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Opto-Electronic Properties and Structural Phase Transition of Filled-Tetrahedral NaZnAs

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Abstract : We predict structural, phase transition as well as opto-electronic properties of the filled-tetrahedral (Nowotny-Juza) NaZnAs compound in this study. Calculations are carried out by employing the full potential (FP) linearized augmented plane wave (LAPW) plus local orbitals (lo) scheme developed within the structure of density functional theory (DFT). Exchange-correlation energy/potential (EXC/VXC) functional is treated using Perdew-Burke and Ernzerhof (PBE) parameterization for generalized gradient approximation (GGA). In addition to Trans-Blaha (TB) modified Becke-Johnson (mBJ) potential is incorporated to get better precision for optoelectronic properties. Geometry optimization is carried out to obtain the reliable results of the total energy as well as other structural parameters for each phase of NaZnAs compound. Order of the structural transitions as a function of pressure is found as: Cu2Sb type → β → α phase in our study. Our calculated electronic energy band structures for all structural phases at the level of PBE-GGA as well as mBJ potential point out; NaZnAs compound is a direct (Γ–Γ) band gap semiconductor material. However, as compared to PBE-GGA, mBJ potential approximation reproduces higher values of fundamental band gap. Regarding the optical properties, calculations of real and imaginary parts of the dielectric function, refractive index, reflectivity coefficient, absorption coefficient and energy loss-function spectra are performed over a photon energy ranging from 0.0 to 30.0 eV by polarizing incident radiation in parallel to both [100] and [001] crystalline directions.

Keywords : NaZnAs, FP-LAPW+lo, structural properties, phase transition, electronic band-structure, optical properties
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