Ultracold polyatomic molecules: formation, dynamics, applications

Summary for the general public

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I. RESEARCH PROJECT OBJECTIVES

Advances in cooling and trapping techniques have allowed for the dynamic development of research on the matter at ultralow temperatures, i.e. temperatures below 1 milikelvin, over the last few decades. Cold and ultracold systems attract researchers' attention because the quantum nature of the world clearly manifests under such conditions, and research into such systems provides new insight into the quantum theory of matter and the interaction between matter and light. After spectacular successes in the field of ultracold atoms – obtaining Bose-Einstein condensates and degenerate Fermi gases – the scientific community turned its attention to research on ultracold molecules, and in recent years, the first attempts to produce ultracold polyatomic molecules have been made.

The project aims to propose and theoretically investigate new methods of formation, properties, interactions, dynamics, and applications of ultracold polyatomic molecules in fundamental research. We suppose that new ultracold polyatomic molecules could be produced and could find many new interesting applications in modern physics and chemistry of ultracold quantum matter. Possible applications range from the study of controlled chemical collisions and reactions to precise measurements and quantum simulations of phenomena important to the few- and many-body physics.

II. WORK PLAN

We will use modern *ab initio* techniques of molecular physics and quantum chemistry as well as develop and implement new concepts and methods. We will start by examining the electronic and rovibrational structure of new polyatomic molecules in the context of their effective laser cooling and applications in precision measurements. Next, we will study intermolecular interactions and cold collisions between polyatomic molecules, focusing on systems critical to ongoing experimental works. This will allow us to determine the stability of ultracold gases of polyatomic molecules and the prospects of their evaporative cooling and the implementation of ultracold controlled chemical reactions. We will also study the interactions and collisions of ultracold polyatomic molecules with atoms to determine the possibility of buffer-gas and sympathetic cooling them through collisions with cold atoms. Interactions and collisions will be investigated for both molecules and atoms in ground and excited electronic states. On the other hand, we will explore the possibility of producing and controlling ultracold polyatomic molecules by associating diatomic molecules with external electromagnetic fields. We will propose new precision spectroscopic measurements, which on the one hand, will be complementary to the developed theory, and on the other hand, will allow testing the fundamental laws of physics by comparing the measurement results with theoretical predictions, measuring the spatiotemporal variation of physical constants, or measuring the electric dipole moment of an electron.

III. MOTIVATION

When considering combinations of known atoms, there are more than ten thousand possible diatomic molecules, while the number of possible triatomic combinations exceeds one million and the number of isomers of four-atomic molecules – one billion. The extraordinary variety of polyatomic molecules promise their fascinating properties and applications, prompting the search for new systems that may have properties suitable for study in ultracold physical and chemical experiments. In this project, we will propose and investigate novel ultracold polyatomic molecules that are fundamentally interesting and still poorly understood. Studying cold collisions and chemical reactions at the most elementary quantum level will bring a significant deepening of understanding of the physical foundations of chemistry, and precision spectroscopic measurements of ultracold polyatomic molecules will help to understand their structure better and may shed new light on fundamental physics. The obtained theoretical results will be used to inspire, guide, and explain ongoing and forthcoming experiments. Efforts will result in a better understanding of the world's quantum nature at the microscale, which is essential for all areas of physics and chemistry.