Compact representation of generalized molecular polarizabilities and efficient calculation of polarization energy in an arbitrary electric field

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Abstract

Generalized polarizabilities and the molecular charge distribution can describe the response of a molecule in an arbitrary static electric field up to second order. Depending on the expansion functions used to describe the perturbing potential, the generalized polarizability matrix can have rather large dimension (˜1000). This matrix is the discretized version of the density response function or electronic susceptibility. Diagonalizing and truncating it can lead to significant (over an order of magnitude) speed-up in simulations. We have analyzed the convergence behavior of the generalized polarizability using a plane wave basis for the potential. The eigenfunctions of the generalized polarizability matrix are the natural polarization potentials. They are potentially useful to construct efficient polarizability models for molecules.

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