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Electronic structures and band gaps of $MgGe_xSn_{(1-x)}N_2$ semiconductors

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Wide-band-gap semiconductors such as III-N have been used as innovation components of solid state lighting devices. For instance, AlN is used to make ultraviolet LEDs [Nature 441, 325 (2006)] and GaN is used to make blue LEDs [J. Appl. Phys. 94, 3675 (2004)]. The alternative wide-band-gap semiconductors are crucial to search for other applications. The mixing of group-III elements in binary semiconductors (III-N) are considered to enable turning of band gap energy such as $In_xGa_{(1-x)}N$, but the large lattice mismatch between InN and GaN produces phase separation in their alloys [Opt. Commun. 237, 363 (2004)]. Thus, instead of mixing different group-III elements in binary semiconductors, the ternary compounds (II-IV-N_2) was proposed by replacing the group-III element with two elements of group-II and group-IV [Phys. Rev. B. 94, 125201 (2016)]. In this work, we study the lattice dynamics and electronic structure of nitride semiconductors $MgGe_xSn_{(1-x)}N_2$, where x = 0, 0.25, 0.5, 0.75 and 1 by using density functional theory (DFT) calculations. Only valence electrons were considered exactly while core electronic states were represented via ultrasoft pseudo-potentials. The exchange correlation functional was approximated by the hybrid functional (HSE). The results present lattice constants of $MgGe_xSn_{(1-x)}N_2$ compounds linearly increase with increasing Sn concentrations according to the Vegard's law and the bowing coefficients p_a, p_b and p_c are 0.0429, -0.0194 and 0.0874 Å respectively. We also find that, in the electronic band structure, the N-p dominated valence band shifts down and Ge-s dominated conduction band moves up with increasing Ge concentrations. This computational study will serve a fundamental knowledge for band structure and defect engineering of this new family of wide-band-bap semiconductors.

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