

## **From Coupled Cluster theory to accurate semi-local Kohn-Sham correlation functional**

Most of the research carried out as part of the project focus on the efficient description of the electron correlation effects in many-electron systems in the context of the Wave Function Theory (WFT) as well as on the Density Functional Theory (DFT) method in the Kohn-Sham (KS) implementation.

The DFT methods are currently the most popular and effective methods used in computational quantum chemistry, theoretical chemistry, solid state physics, and nanotechnology. Implementations of such methods are already present in the vast majority of software packages for quantum-chemical calculations and are routinely used in the calculations carried out for systems of atomic, molecular, and large biological systems and nanostructures. The main advantage of DFT methods, is much lower computational cost, as compared with the standard *ab initio* approaches based on the wave function (i.e. WFT), and thus allowing the calculation of much larger systems. The accuracy and efficiency of DFT methods depend directly on the quality of approximations to the exchange-correlation functionals which are used in these methods. Unfortunately most of the known and widely used popular correlation functionals and potentials gives satisfactory results only in some areas of application, and often the quality of the results obtained are unpredictable. Therefore, the search for the correct, more accurate, based on well-established theoretical foundations and relatively simple exchange-correlation functionals in DFT became, since many years a priority task for quantum chemists and physicists.

One of the possible solutions is the use of orbital-dependent functionals in Kohn-Sham DFT methods. This directly leads to the effective potential (OEP) method, which together with KS-DFT constitutes *ab initio* density functional theory. In this approach the combination of the efficiency of DFT with the accuracy and systematic improbability of WFT promises to bring computational chemistry to a new level, allowing the accurate description of the electronic properties of realistic systems. However, to date, this possibility is hindered by technical limitations that prevent the efficient and widespread use of *ab initio* DFT methods in computational chemistry applications. The main problem of the *ab initio* DFT is the cost of numerical calculation cost of this methods, which is even in some cases 3 orders higher than the numerical cost of standard – density dependent KS-DFT calculations.

In this project, we aim facing problem of this high numerical cost of *ab initio* type methods by developing new class density dependent semi-local correlation functionals, which are compatible with orbital-dependent exchange-only OEPx/KLI/LHF functionals. This will allow applying new class of methods to new, much wider problems in computational chemistry.

All solutions will be implemented in state of art quantum chemical computational systems e.g. ACES2 and libx library. Certainly at the intermediate and final steps of this project, we will perform detailed assessment of the new developed methods by performing several test for standard quantum chemistry benchmarks. The project will also allow for the search for new, more advanced methods describing correlation effects and developing of new functionals in both *ab initio* DFT and the standard KS-DFT.