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First-principles Study of Electronic and Thermal Transport Properties of $Pb_{1-x}M_xTe$ (M=Mg, Ca, Sr, Ba)[1] YI XIA, MARIA CHAN, Argonne National Laboratory — PbTe is an excellent thermoelectric material because of high power factor and low lattice thermal conductivity. Recent studies by Kanatzidis et al. showed significant enhancement in the ZT of PbTe doped with Na, Mg and Sr. However, fundamental understanding of the contribution of various mechanisms to the enhancement of ZT is far from satisfactory. In this talk, we will discuss first principles density functional theory (DFT) investigations of the electronic and lattice aspects of thermal transport in doped PbTe. Electronically, we studied the effects of alloying elements (Mg, Ca, Sr and Ba) on electronic band structures and transport coefficients of PbTe. We investigated the difference between direct and Wannier interpolations, and effects of exchange-correlation functional and spin orbit coupling, in terms of band velocities and electrical conductivity. Carrier lifetimes of pristine PbTe due to electron-phonon interaction will also be reported. We also calculated lattice thermal conductivity (KL) of pristine MTe. Comparison between single mode relaxation time approximation and iterative solution of Boltzmann transport equation is made. Extracted 2nd- and 3rd-order force constants were further utilized to illustrate the mechanism of phonon softening in KL reduction.

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