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Analysis of the large reduced density gradient limit for the exchange energy JOSE GAZQUEZ, Universidad Autonoma Metropolitana-Iztapalapa, JORGE M. DEL CAMPO, Universidad Nacional Autonoma de Mexico, JUAN PACHECO-KATO, Universidad de Guanajuato, SAM TRICKEY, University of Florida, ALBERTO VELA, Cinvestav — Electronic structure calculations have become very important for the analysis, at the microscopic level, of a wide variety of systems in physics, chemistry and biology. The Kohn-Sham version of density functional theory has played a fundamental role in such development. In particular, the generalized gradient approximation (GGA) has proven to be a very useful tool in electronic structure studies of complex systems, because it leads to a reasonable description of many properties, at a moderate computational effort. However, it is desirable to improve beyond the actual limits of accuracy. In this work we will present an analysis of the GGA in the regions of small and large values of the reduced density gradient. Then, taking as starting point the PBE and RPBE functionals, the large reduced density gradient limit will be incorporated, in order to show that it induces small, but subtle changes that lead to a better description of several molecular properties.

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