Description for the general public

Chemical reactions constitute the essence of chemistry. They are key elementary processes of practical application in, among others, chemical engineering, technology, biotechnology or materials analysis. In the most simplified picture, the chemical reaction is a process leading to breaking and formation of chemical bonds between atoms. From the quantum-mechanical perspective it is an exceptionally complex process with the simultaneous dynamics of electrons and nuclei which in most cases cannot be studied satisfactorily within the Born-Oppenheimer approximation. The complexity of the coupled motions of electrons and nuclei in the course of a chemical reaction implies that nearly exact quantum-chemical studies of reactive processes are still restricted to very small systems with no more than three or four atoms involved. Theoretical calculations are often prerequisite to interpret the result of experiments which nowadays can be carried out with an extremely high precision. Theory input is also needed to identify the basic molecular mechanisms of the reactive collisions. The knowledge of the detailed dynamics and mechanisms of the reactions paves the way for controlling this process, in principle, even to such a degree that only one of many possible outgoing channels will be populated. Achievement of such a level of control of a chemical reaction that it leads to only one desired, preselected product should be considered as an ultimate goal of studies on the chemistry and physics of elementary molecular processes.

An other phenomenon of primary importance in chemistry, physics, and biology are intermolecular forces. Intermolecular potentials determine the properties of non-ideal gases, (pure) liquids, solutions, molecular solids, and the behaviour of complex molecular ensembles encountered in biological systems. They describe the so-called non-bonded contributions, as well as the special hydrogen bonding terms, that are part of the force fields used in simulations of processes as enzyme-substrate binding, drug-receptor interactions, etc. A few examples showing important applications of intermolecular potentials include the Monte Carlo and molecular dynamics simulations of biological systems, drug design, studies of processes in the earth's atmosphere, and interstellar chemistry.

These two seemingly distinct problems have one in common - demand for an accurate description of the electron correlation, both the static and the dynamic components. The natural approach to achieve this goal is to use explicitly correlated calculations with a new formula for the so-called correlation factor. Therefore, the main objectives of the project are to devise, implement, benchmark and present pilot applications of the so-called *range-separated* correlation factor in the explicitly correlated quantum chemical calculations, and apply all newly developed methods to predict and interpret high-resolution experimental data.