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**Localized Hartree-Fock density-functional calculation of atomic inner-shell excitation**[1] ZHONGYUAN ZHOU, SHIH-I CHU, Department of Chemistry, University of Kansas, Lawrence, KS 66045 — We present a spin-dependent localized Hartree-Fock (LHF) density-functional theoretical (DFT) approach for the accurate calculation of the electronic energies of atomic inner-shell excited states. In this approach, electron spin-orbitals are obtained by solving Kohn-Sham (KS) equation with a spin-dependent LHF exchange potential and Lee-Yang-Parr correlation potential. A generalized pseudospectral (GPS) technique, allowing non-uniform spatial discretization, is used for high precision solution of the LHF-DFT equations. The method is applied to the study of the inner-shell excitation energies for both closed-shell (Be and Ne) and open-shell (Li, B, and O) atoms. Our calculated results are in very good agreement with available theoretical and experimental data.

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