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Structure and electronic properties of $\mathbf{Zn_xSn_{1-x}O_{2-x}}$ ANINDYA ROY, YANSHA JIN, TONGHU JIANG, MICHAEL FALK, Johns Hopkins University — Using first-principles based hybrid-exchange calculations we look at the structural and electronic properties of Zn-Sn-O system. The oxides represented by $Zn_xSn_{1-x}O_{2-x}$ has end members ZnO and SnO_2. These relatively well studied, native n-type semiconductors are technologically important. Intermediate oxides corresponding to x =2/3 and 1/2 have been synthesized: spinel Zn_2SnO_4 and rhombohedral $ZnSnO_3$. These mixed oxides are functionally promising for their potential as ferroelectrics, transparent conducting oxides, thermoelectrics etc. Previously, *ab initio* calculations investigated the structures, electronic and thermodynamic properties of these mixed oxides. However, we considerably improve our understanding of band gap values and band structure of these compounds using hybrid-exchange method. We also perform band alignment calculations, estimate work function of these intermediate oxides, and compare those values to that of the end members and to the experimental results. The existence of Zn_2SnO_4 in the spinel structure allows a number of configurations which correspond to normal, partially inverted, or inverted spinel forms. We use cluster expansion method to identify energetically most stable form before calculating other properties.

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