Controlled ultracold collisions and chemical reactions of atoms and molecules with complex structure

The aim of chemistry as a science is to gain an understanding of chemical reaction mechanisms and their optimal design. For this reason, gaining this understanding at the most basic, microscopic level, 'from first principles' is fundamentally important. A proof for this are the Nobel prizes given in this field – to Herschbach, Polanyi and Lee in 1986, to Zewail in 1999 and Karplus and Warshel in 2013. The perfect conditions to to study the mechanisms of chemical reactions are since recently provided by the so-called ultracold chemistry, which makes it possible to trap the reactants in external fields, collide them at a given kinetic energy and to accurately study the reaction products.

The aim of this project is to provide tools to control the collisions and chemical reactions in systems that are currently at the forefront of ultracold chemistry research. In particular we will be interested in the possibility to control the interactions between colliding atoms or molecules and to control the collisional cross-sections (which have an impact on the speed of the chemical reaction) and the production of molecules. We will investigate the possibilities of such control by means of magnetic fields, laser radiation and we will accurately calculate the expected reaction products.

Our research will be theoretical in nature and will rely on pursuing the so-called numerical calculations, or, to simplify, computer simulations of the investigated systems. To do so we will be solving different forms of the so-called Schrödinger equation, which makes it possible to describe the motion of particles in the microworld. We will take quantum effects into account both in the calculations of the structure of the molecules we are interested in, as well as in the simulations of collisions of the molecules and their chemical reactions. It is worth noting that such calculations require tremendous computational power and therefore we will need to use an appropriate supercomputer – in our case one provided by the PLGrid infrastructure. This project will also be a challenge from programming point of view – to do these calculations we will implement a special modular computational environment which will be the tangible outcome of the project.