One of the most important puzzles in quantum chemistry is the proper description of the interaction between molecules. As a matter of fact each chemical reaction, which is bond rearrangement between molecules, starts when molecules are far apart and are approaching each other. It turns out that even for modern quantum chemistry such description is challenging and it is very hard to provide proper description of potential energy in systems where molecules are subject to bond-breaking, contain transition metals or unpaired electrons. One can say that this is due to the fact that in the quantum world it is possible that such molecule is in a „mixed state" and in a way, is confused what is its electronic configuration, or, how the electrons are distributed within a molecule.

In this project we will develop the toolbox which provides the detailed information about the interactions of such „confused molecules" which in theoretical chemistry we refer as to „multireference character molecules". We propose to develop such method of study of molecular forces which catches essential physics and provides analysis tool for detailed studies of molecules in „exotic states". Such analysis tool is very important, since the molecular interactions are very sensitive to methods and details of calculations, it is enough to say that they can be many orders of magnitude smaller than total energies of molecules. The method we will develop is referred to as symetry-adapted perturbation theory (SAPT) and treats the interaction between molecules as small perturbation of the whole system. The method provides deep insight into the mechanism of the interaction. For example, we can recognize how large is interaction due to the overlap of molecular charges, how large is the contribution of mutual polarization of monomers, how strong is the repulsion between molecules as they approach each other. The SAPT method performs extremely well for „normal molecules", however it still has not been generalized for molecules of multireference character.