Description for General Public

Exploring biological phenomena at molecular scale is oftentimes indispensable to develop new drugs and intelligent materials. Most of relevant system properties are affected by intermolecular interactions with nearby environment such as solvent or closely bound electronic chromophores. Studying molecular aggregates requires rigorous and accurate *Quantum Chemistry* methods, the computational cost of which grows extremely fast with the number of electrons in the system. Therefore, it is of particular importance to develop mathematical models to simplify equations and implement them in a form that is relatively cheap but still provides high accuracy and reliability.

This Project will focus on finding a unified way to simplify various equations of Quantum Chemistry of *extended molecular systems*, i.e., molecular aggregates such as interacting chromophores and molecules solvated by water and other solvents. Indeed, one of the important difficulties encountered in Quantum Chemistry of large systems is the need of evaluation of special kind of numbers known as *electron repulsion integrals*, or in short, ERI's. In a typical calculation, the amount of ERI's can be as high as tens or even hundreds of millions (!) that unfortunately prevents from application of conventional methods when the number of particles in question is too large. In the Project, the complicated expressions involving ERI's shall be greatly simplified to reduce the computational costs as much as possible while introducing no or minor approximations to the original theories.

The generalized one-electron potentials (OEP's), developed in the Project, will be utilized for two important fields of Quantum Chemistry. First Project is related to the energy transfer at the very short distances between molecules that are present in molecular factories used by nature in the process called *photosynthesis*. In that process, chemical energy is produced directly from sunlight, water and carbon dioxide. Understanding photosynthesis is of key importance in designing novel materials that can absorb sunlight with very high efficiency. Second, the Project will study special kind of *repulsive forces* occurring between molecules, as well as *small deformation of molecular shapes* in the presence of other molecules. These aspects can be helpful in developing new methods to perform accurate simulations of how molecules move in nature, or in other words, what is their dynamics.