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Structural, Electronic, Mechanical and Thermodynamic Properties of Ternary NaVS2: DFT Study

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Structural, Electronic, Mechanical and Thermodynamic Properties of Ternary NaVS2: DFT Study
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Abstract:
Sodium-ion batteries have recently gained a lot of attention because they are environmentally benign and less expensive. The impact of Na atom deintercalation on olivine NaVS2 was examined for potential usage as a cathode material in Na-ion batteries. In this study, first-principle approach was employed to investigate ternary NaVS2 using plane wave pseudopotential method with different exchange correlation functions, GGA-PBE, GGA-PBEsol and LDA. Results revealed that trigonal NaVS2 phase are thermodynamical stable with $\Delta Hf < 0$. Optimized lattice parameters computed with GGA-PBE functional was found to be in good agreement with previous results. Furthermore, the partial density of states and the Mulliken population analysis were investigated to understand electronic properties and the effect of deintercalation on NaVS2 phases. In addition, the elastic properties were calculated to measure the mechanical stability of the structures.

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

No

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