DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

The accurate computational description of complex polyatomic systems became an important tool supplementing experimental studies, chemistry and materials science. Those methods can be directly used to verify scientific hypotheses, to access the data not available directly in experimental measurements, as well as to make some predictions. Within more than 50 years many computational schemes and method has been develop in order to study the electronic structure and physical and chemical properties of ordinary matter (atoms, molecules and solids). Among them, density functional theory (DFT) has the highest accuracy/computational-cost ratio and it has therefore gained large popularity. In fact, DFT calculations strongly contributed to the new revolution in science and technology, boosting new experiments and progress in nano-/bio-science.

The DFT is exact theory in principle, but in practice the final quality of the results strongly depends on approximations of the exchange-correlation (XC) and, in some formulations, the non-interacting kinetic energy (KE). In case of XC functionals, many useful approximations have been proposed. On the other hand, for the KE, despite a long-lasting research effort, really accurate and efficient approximations are still lacking. For this reason, the most popular computational scheme within DFT, the Kohn-Sham one, avoids the direct use of the KE functional, by introducing auxiliary single-particle orbitals to account for the non locality of the KE. Nevertheless, the KE functional is still a key quantity in DFT research, since its study and understanding has important consequences both at the practical and conceptual level. In fact, KE is one of the most important contributions to the total energy and therefore, an important advances in this field are required. This is especially important because recently renewed interest in methods which directly employ KE functionals and potentials such as orbital-free DFT and many embedded methods such as subsystem DFT, where the KE must be expressed as a pure, explicit density functional.

Thus the main objective of this project is the develop new and accurate density-dependent form of KE functional specific to those formalisms, their computer implementation, and applications in the real nano-, and biologically important systems. This will be done by utilization of well know tools and methodologies used, to date, to construct XC functionals and potentials. In more details, we plan to apply the optimized effective potential (OEP) method to derive exact kinetic potentials for different atoms and molecules. This potential will be then mapped onto the subspace defined by several (semi)local density descriptors (e.g. Thomas-Fermi KE, the reduced gradient and Laplacian of the density) to derive accurate (semi)local approximations of KE potential. Moreover, we will use linear path integral technique, to reconstruct the KE functionals from accurate model potentials. Additionally we will also investigate the non-additive KE potentials used in the subsystem formulation of DFT using the "so called" density condition, previously used in the framework of "ab initio" DFT.

The outcome of this project will definitely find practical applications in theoretical and computational chemistry and physics. Furthermore, it will push the knowledge in the field beyond the actual limits enhancing significantly the applicative power of the methods (e.g. subsystem DFT). It will also set a new standard for the theoretical development and provide powerful and practical tool for many future applications in different fields of computational chemistry and materials science. Most importantly project will contribute to our deeper understanding of the methods which are used for the theoretical description of the properties of many-electron systems.