In recent years interest of both physicists and chemists in the investigation of the physical properties of confined quantum systems has 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, quantum dots or simple molecules in quasi-2D or 2D regimes. The spatial confinement of particles lies behind the effect of quantization. This statement can be proofed based on a simple toy example of one particle trapped in the box potential whose energy levels become in these circumstances discrete, contrary to its free counterparts which appear in the continuum. The quantum confinement also 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. 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.

One of the most crucial points when analyzing quantum confined systems is the choice of accurate model and quantum chemical method which allow to describe correctly the changes in the electronic wavefunction due to the effect of confinement. In recent years in most studies, the electronic wavefunction of the system subjected to confinement was span by a set of Gaussian-type orbitals (GTO) belonging to the most widely utilized basis sets in the quantum chemical codes. This allows to study systems in soft confinement regimes by various wave function theory (WFT) and density functional theory (DFT) methods. The spatial electron confinement, in turn, is usually modeled by isotropic 3D, 2D, or 1D harmonic oscillator potential (with small oscillatory strength parameter ω) introduced to N-electron Hamiltonian. However, for larger values of confinement strength (strong quasi-1D/2D regime) or when harmonic potential becomes anisotropic, the common strategy is to supply standard GTOs with, specially designed anisotropic GTOs (aniGTO) in order to guarantee that the wavefunction spans both Culombic and harmonic oscillator eigenstates. We note that these basis sets are not implemented in any of the popular codes, thus not allowing to routinely study of systems under various confinement with standard WFT and DFT methods.

The first goal of the project is to implement the aniGTOs in *libint* library what will allow their general utilization in novel quantum chemistry codes such as PSI4. Next, we will focus on the development and validation of existing WFT and DFT methods for the study of atoms, molecules, and molecular complexes subject to soft and strong spatial electronic confinement. Using accurate WFT methods (e.g. the coupled-cluster methods) we will create a database of confined chemical systems, which will be used to assess and improve the performance, and develop new, advanced DFT methods describing correctly the crossovers from 3D to 2D and 1D (second goal). We note, that most of the standard DFT methods fail badly in the description of dimensional crossovers mentioned before, thus not allow to model systems with strong quasi-2D or quasi-1D characteristics. The problem lays in the construction of the standard exchange-correlation energy functionals which cannot be used directly in low-dimensional regimes due to various limitations. Thus, the dimensional crossovers still remain one of the most difficult open problems in DFT.

The above theoretical and computational work can lead to open a new field of research of high scientific interest. The outcome of the project will explain how the chemical interactions depend on the confinement strength, will unravel the behavior of confined finite systems, and will predict experimental applications. Moreover, an analysis of various theoretical methods can unravel numerous new physicochemical properties of the systems under consideration e.g. the change in reactivity of atoms and molecules.