Reduction of Hartree–Fock Wavefunctions to Kohn–Sham Effective Potentials Using Multiresolution Analysis.

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Abstract

We present a highly accurate numerical implementation for computing the Kohn–Sham effective potentials for molecules based on a Hartree–Fock wavefunction and density,[?] following the RKS approach of Staroverov and co-workers.[1] Potentials and orbitals are represented in a multiresolution wavelet basis, avoiding basis set incompleteness-related issues. Together with the RKS method, the often occurring problems of oscillating potentials are removed. The MRA implementation of the RKS method allows the generation of molecular Kohn–Sham potentials of benchmark quality. Numerical data for atoms up to Kr and a number of molecules are given, with a special emphasis on the role of nodal planes in the calculations, as showcased in HCN and benzene.

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[1] J. B. Stückrath and F. A. Bischoff, J. Chem. Theor. Comp. **17**, 1408 (2021).

[2] S. V. Kohut, I. G. Ryabinkin, and V. N. Staroverov, J. Chem. Phys. **140**, 18A535 (2014).