

Abstract Submitted
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Structure and Properties of Sn_2Se_3 , a mixed valent tin selenium compound.¹ GUANGZONG XING, YUWEI LI, Univ of Missouri - Columbia, XIAOFENG FAN, LIJUN ZHANG, Jilin University, DAVID SINGH, Univ of Missouri - Columbia — Sn_2Se_3 is a possibly expected phase based on analogy with Sn_2S_3 but it has never been reported. It is of interest due to reported phase change memories using this composition using transitions between an amorphous phase and an unknown crystalline phase. We identify the crystal structure Sn_2Se_3 and report its properties at ambient pressure based on the ab initio evolutionary methodology for crystal structure prediction implemented in the Calypso code. We find a structure based on Sn-Se ribbons with clear Sn(II) and Sn(IV) sites similar to the structure of Sn_2S_3 . Compared with the known phase SnSe ($Pnma$) + SnSe_2 ($P-3m1$), the energy is only 2.3 meV/atom higher. The electronic structure of this phase shows mixed valent tins Sn^{2+} and Sn^{4+} in this compound. A small band gap of 0.023 eV is obtained from the band structure consistent with the small resistance reported by Kyung-Min Chung *et al.*

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