Reliable quantum chemical modeling of electronic structures plays a pivotal role in understanding and predicting the physicochemical properties of atoms, molecules, and materials. Examples are theoretically predicted molecular structures, bonding patterns, complexation energies, reaction energies, vibrational and electronic spectra, chemical shifts, and molecular orbitals. In general, we observe the trend that quantum chemistry allows us to study molecular systems of growing size and provides increasingly accurate data. Such a rapid progress is driven by three main factors: (i) the increase of computer power, that is, computer clusters equipped with large amounts of memory and more efficient and multi-threaded processors, supported by graphics processing units, (ii) the progress in quantum chemical software development, and (iii) the development of novel quantum chemistry methods.

Over the past decades, two major groups of quantum chemistry methods emerged. One group is based on density functional theory (DFT)—or its approximate variants—and uses the electron density as building block. The second group of methods is known as wave function theory (WFT), which as the name implies uses the electronic wave function as the main constituent. While DFT is, in general, more efficient and applicable to larger systems, WFT provides more reliable results. One way to combine the advantages of both groups of methods is to couple WFT and DFT together using so-called *embedding techniques*. However, this task is immensely difficult as we need to combine efficient and robust WFT approaches that are computationally feasible for larger systems. The main purpose of the proposed research project is to develop and efficiently implement a new family of WFT-in-DFT methods that uses various pair coupled cluster doubles-based models as the WFT component. Specifically, pair coupled cluster doubles-based methods have been shown to provide reliable and accurate electronic structures and properties for many challenging systems. Compared to conventional WFT models, like conventional coupled cluster theory, they are computationally cheaper and do not fail in cases where the correlated motion of electrons is difficult to describe, especially within conventional coupled cluster methods. In this research project, we will combine the advantages of both DFT and different variants of pair coupled cluster doubles, which will pave the way for studying many challenging problems of present day quantum chemistry, including large scale modeling of molecular interactions and compounds of industrial significance like uranium clusters encountered in nuclear waste.