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Electronic structure of ferroelectrically distorted PbTe[1] MAL-SOON LEE, Michigan State University, MERCOURI G. KANATZIDIS, Northwestern University, S.D. MAHANTI, Michigan State University — PbTe is one of the most promising thermoelectric materials. The electronic transport properties of the p-doped system are generally explained based on the nearly degenerate pockets near L and along Σ at high temperatures, where the energy at the L point decreases with increasing temperature and approaches the Σ point maxima. Recently, Bozin et al. showed that structure of PbTe is ferroelectrically distorted at high temperatures.[2] Following this experiment, a lattice dynamics study using first-principle molecular dynamics simulations have shown an increase of the band gap with increased temperature as seen experimentally.[3] Motivated from these studies, we have performed electronic structure calculations to investigate the effect of structural distortion and expansion on the band structure. We observe that the ordering of energy levels changes dramatically with distortion. In addition to these results we will also discuss how this can affect the electronic transport properties at high temperatures.

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[3]Y. Zhang, X. Ke, P. R. C. Kent, J. Yang, and C. Chen, Prys. Rev. Lett. 107, 175503 (2011).

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