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Scattering of charge carriers and phonons in thermoelectric devices GIUSEPPE ROMANO, LEE JOO-HYOUNG, JEFFREY GROSSMAN, Massachusetts Institute of Technology — We investigate the effects of the scattering of charge carriers and phonons on the figure of merit of thermoelectric devices. Despite many efforts devoted to the optimization of the figure of merit ZT, the commercial diffusion of such systems is still limited due to their low efficiency. The main problem behind the engineering of ZT is the interdependency between the Seebeck coefficients, electrical conductivity and thermal conductivity. ZT could be maximized by either increasing the Seebeck coefficient or decreasing the thermal conductivity. While the first approach involves the distortion of the electronic density of states [1], the thermal conductivity can be lowered by inserting nonporous in the bulk materials [2]. Recent works have shown a detailed comparison between np-Ge and np-Si material and investigated the effect of the porosity on ZT [3]. Here we couple classical molecular dynamics and continuous simulation to study the phonon-phonon, phonon-pore, electron-phonon and phonon-boundary scattering and their effects on the electrical and thermal conductivities. The knowledge gained about material properties is then used to perform simulations of thermoelectric devices.

[1] PRL **104**, 016602 (2010)
[2] PRB **80**, 155327 (2009)
[3] APL **95**, 013106 (2009)

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