Abstract Submitted
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Computational characterization of optical and thermodynamic properties of bulk zinc stannate (Zn2SnO4)[1] GRIGORY KOLESOV, Univ of Wyoming — Zn_2SnO_4 (ZTO) is an important material with a wide band gap. It is often used in novel device designs such as quantum dot- and die-sensitized solar cells. The crystal structure of ZTO is inverse spinel, with the general formula AB_2O_4. In inverse spinel A and B atoms share the occupation of octahedral sites 0.5/0.5, while the exact occupation is often unknown. Here we study configuration space of ZTO with DFT and derive cluster expansion model. We find temperature dependence for the occupation of octahedral sites and demonstrate that the lowest energy ground state configuration is stable at the normal range of temperatures. Because of the large unit cell (56 atoms) the calculation of optical properties with many-body methods appeared to be impractical and we compute band structure with DFT using Tran-Blaha correlation functional. The optical band gap we obtain with this method matches experimental value.

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