Is There a Consistent Density Functional Theory?

R. J. Bartlett, A. Perera, and P. Verma

Quantum Theory Project, Department of Chemistry and Physics,
University of Florida, Gainesville, FL 32611-8435, USA.

The meaning of a consistent KSDFT is one whose functional provides accurate total energies and related properties, while its potential, has the property that its eigenvalues are good approximations to all the principal ionization potentials of a molecule, not just the homo. There is no currently used KSDFT method that is consistent, except the ab initio dft method we have been pursuing. Hence, the latter demonstrates that such an effective one-particle theory exists, and its numerical results for a variety of properties are superior to more conventional GGA, hybrid, and other KSDFT methods. In our opinion the weak link in current KSDFT is the inaccuracy of the potential, so we have addressed that issue several ways. We will discuss some of them here.

[1] P. Varma and R. J. Bartlett, J. Chem. Phys. **136**, 044105 (2012).

[2] P. Verma, A. Perera, and R. J. Bartlett, Chem. Phys. Letts. **524**, 10 (2012).

[3] R. J. Bartlett, Wiley Interdisciplinary Reviews – Computational Molecular Science **2**, 126 (2011).

Contact: bartlett@qtp.ufl.edu