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Design of Thermoelectric Materials using First-principles Computations of Electron and Phonon Transport Properties

Boris KOZINSKY
Bosch Research and Technology Center, Cambridge, MA, U.S.A.

Abstract:

More than 60% of energy in a typical passenger vehicle is wasted as heat, and there are active efforts to recover that energy using thermoelectric systems. Understanding the atomic-level origins of thermoelectricity is necessary in order to design and optimize higher-performing materials, and we demonstrate that ab-initio computation is a valuable tool, complementary to experiments. By developing advanced methods to treat electronic and thermal transport in doped semiconductors at high temperature, we are able to perform rapid screening of new thermoelectric compositions and discover new thermoelectric alloys with leading performance.