Generalized Localized Hartree-Fock Density Functional Theory for Calculation of Excited-state Electronic Energies of Diatomic Molecules[1] ZHONGYUAN ZHOU, SHIH-I CHU, Department of Chemistry, University of Kansas, Lawrence, KS 66045 — We present a spin-dependent localized Hartree-Fock (SLHF) density-functional theoretical (DFT) approach for the accurate calculation of electronic energies of diatomic molecular excited states. In this approach, electron spin-orbitals are obtained by solving Kohn-Sham (KS) equation with the SLHF exchange potential and Perdew-Burke-Ernzerhof (PBE) generalized-gradient correlation energy functional. A generalized pseudospectral (GPS) technique, allowing non-uniform spatial discretization, is used for high precision solution of the SLHF-KS equations. The method has been applied to the calculation of electronic energies of excited states of H_2, O_2, and N_2. The results are in good agreement with available theoretical and experimental data.

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