Non-empirical exchange-correlation parameterizations based on exact conditions from Correlated Orbital Theory

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Exact conditions provided by the Correlated Orbital Theory (COT) [1] have been applied to propose non-empirical parameterizations for methods based on Density Functional Theory (DFT). We pursued an approach with minimum parameterization of exchange-correlation functionals with long-range corrections [2]. Improvements have been observed in the description of reaction barrier heights and electronic excitation energies. These new functionals also presented nice results for challenging charge-transfer excitations. However, the most important achievement provided by these functionals was the excellent description of vertical electron affinities by using only the negative of appropriate virtual orbital eigenvalues, with resulting mean absolute deviations around 0.1 eV.

[1] R.J. Bartlett, *Chem. Phys. Lett.* **484** (2009) 1-9.

[2] T. Yanai, D.P. Tew, N.C. Handy, *Chem. Phys. Lett.* **393** (2004) 51-57.

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