NEW WAYS TOWARDS PRODUCTION AND CONTROL OF ULTRACOLD POLYATOMIC MOLECULES

Systems composed of atoms, molecules, and ions takes a fundamentally important place in chemistry as a science. The knowledge about their composition, structure, energy spectrum, properties, and reactivity allows not only for a better understanding of nature but also brings numerous practical applications. Under the perfect conditions, the system may be coherently controlled with the accuracy of the single quantum state, which is one of the main challenges for the development of modern technology based on quantum mechanical laws. Candidates ideally suited for this purpose are low-temperature gases trapped in the external potentials; they may be insulated from the environment as well as they manifest, usually inaccessible in hotter systems, many physical consequences of wave-particle duality, in particular, wave nature of matter. The importance of ultracold gases was best proven by Nobel prizes in Physics awarded for the development of cooling and trapping of atoms with laser light in 1997 and observation of Bose-Einstein condensates in 2001. Recently, ultracold atoms in optical lattices paved the way for the realization of toy models of quantum simulators, and clocks built using cold atomic clouds have allowed pushing the frontier for measurement science.

In comparison to atoms, molecules have even more advantages for quantum control. For example, ultracold molecules can be polarized leading to the internal electric field recently finding unique applications in searching for new physics beyond the Standard Model. However, the preparation of molecules in the ultracold regime is a typically difficult task because, in contrast to atoms, they have rotational and vibrational levels associated with each electronic state. These problems are compounded by the fact that many molecules with potentially enhanced sensitivity to new physics are polyatomic, heavy, and chemically weakly bound. Only recently, two groups from Caltech and Harvard have demonstrated triatomic molecules in the micro Kelvin regime: monohydroxides of alkaline-earth (SrOH) and earthlike-metal radicals (YbOH). These systems will play a key role in detecting electric dipole moment and violating of charge-parity symmetry shedding light on the asymmetry between matter and antimatter in the universe.

The aim of this project is a theoretical investigation of interactions and nonreactive collisions between closed-shell atoms and heavy triatomic molecules being currently at the forefront of ultracold matter studies. We propose the X-XOH (X=Ca, Hg, Sr, Yb) system which is in direct response to current laser cooling of SrOH and YbOH molecules. Special attention will be put on whether these systems can be controlled by experimentally accessible parameters using external magnetic and electric fields. The primary tool for such manipulation is the Feshbach resonance, which requires collisions in a single partial-wave (s-wave) regime. Specifically, this regime occurs at temperatures well below micro Kelvin for molecules what means that new cooling approaches must be proposed to reach a regime, where Feshbach resonances could be observed. For this reason, it would be very interesting to explore prospects for sympathetic cooling of the molecule into a single partial-wave regime.