REGULAR ARTICLE

Static polarizability and hyperpolarizability in atoms and molecules through a Cartesian-grid DFT

Tanmay Mandal[1] · Abhisek Ghosal[1] · Amlan K. Roy[1]

Abstract

Static electric response properties of atoms and molecules are reported within the real-space Cartesian-grid implementation of pseudopotential Kohn–Sham density functional theory. A detailed systematic investigation is made for a representative set of atoms and molecules, through a number of properties like total ground-state electronic energies, permanent dipole moment (μ), static average dipole polarizability ($\overline{\alpha}$). This is further extended to first hyperpolarizability (β) in molecules. It employs a recently developed non-uniform grid-optimization technique, with a suitably chosen fixed initial applied field. A simple variant of the finite-field method, using a rational function fit to the dipole moment with respect to electric field, is adopted. We make use of Labello–Ferreira–Kurtz basis set, which has performed quite well in these scenarios. To assess the efficacy and feasibility, four XC functionals such as LDA, BLYP, PBE and LBVWN are chosen. The present results are compared with available literature (both theoretical and experimental) values, whenever possible. In all instances, they show excellent agreement with the respective atom-centered-grid results, very widely used in many quantum chemistry programs. This demonstrates a viable alternative toward accurate prediction of response properties of many-electron systems in Cartesian coordinate grid.