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Time-dependent localized Hartree-Fock density-functional theory for photoionization processes of excited states of atomic systems[1]
ZHONGYUAN ZHOU, SHIH-I. CHU, Department of Chemistry, University of Kansas, Lawrence, KS 66045 — We propose a time-dependent localized Hartree-Fock density-functional approach for the treatment of photoionization processes of excited states of atomic systems. In this approach, Kohn-Sham (KS) equation with a spin-dependent localized Hartree-Fock (SLHF) potential being used as its exchange potential is solved to obtain electron spin-orbitals and orbital energies from which linear response function induced by an external radiation field is calculated and photoionization process is studied. The SLHF potential has good long-range behavior and thus allows one to treat the high-lying Rydberg states accurately. For demonstration, we apply this approach to calculate photoionization cross sections, linewidths, and resonance parameters of Ne. The results are in good agreement with experimental data and other theoretical calculations. We also present for the first time the photoionization cross sections of highly excited and inner-shell excited states of Ne.

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