Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Self-interaction corrected Kohn–Sham potentials VIKTOR STAROVEROV, Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7, Canada — Exchange-correlation potentials derived from conventional density-functional approximations fail to exhibit the slow Coulombic decay—a problem that is related to the self-interaction error in the potential. We show how the self-interaction error of standard semilocal approximations can be effectively reduced by employing modified electron densities to construct the corresponding Kohn–Sham potentials. Using this correction scheme in the framework of adiabatic time-dependent density-functional theory we obtain significantly improved electronic excitation energies, especially for Rydberg states.

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Date submitted: 09 Nov 2011 Electronic form version 1.4