

Abstract Submitted  
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**First-principles studies of physical properties of IV-VI derived semiconductor heterostructures and superlattices for thermoelectric applications** PABLO D. BORGES, Universidade de Vicosa, Brazil, JOHN E. PETERSEN, LUISA SCOLFARO, THOMAS H. MYERS, Texas State University — Doped PbTe is of great interest in high temperature thermoelectric devices. Looking at the qualitative improvements of the figure of merit, here we study the crystal and electronic structure of bulk PbTe, Thallium and Bismuth delta-doped layers in PbTe along the [100] crystalline directions and PbTe/SnTe heterostructures. The thermoelectric properties as a function of carrier concentrations and temperature were studied by solving the semiclassical Boltzmann transport equations in conjunction with ab initio electronic structure calculations, performed within Density Functional Theory. Based on maximally-localized Wannier functions basis set and the ab initio band energies, results for the Seebeck coefficient and figure of merit are presented and compared with available experimental data. Most cases showed good agreement between the calculated properties and experimental available data. Our predictions for temperature and concentration dependences of the figure of merit revealed a promising use of PbTe derived superlattices and heterostructures for thermoelectric devices applications.

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