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Electronic structure calculation of atoms and molecules through a DFT approach in the AMLAN K. ROY, Department of Chemistry, University of Kansas, Lawrence, KS, 66045 — In this follow-up of the recently proposed work [1] on the pseudopotential calculation of atoms and molecules using cartesian coordinate grids (CCG) detailed results are presented to demonstrate the usefulness and applicability of the same. About 50 molecules and 10 atoms are studied systematically, for both local and non-local exchange-correlation combinations, utilizing the Hay-Wadt type effective core potentials. The localized gaussian basis set, the electron density as well the various two-body potentials are constructed directly on the grid. Thorough comparison on the total energy, individual energy components, eigenvalues, atomization energies and the potential energy curves with the widely used quantum chemistry programs reveals that these two results are virtually identical for all practical purposes. Additionally the highest occupied molecular orbital energies for a series of molecules show significant improvements by using the LB (van Leeuwen-Baerends) exchange potential, compared to both LDA or the BLYP results.

[1]A. K. Roy, Int. J. Quant. Chem. **108** 837 (2008).

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