

Abstract Submitted  
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**First-principles investigation of the band gap evolution in (Pb,Sn)Te**<sup>1</sup> XING GAO, MURRAY DAW, Dept of Physics & Astronomy, Clemson University — The electronic structure of Sn-doped PbTe is interesting because of the so-called band inversion in its two end members, PbTe and SnTe [1,2]. Although, the electronic structure of these two compounds have been extensively studied by first-principles calculations, to our best knowledge, there are no direct first-principles calculations of the band gap evolution through the full range of alloying. We report a study of the electronic structure of this material through the full range of alloy content, combining SQS [3] and LDA. Our results show that disorder plays an important role in the electronic structure of this alloy.

[1] Dimmock, Melngailis, and Strauss, Phys. Rev. Lett. 16, 1193 (1966).

[2] Tung, and Cohen, Phys. Rev. 180, 823 (1969).

[3] Wei and Zunger, Phys. Rev. B 55, 13605 (1997).

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