Limitations and Perspectives of Contemporary Density Functional Approximations

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By presenting the development, performance and selected applications of a series of exchange-correlation functionals, or density functional approximations, that we have recently proposed[1-7] I will show the limitations that these approximations have and I will discuss the possible consequences of using them in molecular modeling. These functionals have been designed by constraint satisfaction focusing on the role played by the non-uniformity of the electron density, the Lieb-Oxford bound, the behavior of the enhancement functions for large gradients and the correct description for the hydrogen atom. Using these constraints I will present some of the GGAs, meta-GGAs and global hybrids that we have developed using the previously mentioned constraints. A functional designed to recover the correct asymptotic behavior on the exchange potential will also be presented. The application of these functionals to the conformational ordering of amino acids and prediction of the heats of formation of some interesting organic substances will be presented. The functional with correct asymptotic behavior of the exchange potential will be used to calculate polarizabilities and hyperpolarizabilities and it will be shown that it provides very encouraging results, both, for the static and frequency dependant cases.

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