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First principle study of structural and thermodynamic stability of ternary NaVSe2

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Ternary AIIBIVCVII structures have received a great deal of attention from both technological and scientific perspectives due to their optoelectronic properties and both p- and n-type electronic conductivity. Among them, NaVSe2 dichalcogenide compound promises excellent intercalation and high conductivity. However, details on the structural, and electronic properties of NaVSe2 remain limited, especially at the atomistic scale. The present study employed density functional theory approach using different functionals such as GGA-PBE, GGA-PBEsol, and LDA to investigate the structural, thermal, and electronic stability of NaVSe2. The results showed that the ΔHf <0 for NaVSe2, which implies that the phase is thermodynamically stable. In addition, it was found that GGA-PBE functional is the most suitable function than GGA-PBEsol and LDA functional. Moreover, the partial density of state was computed wherein Se 4p states contribute mainly to the valance band whilst the conduction band mainly consists of V s- and Se -p states.

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

No

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

N/A

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