Description for the general public

Molecules cooled to temperatures below $T = 10^{-3}\,\mathrm{K}$ allow for tackling questions touching upon the very fundamentals of quantum mechanics. They are promising candidates in novel applications, ranging from ultracold chemistry and precision measurements to quantum computing. Cold and ultracold molecules are thus opening up new and exciting areas of research in chemistry and physics due to their manifestly quantum nature.

The positions of lines and intensities in the molecular spectra at ultralow temperatures can be measured with an unprecedented accuracy since the Doppler broadening effects on the spectral lines are almost absent. Such precision measurements represent a big challenge for theory, and will certainly lead to new theoretical and computational developments. Precision measurements of the molecular properties and interactions may also give insights into the fundamental aspects of modern physics, such as experimental verification of theories going beyond the standard model. The time variation of the fundamental constants or the permanent electric dipole moment of electron are very good examples where methods of molecular physics at ultralow temperatures can be applied in fundamental science. Ultracold molecules can also be used in high-resolution spectroscopic experiments as an indirect probe of interatomic interactions at very large interatomic distances including the relativistic and QED effects.

The role of a quantum chemist in the field of molecular physics at ultralow temperatures is (*i*) to provide the experimentalists with predictions of various physical processes that will lead to an effective production of ultracold molecules, (*ii*) to predict accurate data characterizing the spectroscopic and scattering properties of relevant molecules and collisional complexes, and (*iii*) to interpret the available experimental data. The main objective of the proposed research will cover the three areas briefly introduced above and will focus on the the theoretical predictions for state-selective production of molecular ions.

A proper realization of the above mentioned goal will require new developments in the electronic structure theory. These will go in three directions: increase the accuracy of the approximate methods to compute the electronic structure data such as the potential energy surfaces, spin-orbit and nonadiabatic coupling matrix elements, one- and multi-photon transition moments, and dynamical Stark shifts by explicitly correlated methods with Slater orbitals Kołos-Wolniewicz basis functions.