

Non-covalent intermolecular interactions, although very weak, determine many physicochemical processes. These include aggregation of molecules, solvation, or bulk properties such as viscosity. Chemical reactions start when molecules experience attractive forces between them. Thus, being able to describe these forces is vital for understanding many phenomena in chemistry and molecular physics. In other words, the dynamics of chemical processes govern the shape of the potential energy surface of the system. The interaction energy is easy to define, as the difference between the energy of a "super-system" that contains two molecules, and the sum of the energies of two molecules at infinite separation. In practice, it is not so straightforward, since the interaction energy is orders of magnitude smaller than the values that need to be subtracted from each other (total energies). Ideally, we would like the calculation of interaction energy directly using the wave functions of monomers: in such a scenario, the calculation cost is lower, we have better control of calculation accuracy. This scenario is realized in the so-called Symmetry-Adapted Perturbation Theory (SAPT) in which as the zero-order function one takes the product of wavefunctions interacting molecules. SAPT also forces correct permutation symmetry of electrons in the system, which is indistinguishable particles. Currently, SAPT applies to is very well suited for a variety of application which ranges from small molecular systems, such as atmospheric chemical compounds, to large molecules in molecular crystals. What still causes many problems for theorists is to accurately describe interactions of unstable molecules, radicals and molecules in excited states. There are many such situations in nature: oxygen in the atmosphere is such a molecule. In the case of chemical reactions, we always deal with the interaction of fragments of molecules with each other.

In this project, we would like to develop new theories that correctly describe non-covalent intermolecular interactions in a situation where the constituent molecules are easy to polarize, exchange charges and at the same time interact with a solvent, or atmospheric gas. One of the most challenging tasks is the correct description of the so-called induction effects in the system, i.e. phenomena of mutual polarization of molecules. Also, developed the theory can be applied to the situation when one of them is in a (quasi)degenerated state, i.e. when the energies of the neighbouring molecule are close. We will also give a new formulation of theories of molecular properties (such as dipole moment) induced by interaction. Such properties are critical to the description of the spectra of the molecules in environments and their interaction with light.

The final part of the project includes the application of the theories introduced to study potential energy surfaces in a system with astrochemical relevance. For example, the collision of atoms with the OH + ion radical or the OH or SH radicals with organic molecules - these studies are of fundamental importance for understanding mechanisms of water reactions in the Space. In addition, new theories will be applied to the interaction of oxygen in the electronically excited state with other molecules in the atmosphere, such as nitrogen or CO<sub>2</sub>.