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A grid-based DFT method for the electronic structure calculation of many-electron systems AMLAN K. ROY, SHIH-I. CHU, Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA — We propose a new simple pseudopotential density functional method along with its implementation for the efficient and accurate treatment of electronic properties of molecules. The atom-centered localized gaussian basis sets, the electronic density as well as the various potentials are directly set up in a real uniform grid of three-dimensional cubic box. The nonrelativistic Kohn-Sham equation is solved within a linear combination of atomic orbitals-molecular orbitals (LCAO-MO) framework on grid using the standard self- consistent procedure. As a first step, simple local XC functionals and Hay-Wadt-type pseudopotentials are employed. As an illustration, we compare the total energy, eigenvalue, potential energy curve, the equilibrium bond length and vibrational frequency for Cl_2 and HCl molecule, which show very good agreement with the reference data. This provides a simple practical route to accurate molecular quantum mechanical calculations.

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