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First-principles calculation of alloy scattering of n-type carriers in SiGe FELIPE MURPHY-ARMANDO, Tyndall National Institute, University College Cork, Ireland, STEPHEN FAHY, Tyndall National Institute and Department of Physics, University College Cork, Ireland — Starting from a virtual crystal approximation (VCA) for the band structure of the $\text{Si}_{1-x}\text{Ge}_x$ alloy host, calculated in first-principles density functional theory, we find the scattering matrix for intra-valley and inter-valley n-type carrier scattering by a Si or Ge substitutional atom in a lattice of VCA atoms. The scattering matrix is calculated from energy splitting in large supercells (containing up to 127 VCA host atoms and one Si or Ge atom) of degenerate levels corresponding to the L, X and other points in the Brillouin zone. Atomic relaxation is found to have a substantial effect on the scattering matrix elements. Using supercells containing more than one Si or Ge atom, we test the accuracy of the approximation, in which each Si or Ge atom is considered to contribute independently to the carrier scattering matrix. The carrier mobility is calculated from the scattering rate using the Boltzmann transport equation. The results are compared to experiment.

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