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Anisotropic lattice thermal conductivity for chain tellurium HUA PENG, NICHOLAS KIOUSSIS, Department of Physics, California State University, Northridge, California 91330-8268, USA, DEREK STEWART, Sensors Materials & Technology, HGST, San Jose Research Center, San Jose, California 95135, USA — Trigonal tellurium is elemental crystal consisting of two kind of boding: weak interchain van der Waal's forces and strong covalent intrachain boding. Using the ab initio calculations combined with the phonon Boltzmann transport equation we calculate the temperature and pressure dependent lattice thermal conductivity of chain tellurium. The heat transport along and perpendicular to the chain has large anisotropic character, and also for the gruneisen parameter and phonon velocity. The three-phonon scattering rate of the acoustic branches and the phonon mean free path of tellurium are also investigated, which are important for the nanostructure thermoelectric material developing.

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