SEMINAR ANNOUNCEMENT

Tuesday, 16th of February 2015 at 11:30
UPC campus nord, B4-212 (aula seminari)

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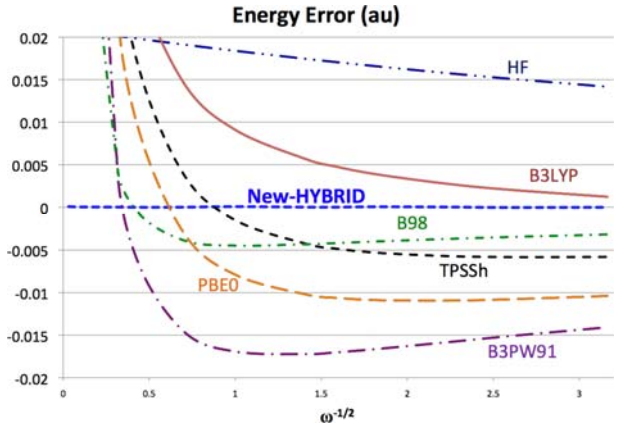
"Harmonium atom as a calibration and development tool in DFT"

Abstract

The construction of energy functionals in DFT is a complicated task because there are very few conditions known about the exact functional and they are diffcult to impose in functional expressions. Despite these difficulties in the last years quite many functionals have been put forward, broadening the choice of methods in computational chemistry. In this regard, new theoretical models to explore and calibrate the existing zoo of functionals and construct new expressions are required. Harmonium atom is a model system that replaces the usual electron-nuclear attraction by a harmonic interaction tuned with the confinement parameter strength (ω). The model is realistic as far as the electron correlation is concerned and presents a continuous transit from weak electron-correlation regimes (large ω) to strong-correlation regimes (small ω), thus being a formidable test bed for density functional methods. In this talk, several popular density functionals will be analyzed in the two lowest-lying energy states of three-electron harmonium atom. None of the functionals tested (including a wide variety of LDA, GGAs, meta-GGAs and range-separated functionals) are accurate in the whole range ω values, failing short in the description of the weak correlation limit. Finally, it is shown that new hybridized functional expressions can remedy this pitfall attaining ten μ-hartree accuracy for the whole range of confinement strength values.



[1] E. Matito and J. Cioslowski, in preparation.
[2] E. Matito, J. Cioslowski and S. Vyboishchikov, Phys. Chem. Chem. Phys. 12, 6712 (2010); J. Cioslowski and E. Matito, J. Chem. Theory Comput. 7 915 (2011)
[3] J. Cioslowski, K. Strasburger and E. Matito, J. Chem. Phys. 136 194112 (2012); ibid 141 044128 (2014)