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**FULL PAPER**

## Density functional electric response properties of molecules in Cartesian grid

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### Abstract

Within the finite-field Kohn-Sham framework, static electric response properties of diatomic molecules are presented. The electronic energy, dipole moment ( $\mu$ ), static dipole polarizability ( $\alpha$ ), and first-hyperpolarizability ( $\beta$ ) are calculated through a pseudopotential-DFT implementation in Cartesian coordinate grid, developed in our laboratory earlier. We engage the Labello-Ferreira-Kurtz (LFK) basis set; while four local and nonlocal exchange-correlation (LDA, BLYP, PBE, and LBVWN) functionals have been adopted. A detailed analysis of *grid convergence* and its impact on obtained results is presented. In each case the *electric field optimization* was carefully monitored through a recently prescribed technique. For all three molecules (HCl, HBr, HI) considered, the agreement of all these quantities with widely successful and popular atom-centered-grid procedure, is excellent. To assess the efficacy and feasibility, companion calculations are performed for these on a representative molecule (HCl) at distorted geometries, far from equilibrium. Wherever possible, relevant comparison is made with available *all-electron* data and experimental results. This demonstrates that Cartesian grid provides accurate, reliable results for such properties of many-electron systems within pseudopotential representation.