Potential-based density-functional methods

Viktor N. Staroverov

Department of Chemistry, The University of Western Ontario,
London, Ontario N6A 5B7, Canada

I will survey some recent advances in the theory of model exchange-correlation potentials and show how, by thinking of density-functional methods in terms of Kohn–Sham potentials, one can arrive at new physical insights and better approximations for computing molecular properties. The following topics will be discussed: determination of energy values and development of energy functionals from Kohn–Sham potentials [1, 2], construction of model potentials that are functional derivatives [3, 4], accurate prediction of Rydberg excitation energies using a shape-correction scheme based on fractionally depopulating the HOMO [5, 6], and development of new model potentials for exchange and correlation [7, 8].

References

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