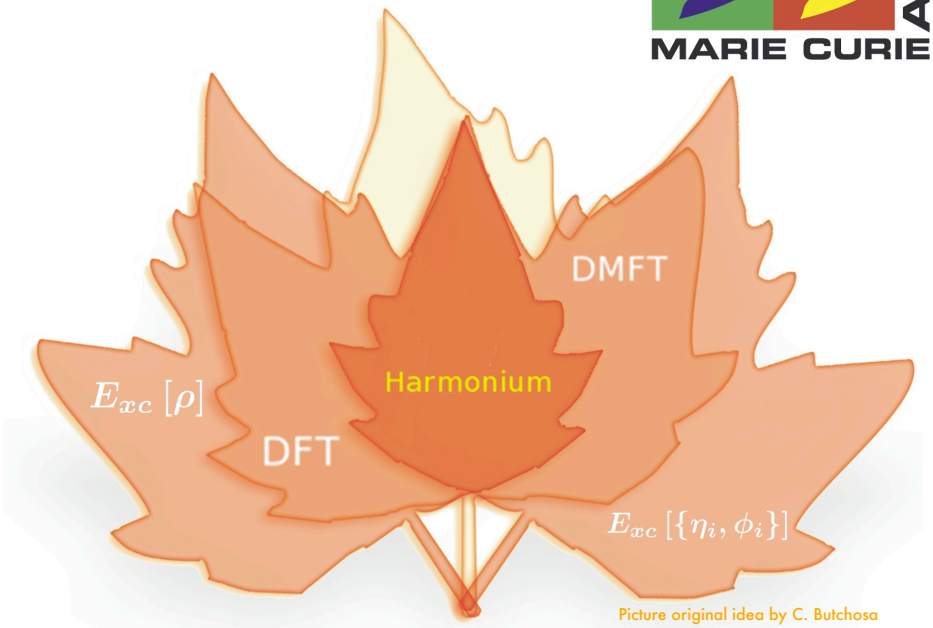
NewDFTfunct

DEVELOPMENT OF NEW NON-EMPIRICAL DFT FUNCTIONALS

DR. EDUARD MATITO

MARIE CURIE ACTIONS



Picture original idea by C. Butchosa

Harmonium atom is the model system that will be used for the calibration and development of new functionals in DFT and DMFT.

Development of new DFT and DMFT functionals.

Quantum chemistry is a branch of chemistry that uses the results of quantum mechanics to analyze chemical problems. It can be divided into Theoretical and Computational Chemistry.

Theoretical Chemistry (TC) develops and improves tools and methods based on quantum mechanics, which Computational Chemistry (CC) uses to analyze chemical systems.

CC has a wide range of applications, from purely chemical to nano- or bio-oriented chemistry problems. The size of the species involved in these studies exceeds the computational cost affordable with classical TC tools and, for this reason, the so-called Density Functional Theory (DFT) has became the preferred tool of CC to address their studies.

Unfortunately, most DFT functionals are highly specific to particular chemistry problems and lack the desirable accuracy in a wide range of problems. In addition, the development of new functionals is particularly difficult and mostly relies on the parameterization of existing functionals. On the other hand, the emerging theory known as Density Matrix Functional Theory (DMFT) permits an easier approach to functional development, but its application is still on its infancy.

This project, financed by the FP7 (research program of the EU) is a mainly theoretical-chemistry project aimed at the development of new DFT and DMFT functionals, with wider applicability in chemistry. In particular, we will use a model system known as Harmonium Atom (HA) as the workhorse for the construction of new non-empirical functionals.

The project aims at the development of new computational tools to solve chemical problems

This project pursues the goal to construct new DFT and DMFT functionals employing a very genuine strategy, and holds the promise to provide relevant results for the fields of both theoretical and computational chemistry.

Call: Master and PhD grant

- Grant: Master (1year) + PhD (3 years)
- Supervisors: Dr. Matito and Prof. Solà
- Requirement: Chemistry or Physics degree
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Perform a Master and PhD thesis at the Institute of Computational Chemistry and Catalysis (IQC²)

UdG

The IQC² offers a Master on Computational and Theoretical Chemistry and/or a PhD thesis (total up to 4 years) to work on the aforementioned project. This grant is under the umbrella of the Career Integration Grant (CIG) project 'Development of New Non-Empirical DFT Functionals' granted to Dr. Matito and financed by the Marie Curie actions (FP7 program). Prof. Solà and Dr. Matito, at the IQC² in the University of Girona (Catalonia, Spain) will be the PhD supervisors. Candidates should have a degree in Chemistry or Physics and send their CV to the e-mail address above.