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Enhancement of the thermoelectric figure of merit by distortions of the dispersion relation

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A doubling of the thermoelectric figure of merit (zT) of p-type PbTe above 700 K has been recently demonstrated (1) in thallium-doped material. The effect comes about because an electronic energy level of the Tl atoms resonates with the valence band of PbTe. This creates an excess density of states, g(E), at a specific energy about 60 meV below the valence band edge, which in turn gives a thermoelectric power at that carrier concentration about three times higher than that of similarly-doped p-type PbTe. In this talk, we will review the mechanisms by which this distortion of the g(E) function, from the normal $E^{1/2}$ form valid for parabolic bands in three dimensions into a spike-like function, increases the thermoelectric power and thus zT. We further derive a set of criteria for the excess g(E) to improve zT. We will discuss the applicability of this approach to other electronic levels in PbTe first, and then describe the more general quest for such energy levels in other thermoelectric semiconductors. (1) J. P. Heremans et al., Science **321** 554 (2008)