

Scientists aim to understand better the structure of various molecules, their interactions, and the influence of various external factors on their properties. Research conducted in an ultracold temperature regime is a new approach to studying exotic phenomena in atomic and molecular systems. At 1K and smaller temperatures, the wave nature of matter is much more revealed, and quantum description becomes necessary. Several Nobel prizes have honoured research on ultracold matter, including producing atomic Bose-Einstein condensate and developing laser cooling and trapping techniques. Polyatomic molecules pose a more significant challenge in effective cooling and entrapment than atoms or diatomics because they possess additional rotational and vibrational degrees of freedom. However, the complexity of their structure and interactions is why the world of science paid attention to them. The ability to precisely control polyatomic molecules is a tool for many interdisciplinary research projects in quantum simulations and computing, mechanisms of chemical reactions and ultraprecise spectroscopy.

As part of the project, we will use and develop quantum chemistry and molecular physics methods. We will carefully examine the electronic structure of selected molecular systems consisting of atoms of alkali metals, alkaline earth, lanthanides and actinides of the periodic table. As part of quantum-chemical calculations, we will determine the interaction potentials and physicochemical properties of various electronic states of selected molecules. This will help determine whether a particular system can be cooled to the milliKelvin regime. In the next step, we will theoretically investigate the sensitivity to very exotic effects in molecules related to breaking nature's fundamental symmetries. One of them is a violation of the CP symmetry. As a result, elementary particles such as negatively charged electrons may exhibit an electric dipole moment. A thorough understanding of the nature of these phenomena will be fundamental to understanding the laws governing the Universe and a more complete understanding of its evolution.

The multitude of combinations of connections between atoms is a source of richness in multiatomic systems. This provides solid grounds for claiming that these systems still have many fascinating phenomena to discover. They can contribute to a better understanding of the world around us and the development of many modern technologies based on quantum theory. The completed project will significantly contribute to understanding chemistry and physics at the most fundamental level. Moreover, it will be a source of scientific inspiration for further research in physics beyond the Standard Model, e.g. explaining the asymmetry of the ratio of matter to antimatter in the Universe.