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Electronic structure and thermoelectric transport properties of Tellurium from Boltzmann transport theory HUA PENG, NICHOLAS KIOUSSIS, Department of Physics, California State University, Northridge, California 91330-8268, USA — Tellurium has a trigonal structure consisting of isolated helical chains parallel to c axis. Density functional theory combined with Boltzmann transport theory was applied to investigate the electronic and thermoelectric transport properties of Tellurium in the rigid band model. Calculation results showed that p-type doping gives a higher ZT and larger anisotropic behavior than n-type doping does. From the electronic structure, we find that the light band spitted from the spin-orbit coupling can contribute high mobility, while the drastically increased density from the heavy band bring a large asymmetry for the transport distribution function, which is benefit for the Seebeck coefficient. Besides, the band near the valence band maximum H point have a saddle-shape band structure along c direction, and smaller effective mass along this direction than other two directions. The overall result is good thermoelectric property for p-type doping tellurium along c direction. So, our calculation results suggest that in experiment, people can get a high ZT in tellurium by doping with small covalent electrons elements with a texture along [001] direction.

Hua Peng
Cal State Univ - Northridge

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