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First-principles calculation of anharmonicity induced phonon lifetimes in FeSi[1] MOSES NTAM, JIANJUN DONG, Auburn University, OLIVIER DELAIRE, PAUL R. KENT, Oak Ridge National Laboratory — FeSi has attracted a lot of interest as a promising thermoelectric material for refrigeration applications. We present a first principle calculation of phonon lifetimes of FeSi based on our newly developed computational technique which combines first-principles density functional theory (DFT) and quantum scattering theory. Phonon lifetimes are calculated within the Fermi's golden rule using third order lattice anharmonicity tensors and vibrational phonon frequencies as inputs. Second order force constant matrices and third order lattice anharmonicity tensors are extracted using a real space supercell technique within the local density approximation (LDA). We compare our calculated phonon spectrum and lifetimes with recent neutron scattering measurements of phonon dispersions and linewidths. Finally we use the calculated phonon lifetimes to estimate the thermal conductivity of FeSi using kinetic transport theory.

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