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Density functional theory study of Ti-doped NaMnO2, a cathode material for sodium-ion battery

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Due to the accessibility of Na resources and comparable performance to lithium-ion batteries, rechargeable sodium-ion batteries are popular for large-scale electric energy storage and smart grids. attributed by its benefits, NaMnO2 is a promising cathode material for Na-ion rechargeable batteries. However, Na has a lower ionization potential than Li, resulting in lower operating voltages and energy densities than LIBs. Na+ ions are heavier and larger than Li+ ions, resulting in slow diffusion within a solid electrode during SIB cycling and often larger electrode volume expansion. In this study, we used the cluster expansion formalism to investigate the Ti-doped NaMnO2 phase stabilities, predicting the stable multi-component crystal structures and ranks metastable structures by enthalpy of formation while maintaining the predictive power and accuracy of first principle density functional theory method. The binary diagram produced 30 new structures of stable phases from which only five structures are stable. The stable structures obtained from the binary diagram have different space groups, different lattice parameters, the same Wyckoff positions and a different energy of formations. The optimised structures have a cross validation score of 1.1 meV which is an indication of a good cluster expansion because it has CVS lesser than 5 meV per active position.

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

YES

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

PhD

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