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First-principles calculation of phonon scattering of n-type carriers in SiGe alloys FELIPE MURPHY ARMANDO, STEPHEN FAHY, Tyndall National Institute, University College Cork — We calculate the scattering matrix due to phonons in a $Si_{1-x}Ge_x$ random substitutional alloy using first principles density functional theory. The electron-phonon matrix elements are obtained from linear response theory in supercells containing up to 128 atoms. We calculate the n-type carrier mobility from the scattering rates of phonon and alloy scattering using the Boltzmann transport equation. Results are compared to experiments.

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