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

Project title: New computational methods for the quantum chemistry realm.

1.1. Project goal: The KS-DFT is one of the most used methods in electronic calculations and finds large applications in computational chemistry due to its ability to describe ground state electronic structure, mechanical and optical properties, and inter-atomic forces in systems containing hundreds and sometimes thousands of atoms. However, the overall accuracy relays on approximations of the XC energy functional, which is a fundamental physical quantity, which incorporates all the quantum many-body effects beyond the simple Hartree approximation. In the last decades, tremendous work has been done in order to construct accurate XC density functionals which are commonly classified in the so-called Jacob's ladder of accuracy. All semi-local (LDA, GGA, meta-GGA) and hybrid density functionals work quite well applied for atoms, molecules, bulk solids, and solid surfaces in 3D. They even give quite reasonable results for mild quasi-dimensional regimes where the presence of spatial confinement has a rather small effect on the performance of DFT methods (see Ref. [35] and references therein). However, all popular functional approximations (including hybrids), fail badly for systems approaching stronger quasi-low-dimensional regime. This is due to the high inhomogeneity of the electron density raising along the confined direction. This regime is, in fact, essential for real-life applications (note that in the real world, the true 2D limit, is just an extreme, theoretical limit). Hence, the theoretical systems require further progress of DFT, and this proposed work can solve these problems. Thus, one important objective of the proposal is to construct a novel class of ground-state density functionals, equally accurate for 3D, quasi-2D, and quasi-1D systems, that incorporates many exact conditions, and important model systems, such as 3D, 2D, and 1D homogeneous electron gases (HEG). We expect that new functionals will provide the results which are comparable with ab initio WFT approaches at much reduced computational cost.

1.2. Outline: The quantum confinement substantially alters the electronic structure of quantum systems (e.g. atom, molecules, and solids) as compared to their corresponding free state counterparts. This is exhibited in the changes in electronic energy levels, electronic shell filling, orbitals what, in consequence, affect their physical as well as chemical properties such as energetics, reactivity, response properties, etc. Therefore, the chemistry of confinement systems may drastically change. In recent years interest, both physicists and chemists in the study of the physical properties of confined quantum systems have increased with advances experimental techniques which allow to study e.g. atoms or molecules encapsulated in cages like fullerenes, nanotubes or zeolites, atoms, and molecules under pressure or quantum dots or simple molecules in quasi-2D or 2D regimes. The reduction of spatial dimensionality from three dimensions (3D) to 2D and 1D has been often used as an efficient strategy to promote the occurrence of new phenomena. Despite the large scientific effort on this topic, most of the studies and practically all applications have concerned confined extended systems, even if the practical realization of electronic confinement in chemical applications can also be achieved. The study of chemistry under

electronic confinement is a challenging topic because the dimensional crossovers (from 3D to 2D and 1D) are one of the most difficult theoretical and computational problems.

1.3. Work plan

- Design and development of new methods and theoretical mathematical and numerical tools for quasi-1D/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 *(max. 10 listed, as a suggestion for a PhD candidate)*

[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