications induced by the dopant. As a result, the total volume of the $NaMnPO_4F$ unit cell shown a slight increase, aligning with the development of a more open framework that could enhance sodium-ion diffusion. Mechanical stability was validated via calculations of elastic constants, with all stability criteria met. Fluorine doping markedly enhanced resistance to shear deformation, and the material exhibited a Pugh's ratio over 1.75, signifying ductile behavior. This differs from the fragile characteristics typically seen in undoped equivalents and indicates enhanced mechanical reliability during cycling settings. This study demonstrates that the incorporation of fluorine into $NaMnPO_4$ boosts electronic conductivity via band gap reduction and PDOS modification while also facilitating advantageous structural expansion and better mechanical properties. These results confirm $NaMnPO_4F$ as a mechanically robust and electronically conductive cathode material appropriate for advanced sodium-ion battery applications.

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