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Stability, electronic and optical properties in ternary nitride phases of MgSnN2: A first principles study[1] BISHAL DUMRE, University of Toledo, DANIEL GALL, Rensselaer Polytechnic Institute, SANJAY KHARE, University of Toledo — We studied the disordered-rocksalt, orthorhombic and disordered-wurtzite phases of the ternary nitride semiconductor MgSnN2 from first principles methods using density functional theory (DFT). We find that MgSnN2 is mechanically and dynamically stable in all three phases. However, COHP analysis suggests that the disordered rocksalt structure has anti-bonding states below the Fermi level between -5 eV to -2 eV as compared to the bonding states in other two phases, indicating thermodynamic metastability. Computed lattice constant and electronic band gap values of 4.56 and 2.69 eV of MgSnN2 in disordered rocksalt structure compare well with experimentally reported values of 4.48 and 2.3 eV respectively. Furthermore, band gaps were computed in MgSnN2-xOx, with x = 0.5, 1.0, 1.5, 2.0, to elucidate the role of possible oxygen impurity. Of the three phases, disordered-rocksalt structure shows the lowest charge carrier effective masses. Moreover, this phase has promising absorption coefficient and reflectivity to be used as the absorber layer of tandem solar cells in the higher energy region of the visible portion of the solar spectrum. The other two phases can be utilized as a window layer of solar cells owing to their larger band gap values of 4.36 eV and 4.86 eV respectively.

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