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Phonon dispersion relations for unstrained $Si_{1-x}Ge_x$ via density functional theory MD HOSSAIN, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA, JONATHAN FREUND, HARLEY JOHNSON, Department of Mechanical Science and Engineering,University of Illinois at Urbana-Champaign, IL 61801, USA — Phonon dispersions for the $Si_{1-x}Ge_x$ alloy system are computed using localized basis density functional theory. Including interactions up to third-nearest-neighbors and the effect of atomic randomness, phonon dispersion for the full Brillouin zone of a supercell containing 8 atoms is computed for 8 different compositions. Frequencies are found to be in excellent agreement with available experimental results for both crystalline Si and Ge. Results are compared with a 64-atom supercell calculation for optical frequencies to show any possible effect of supercell size on the phonon calculation. The atoms in the calculation are relaxed to a force tolerance of 0.0001eV/Å, which is found to be important to correctly determine the dispersion near the Γ- and X-points of the Brillouin zone where q-convergence is harder to achieve. The highest optical phonon frequencies are observed to vary nonlinearly with composition, a fact not investigated before using computational methods.

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