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Parametrization and performance appraisal of the analytic and variational Xα method RAJENDRA ZOPE, George Washington University, BRETT DUNLAP, Code 6189, US Naval Research Laboratory — The linear combination of atomic orbitals, analytic and variational implementation of Slater's Xα method that allows arbitrary scaling of the exchange-correlation potential around each atom has been formulated. The method is numerical integration free, and thus delivers machine-precision energies that are stationary in all respects. One choice of scaling uses the αs that give exact atomic energies. We present the results of a performance assessment of this method by calculating the atomization energies and total energies of the G2 and extended G2 sets of molecules. Similar calculations for uniform α are also appraised. Minimizing the mean absolute error in both the Xα energies and the Hartree-Fock energies shows that Slater's exchange functional with $\alpha = 0.7091$ performs significantly better than the Gáspár-Kohn-Sham exchange functional for these molecules and for equally weighted atoms H-Kr. The Office of Naval Research, directly and through the Naval Research Laboratory, and the DoD's High Performance Computing Modernization Program, through the Common High Performance Computing Software Support Initiative, Project MBD-5, supported this work. The calculations were performed at the Army Research Laboratory Major Shared Resource Center (ARL MSRC).

Brett Dunlap
US Naval Research Laboratory

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