# Development and Applications of Potential-Based Density-Functional Theory

*Viktor N. Staroverov*

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

I will survey recent advances in the theory of Kohn–Sham effective potentials and show how, by thinking in terms of these quantities, one can obtain new physical insights and better density-functional approximations for computing molecular properties. Topics include: development of energy functionals from Kohn–Sham potentials, accurate prediction of excitation energies, and a new tool for studying chemical reactivity called the average local electron energy.

*References*

1. I. G. Ryabinkin and V. N. Staroverov, "Average local ionization energy generalized to correlated wavefunctions", *J. Chem. Phys.* **141**, 084107 (2014).
2. I. G. Ryabinkin, A. A. Kananenka, and V. N. Staroverov, "Accurate and efficient approximation to the optimized effective potential for exchange", *Phys. Rev. Lett.* **111**, 013001 (2013).
3. A. P. Gaiduk, D. Mizzi, and V. N. Staroverov, "Self-interaction correction scheme for approximate Kohn–Sham potentials", *Phys. Rev. A* **86**, 052518 (2012).
4. A. P. Gaiduk, D. S. Firaha, and V. N. Staroverov, "Improved electronic excitation energies from shape-corrected semilocal Kohn–Sham potentials", *Phys. Rev. Lett.* **108**, 253005 (2012).
5. P. D. Elkind and V. N. Staroverov, "Energy expressions for Kohn–Sham potentials and their relation to the Slater–Janak theorem", *J. Chem. Phys.* **136**, 124115 (2012).
6. A. P. Gaiduk and V. N. Staroverov, "A generalized gradient approximation for exchange derived from the model potential of van Leeuwen and Baerends", *J. Chem. Phys.* **136**, 064116 (2012).
7. A. P. Gaiduk and V. N. Staroverov, "Construction of integrable model Kohn–Sham potentials by analysis of the structure of functional derivatives", *Phys. Rev. A* **83**, 012509 (2011).
8. A. P. Gaiduk and V. N. Staroverov, "Explicit construction of functional derivatives in potential-driven density-functional theory", *J. Chem. Phys.* **133**, 101104 (2010).