

Abstract Submitted
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Phonon thermal transport in transition metal and rare earth nitride semiconductors from first principles¹ DAVID BROIDO, CHUNHUA LI, Department of Physics, Boston College — The thermal properties of four transition metal and rare earth nitride compounds: ScN, YN, LaN and LuN, have been studied using a first principles approach. The phonon dispersions for the four compounds show large LO-TO splittings and soft TO modes, which results in strong anharmonic scattering between acoustic and optic phonons that reduces the lattice thermal conductivities, k_L , of these compounds. The particularly soft TO mode at Γ in LaN gives it a much lower k_L than the other compounds. The room temperature k_L value for LaN of only $6 \text{ Wm}^{-1}\text{K}^{-1}$ is four times smaller than that of LuN in spite of the latter having larger average atomic mass, similar acoustic phonon velocities, and similar mode averaged Grüneisen parameters. Electronic structure calculations using the HSE06 hybrid functional including spin-orbit coupling show that LaN has highly anisotropic conduction and valence bands in the vicinity of the band extrema. These features combined with its small k_L make LaN a potentially viable thermoelectric material.

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