Sanibel Symposium 2017
St. Simons Island, GA, USA, February 19-24

Analysis of GGA exchange energy functionals with correct asymptotic behavior of the corresponding potential

José L. Gázquez[a], Javier Carmona-Espíndola[a], Alberto Vela[b] and S. B. Trickey[c]

[a]*Universidad Autónoma Metropolitana-Iztapalapa, Departamento de Química, Av. San Rafael Atlixco 186, Cd. de México, 09340, México.*

[b]*Centro de Investigación y de Estudios Avanzados, Departamento de Química, Av. Instituto Politécnico Nacional 2508, Cd. de México, 07360 México.*

[c]*University of Florida, Quantum Theory Project, Dept. of Physics and Dept. of Chemistry, P.O. Box 118435, Gainesville, Florida 32611-8435, USA.*

The generalized gradient approximation (GGA) to the exchange energy functional of Kohn-Sham theory has become a rather important approach to the description of the electronic structure of atoms, molecules and extended systems. The GGA is usually expressed as the product of the local density approximation and an enhancement factor that is a function of the reduced density gradient, s. The different expressions for the enhancement factor that characterizes this approximation, are generally built to satisfy different constraints that the exact functional satisfies. In the present work we analyze several forms of this factor that lead to an exchange potential with the correct asymptotic behavior and that include the derivative discontinuity effects. These forms provide a good description of properties that depend on response functions and excited states. At the same time, the proposed approximations preserve the basic properties of the enhancement factor in the physically important region, $0 \leq s \leq 3$, so that they also lead to a good description of properties that depend on energy differences.