Research Topic for the ParisTech/CSC PhD Program

Subfield: Theoretical and Computational Chemistry

ParisTech School:ChimieParisTech

Title:Development of new double hybridfunctionals for the description of ground and excited state properties

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Short description of possible research topics for a PhD:
The aim of this PhD work is to develop new approaches rooted on Density Functional Theory enabling the correct description of the structural and electronic features at the ground and excited state of complex molecular systems. In particular, it is well known that currently applied DFT based methods, such as global hybrids, are affected by systematic errors related by the use of approximate exchange and correlation functionals. Our recent works have shown how improved numerical performances are obtained with the so-called Double Hybrids functionals, which combinestandard DFT approaches with a perturbative treatment for correlation energy (MP2 term). These new family of functionals is still much less exploited and developed, though results obtained up to now for the description of difficult chemical casesare very encouraging. The aim of this thesis will be to develop new double hybrid functionalsfollowing the ab-initio (i.e. non-parameterized) philosophy of functionals' development we have applied in the past to develop the popular global hybrid PBE0 and more recently double hybrid derivatives, such as the PBE0-DH. The so-constructed functionals will be implemented in the computer code Gaussian (www.gaussian.com), whose prof. Adamo is one of the co-authors, and tested not only on case study (benchmarks) but also on real chemical systems.

Required background of the student: Theoretical and Computational Chemistry, Chemical Physics or Physical Chemistry.

A list of 5(max.) representative publications of the group:
1) I. Y. Zhang, N. Q. Su, E. Brémond, C. Adamo, X. Xu *Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0,* J. Chem. Phys. 136 (2012) 174103

2) D. Bousquet, E. Brémond, J.C. Sancho-García, I.Ciofini, C. Adamo, *Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets* J. Chem. Theory Comp. 9 (2013) 3444-3452.

3) E. Brémond, J.C. Sancho-García, Á. J. Pérez-Jiménez, C.Adamo*Double-hybrid Functionals from Adiabatic-Connection: the QIDH model* J. Chem. Phys.141 (2014) 031101

4) E. Brémond, M. Savarese, A.J. Perez-Jimenez, J.C. Sancho-Garcia, C. Adamo *Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes* J. Phys. Chem. Lett. 6 (2015) 3540-3545.

5) E.Brémond, I.Ciofini, J.C. Sancho-García, C.Adamo, *Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists* Acc. Chem. Res. 49 (2016) 1503–1513