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First-Principles Study of Ni-Doped NaMnPOF Cathodes: Enhancing Electronic Conductivity and Sodium-Ion Mobility for Advanced SIBs

The development of sodium-ion battery (SIB) technology relies on the development of high-performance cathode materials. Ithis study investigates the structural, electrical, and electrochemical properties of Ni-doped NaMnPO3F cathodes (NaMn1-xNixPO3F, 0 < x < 0.5) through the first-principles calculations based on density functional theory (DFT). The simulations conductedin this study show a slight decrease in the band gap, resulting from the partial substitution of Mn with Ni via doping, indicating enhanced electronic conductivity and improved charge transfer. The Bader charge analysis and partial density of states (PDOS) further suggest a synergistic redox activity between Mn and Ni during sodium de/intercalation.Additionally the calculated formation energies confirm the thermodynamic stability of the doped structures.Overall, the results demonstrate that Ni doping not only stabilizes the olivine-type structure but also enhances the electrochemical performance of $NaMnPO_3F$, positioning $NaMnNiPO_3F$ a promising candidate for high-capacity and high-rate sodium-ion battery cathodes.

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