Development of new density functional approximations

Supervisor(s):
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Duration: 3 years (possibility of one-year extension based on the availability of funding)
Application Deadline: 31/08/2021

Since its appearance, the density functional theory (DFT)[1] has experienced a vast development, establishing nowadays as the most employed tool to tackle many different aspects of the electronic structure of molecular systems. The density functional theory is, in principle, an exact method. It works with functionals, which give the energy or other properties in terms of the electron density *n(r)*. Only a small but essential contribution to the energy, the exchange-correlation (XC) energy, thus far remains unknown as a functional of the density and has to be approximated. In this regard, current density functional approximations are a far cry from predictable, and consequently, they do not show the desirable transferability among properties.

In contrast to the traditional and widespread density functional approximations based on the local expansion of the XC homogeneous electron gas, this Ph.D. project will follow a sort of bottom-up approach in constructing the XC functional. The *main goal* of this thesis is to develop new density functional approximations that do not rely on the homogenous electron gas, which is the primary physical model behind most current approximations. Two different strategies will be followed: (i) *obtaining the XC potential by inverting the Kohn-Sham equation of a simple physical model*, (ii) *developing correlation functionals from a physical-motivated partition of the pair density*.[2] The two-electron Harmonium Atom[3] (2e-HA) will be the physical model used for the former purpose. The HA resembles an ordinary atom in which the external Coulomb potential is replaced by a parabolic one, which depends on a confinement parameter ω. The project will furnish new DFAs and DFA ingredients that will significantly differ from the existing ones and could be used as a starting point to further developments in the context of orbital-free DFT.

The position is opened for candidates holding a degree in Chemistry, Physics, or Mathematics. They are expected to have a solid background in quantum mechanics, high-level mathematics, and a keen interest in computational chemistry. Good command of English, both verbal and written, is mandatory. Experience with Mathematica® and programming (preferably in FORTRAN or C++) is highly desirable but not required.

The successful candidate will join the *Quantum Chemistry Development* group at Donostia International Physics Center (DIPC), led by Eduard Matito. The candidate will be provided with ample office space, all the resources needed to carry out the research and will be encouraged to participate in international conferences. Applicants of all genders and ethnicities are welcome. The deadline to start is January 2022.

Interested candidates should submit an updated CV and a brief statement of interest to the supervisors' email listed above. Reference letters are welcome but not indispensable.

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1 R.O. Jones, *Reviews of Modern Physics* **87**, 897 (2015)
2 M. Via-Nadal, M. Rodríguez-Mayorga, E. Ramos-Cordoba, E. Matito, *J. Phys. Chem. Lett.* **10**, 4032 (2019)
3 N.R. Kestner and O. Sinanoglu, *Physical Review* **128**, 2687 (1965)