1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Quantum chemistry in two dimensions.

1.1. Project goals

The quantum confinement substantially alters the electronic structure of quantum systems (e.g. atoms, molecules, clusters, and solids) as compared to their corresponding free state counterparts (see Ref. [1] and references therein). This is exhibited in the changes in the electronic energy levels, electronic shell filling, and orbitals, which, in consequence, affect their physical as well as chemical properties, such as energetics, reactivity, response properties, etc. There exist only a few studies[2, 3] where authors have considered the interaction properties of atoms confined (1D or 2D) in a small region of space, showing intriguing perspectives. However, the more interesting perspective reviled the work of Loos et al. regarding the chemistry in 1D[4]. The authors have shown that 1D chemistry differs in a number of interesting ways from a 3D counterpart. Within the project we would like to perform a similar study, however, this time focusing solely on the 2D systems. To this end, we will reformulate all known quantum chemistry methods within a 2D theoretical framework and develop a new computer program dedicated to perform this type of calculation.

1.2. Outline

In order to transform quantum chemistry 2 dimensions (2D) we will start from the 2D variant of Schrodinger equations for N-electron systems. Using a similar approach as in 3D and 1D cases we will develop Hartree-Fock, and Kohn-Sham's DFT methods, as well as perturbative approaches such as these obtained within Moller-Plesset perturbation theory. All methods will be implemented in a newly developed quantum chemistry code specially designed to deal with 2D N-electron systems. We will study the numerical stability of the methods, their basis set dependence, and implementation dependence. Most importantly, we will study how 2D chemistry differs from 1D and 3D counterparts. This can be especially important from the standpoint of developing new quantum chemistry methods designed to work in quasi-2D regimes.

1.3. Work plan

- Design and development of new methods and theoretical mathematical and numerical tools for 2D systems
- Numerical implementation of developed methods.
- Performing test calculations for small and medium-sized atomic and molecular systems.
- Study of quantum chemistry in 2 dimensions

1.4. Literature

[1] W. Jaskólski, Phys. Rep 271, 1 (1996).
[2] H. Moritz and et al., Phys. Rev. Lett. 94, 210401 (2005).
[3] A. T. Sommer and et al., Phys. Rev. Lett. 108, 045302 (2012).
[4] P.-F. Loos and et al., Phys. Chem. Chem. Phys. 17, 3196 (2015).

1.5. Required initial knowledge and skills of the PhD candidate

- Basic knowledge about quantum mechanics and quantum chemistry
- Basic knowledge about quantum chemical methods at the level of exchange and correlation effects
- Basic knowledge about Density Functional Theory and Wave Function Theory methods
- Programming skills (e.g.,FORTRAN, C, Python)
- Basis and/or advanced numerical methods knowledge
- Involvement in scientific work
- Good knowledge of written and spoken English

1.6. Expected development of the PhD candidate's knowledge and skills

- Deep knowledge and understanding quantum-chemical methods ranging from DFT methods up to *ab initio* HF, Coupled Cluster, Perturbation Theory
- Acquiring extensive knowledge of description of many-electron systems including electron correlation effects
- Efficient programming at the advanced level, making parallel code, running quantum chemical calculations
- Ability to analyze the results and to draw conclusions
- General knowledge about calculating different properties of many electron system
- Ability to prepare, present and defend own scientific hypotheses and theses