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The influence of band structure on the thermoelectric performance of lanthanum telluride ANDREW F. MAY, California Institute of Technology, DAVID J. SINGH, Oak Ridge National Laboratory, ESPEN FLAGE-LARSEN, University of Oslo, G. JEFFREY SNYDER, California Institute of Technology — The electrical transport properties of the high temperature, n-type thermoelectric material lanthanum telluride ($La_{3-x}Te_4$) will be discussed in detail. The influence of electronic structure on transport has been investigated via density functional calculations on La_3Te_4, which reveal light bands at the conduction band edge and heavy bands approximately 0.3 eV above this minimum. Multi-band transport explains the experimentally observed trend in Seebeck coefficient versus carrier density, which is qualitatively reproduced in the first principles calculations. The optimum doping level is found to correspond to a Fermi energy located near the heavy band minima. Finally, calculations on the single vacancy composition ($x = \frac{1}{4}$) will be utilized to discuss the influence of lanthanum vacancies on the electronic structure and the validity of the rigid band approximation.

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