

Abstract Submitted
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***Ab Initio* Study of Electronic Structure of Defects in SnTe and GeTe.**¹ SALAMEH AHMAD, S.D. MAHANTI, Michigan State University — *Ab initio* electronic structure calculations have been carried out within density functional theory (DFT) in SnTe and GeTe, two well-known narrow band-gap semiconductors, to understand the nature of deep defect states (DDS) introduced by Cd and In impurities substituting for Sn/Ge. These results are compared with similar studies in PbTe¹. The calculations have been carried out using a 64 atom super-cell model containing one defect. The density of states near the top of the valence band (VB) and the bottom of the conduction band (CB) get significantly modified by the defects as found in PbTe. The DDS associated with Indium impurity near the top of the VB is resonant in SnTe and lies in the gap in GeTe; its energy increasing in the order Sn-Pb-Ge. Cadmium on the other hand gives resonance (GeTe) and bound states (on SnTe) near the bottom of the CB, the energy of the DDS increasing from Sn-Pb-Ge. The positions of these DDS can have significant impact on thermoelectric and other transport properties of these semiconductors. 1. Salameh Ahmad, Hoang Khang, and S.D. Mahanti, Phys. Rev. Lett. 96, 056403 (2006); Salameh Ahmad et. al. Phys Rev. B74, 155205 (2006).

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Salameh Ahmad

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