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Title:Modified Corrections for London Forces in Solid-State Density Functional Theory Calculations of Structure and Lattice Dynamics of Molecular Crystals
Authors:King, M.D. (1); Korter, T.M. (1)
Author affiliation: (1) Syracuse Univ, Dept Chem, Ctr Sci & Technol 1 014, Syracuse, NY 13244 USA
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Abstract:Dispersion forces are critical for defining the crystal structures and vibrational potentials of molecular crystals. It is, therefore, important to include corrections for these forces in periodic density functional theory (DFT) calculations of lattice vibrational frequencies. In this study, DFT was augmented with a correction term for London-type dispersion forces in the simulations of the structures and terahertz (THz) vibrational spectra of the dispersion-bound solids naphthalene and durene. The parameters of the correction term were modified to best reproduce the experimental crystal structures and THz spectra. It was found that the accurate reproduction of the lattice dimensions by adjusting the magnitude of the applied dispersion forces resulted in the highest-quality fit of the calculated vibrational modes with the observed THz absorptions. The method presented for the modification of the dispersion corrections provides a practical approach to accurately simulating the THz spectra of molecular crystals, accounting for inherent systematic errors imposed by computational and experimental factors.
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