Title: Structural phase transition and opto-electronic properties of NaZnAs

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Abstract: In this study, we predict the structural phase transitions as well as opto-electronic properties of the filled-tetrahedral (Nowotny-Juza) NaZnAs compound. Calculations employ the full potential (FP) linearized augmented plane wave (LAPW) plus local orbitals (lo) scheme. The exchange-correlation potential is treated within the generalized gradient approximation of Perdew-Burke and Ernzerhof (GGA-PBE). In addition, Tran and Blaha (TB) modified Becke-Johnson (mBJ) potential is also used to obtain more accurate optoelectronic properties. Geometry optimization is performed to obtain reliable total energies and other structural parameters for each NaZnAs phase. In our study, the sequence of the structural phase transition on compression is Cu2Sb-type ? ß ? a phase. NaZnAs is a direct (G-G) band gap semiconductor for all the structural phases. However, compared to PBE-GGA, the mBJ approximation reproduces better fundamental band gaps. Moreover, for insight into its potential for photovoltaic applications, different optical parameters are studied.