

Atomic-Structural Metrics for High Performance Thermoelectrics

Efficient solid state energy conversion based on the thermoelectric (TE) effects, i.e., the Peltier effect for cooling and the Seebeck effect for power generation, has great potentials in many applications. A high performance TE material requires a high Seebeck coefficient α_s , a high electrical conductivity σ_e and a low thermal conductivity k , and its TE quality is described by the figure of merit $Z_e (= \alpha_s^2 \sigma_e / k)$. Identifying or designing materials with a high Z_e has proved to be extremely challenging in the past decades. A theoretic and systematic study of the relationship between atomic-structural features and TE properties will enhance the understanding of the transport mechanism in TE materials. This is very useful for the search and design of high performance thermoelectrics. The goal of this project is to understand the structure metrics of high performance thermoelectrics at multi-scale level.

A comprehensive approach that can predict all the key TE transport coefficients (α_s , σ_e , and k) is developed. Bi_2Te_3 and PbTe are selected for this investigation. First-principles quantum-mechanical calculations based on density functional theory (DFT), molecular dynamics (MD) simulations, and Boltzmann transport equations (BTE), are combined to predict all the TE transport properties. DFT calculations are also used to parameterize the force field of MD, which can in turn predict k_L (the lattice part of k) by combining with the Green-Kubo (G-K) autocorrelation decay method. This modern approach allows for composition variations, site substitutions, and rattler insertion, etc.

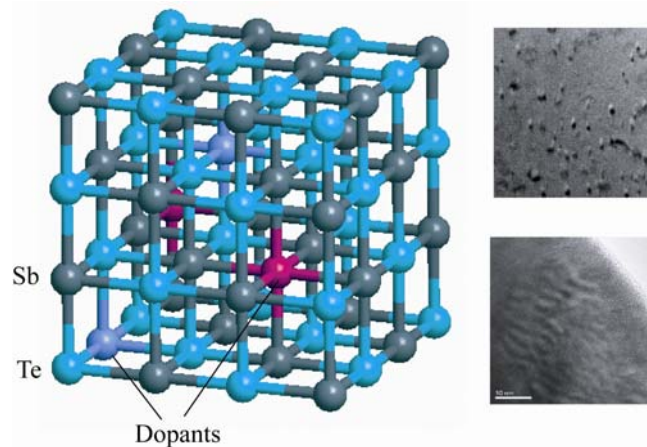


Figure 1. Doped PbTe crystal and the resulting nanostructures.

This approach will also be used to evaluate the thermoelectric performance of “nanocomposites”, which are the hybrid of nanostructures and bulk TE materials. The introduction of nanostructure into bulk TE materials provides opportunities to tailor the electron and phonon transport through structure engineering. As an important part of this project, the characterization of “nanocomposites” will advance our understanding of the TE properties in novel TE materials.

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