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FIRST-PRINCIPLES CALCULATIONS OF ELECTRON AND PHONON TRANSPORT PROPERTIES IN SINGLE CRYSTALS

Gang Chen, Bolin Liao, Sangyeop Lee, and Jiawei Zhou
Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States.

ABSTRACT Electron and phonon transports in crystal solids are of great interests for many applications, from electronic devices and their thermal management, to energy conversion. This talk will summarize recent progresses we are making on first-principles approaches to simulate electron and phonon transport in single crystals geared towards thermoelectric applications. While phonon simulations are becoming mature, electron simulations remain a challenge. We are now able to simulate electron transport from first-principles, including electron-phonon scattering, and with some approximation, also electron-impurity scatterings. The energy dependent relaxation times are then used in the Boltzmann transport theory to obtain the electrical conductivity, Seebeck coefficient and electronic thermal conductivity. Such first-principles approaches led to new insights on phonon and electron transports, such as the role of resonant bonding on thermal conductivity, phonon Poiseuille flow, impacts of electron scattering on phonon thermal conductivity, and phonon drag effects. Detailed modal information on mean free path also provides vital information for nanoengineering materials to improve thermoelectric figure of merit.

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