Cooling and dynamics of polyatomic molecular ions immersed in ultracold atomic gases

Summary for the general public

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I. RESEARCH PROJECT OBJECTIVES

The development of laser and cooling techniques resulted in the birth and successful advances of the field of ultracold matter in recent decades. The revolution in the research at ultracold temperatures, that is temperatures below 1 miliKelvin, started with the creation of the Bose-Einstein condensates and degenerate Fermi gases. After many spectacular successes, the scientific community has drawn its attention to two new areas: the formation and control of ultracold molecules on one hand, and hybrid systems of atomic ions immersed in ultracold atomic gases on the other hand. Here, we combine these two research directions.

The aim of the project is to propose and theoretically investigate properties, interactions, dynamics, and potential applications of polyatomic molecular ions immersed in ultracold atomic gases. The molecular ions can be trapped in the Paul trap, or in the dipole trap, and immersed in a gas of alkali-metal or alkaline-earth-metal atoms cooled down to temperatures below 1 μK and trapped in the dipole trap. The first question, that we will answer, is what happens with molecular ions after immersing them in ultracold atomic gases. We will investigate whether the translational and rotational motions of ions are cooled down, and what conditions have to be met to cool them down efficiently. Next, we will explore in detail ultracold interactions and collisions between polyatomic molecular ions and atoms, as well as ultracold chemical reactions controlled with external laser and magnetic fields. Finally, we will propose the applications of the investigated systems in high precision spectroscopic measurements.

II. WORK PLAN

Fist of all, we will investigate electronic structure of molecular ions, staring with rigid linear anions, and select the most promising systems. We will employ advanced *ab initio* methods of quantum chemistry to calculate potential energy surfaces for several selected molecular ions interacting with alkali-metal and alkaline-earth-metal atoms. This will allow us to characterize and understand interactions in the investigated systems. The calculated potential energy surfaces will be employed in scattering calculations. Ultracold elastic and inelastic collisions, as well as chemical reactions between molecular ions and atoms will be investigated depending on the collision energy, the structure and quantum state of the ion and atom. The comparison of the cross sections for elastic and inelastic scattering will allow us to characterize the cooling process. We will investigate the impact of external laser and magnetic fields on ultracold collisions and chemical reactions. We will propose new control schemes of ultracold collisions and chemical reactions. We will investigate the impact of molecular ions as rotating quantum impurities coupled to Bose-Einstein condensate and degenerate Fermi gas. An in-depth understanding of the considered systems will allow us to propose new high precision spectroscopic measurements, which will be complementary to conducted theoretical studies.

III. MOTIVATION

Molecular ions are important in many areas of chemistry as different as the organic synthesis and astrochemistry. Therefore, the considered systems are interesting from the fundamental point of view. The investigation of ultracold collisions and chemical reactions between molecular ions and atoms on the quantum level will result in better understanding of the physical basis of chemistry, and the high precision spectroscopic measurements of cooled molecular ions will allow one to better understand the electronic and rovibrational structure of molecules. Applications of polyatomic neutral molecules and molecular ions are also expected to be an important part of upcoming experimental research. At the same time, the knowledge about collisions between polyatomic molecular ions and ultracold atoms is very limited, which limits the advances in experimental investigations of these systems. Therefore, the important goal of the project will be to investigate and propose optimal and interesting new experiments on cold polyatomic molecular ions.