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Estimating thermal conductivity and thermoelectricity in $PbTiO_3$ from first principles ANINDYA ROY, Johns Hopkins University — A combination of density functional theory and Boltzmann transport equation is used in this study to calculate the lattice thermal conductivity (κ_L) of $PbTiO_3$ (PTO). We cannot apply this procedure to determine κ_L in presence of imaginary phonon modes ("soft modes"). Hence the tetragonal structure of PTO is used in these calculations, and the predicted κ_L is extrapolated to higher temperature using insights from experiments. The computed κ_L of PTO is low, possibly due to the anharmonicity associated with the ferroelectric/paraelectric transition. Electronic transport parameters such as the Seebeck coefficient and the electrical conductivity are also determined (under constant scattering time approximation in semiclassical Boltzmann theory) for PTO. The low κ_L and the electronic transport parameters together indicate excellent thermoelectric properties of PTO ($zT > 1.5$ at 1000 K). As a technologically important ferroelectric/piezoelectric material, PTO is used in alloys and in layered structures. These morphologies could bring down the κ_L further, improving its thermoelectric performance. Synthesis of electrically conducting samples of PTO would allows us to verify the above predictions.

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