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Ultralow Thermal Conductivity and Novel Thermoelectric Materials

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More than half of the energy produced worldwide is currently lost as heat and recovering even a fraction of that would be beneficial for global climate change. Toward this aim, thermoelectric materials can recover waste heat and convert it to useful energy. However, thermoelectrics are not widely commercially applied due to high cost and low efficiency. The search for new high-performance thermoelectric materials is challenging because they require enhanced electrical properties and low thermal conductivity. A potential route to discover novel high-performance thermoelectric materials can be provided by first-principles calculations [Chen, Pöhls *et al. JMCC*, 2016].

While the electronic properties can be predicted with a high accuracy, accurate prediction of the heat transport is currently not feasible. However, insight of the heat transport can be provided by computing the minimum thermal conductivity. In this study, a new model of minimum thermal conductivity was developed in which the thermal energy is transported between entities of phonons vibrating in a range of frequencies and limited by the phonon mean speed. This model was motivated by understanding the lowest experimental thermal conductivity to date for a fully dense solid (PCBM, κ = 0.07 W K^{-1} m^{-1} at 300 K), which agrees with the present model [Pöhls *et al. PCCP*, 20161].

In a high-throughput screening within 'The Materials Project' the electronic properties of ˜48,000 compounds were calculated and two novel high-performance thermoelectric classes, XYZ_2 (X,Y: rare earth or transition metals, Z: Group VI element) and metal phosphides, show promise. A variable relaxation time was developed using a semi-empirical approach to accurately calculate the temperature-dependent electronic properties.

Three compounds of the XYZ_2 class were synthesized and their computed thermoelectric properties were compared to experiments [Zhu *et al. JMCC*, 2015; Aydemir, Pöhls *et al. JMCA*, 2016]. All compounds exhibited extremely low thermal conductivity and a maximum figure of merit of ˜0.73 was found. Enhanced electronic properties and low heat transport were also predicted for metal phosphides. As an example, NiP_2 was synthesized indicating good agreement with computation and the present model of minimum thermal conductivity [Pöhls *et al. JMCC*, 2017].

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