

The infrared absorption spectrum of Germanium and Silicon calculated from first principles

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In this work, the infrared absorption spectra of Germanium and Silicon are investigated. Due to the inversion symmetry of these crystals, the dominant part of the spectrum is given by two-phonon processes.

To determine this spectrum, one needs the knowledge of the dipole moment of the crystal. By expanding the dipole moment, one realises that the important contribution is given by the nonlinear dipolcoefficients, which are third-order derivatives of the total energy of the crystal with respect to an electric field (once) and atomic displacements (twice). We have applied density-functional perturbation theory up to third order [1,2] to determine these expansion coefficients.

With the knowledge of the nonlinear dipolcoefficients, we have evaluated the susceptibility of the crystal and afterwards the absorption spectrum. Compared with experimental data [3,4] our spectra are excellent. Both the shape and the intensities show a good agreement without using any experimental input.

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