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Hole mobility in SiGe alloys from first principles. SIAN JOYCE, FELIPE MURPHY-ARMANDO, Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland, STEPHEN FAHY, Tyndall National Institute and Dept. of Physics University College Cork, Ireland — First principles density functional theory is used to calculate the mobility of holes in $Si_{1-x}Ge_x$ alloys as a function of alloy composition. The alloy host is modelled within the virtual crystal approximation (VCA) using supercell techniques. The scattering matrix for carrier scattering in the presence of a Ge or Si substitutional atom in the VCA lattice is determined from the resultant energy splitting in the valence bands. The effect of the spin-orbit interaction is included in these calculations. The mobility is obtained from the scattering rate using the Boltzmann transport equation in the relaxation time approximation.

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