Spectroscopy, formation, and application of ultracold highly polar KAg and CsAg molecules: theory and experiment

Summary for the general public

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I. MOTIVATION

Ultracold polar molecules are a perfect platform for investigating the fundamentals of quantum physics and chemistry. Diatomic molecules possessing permanent electric dipole moments (PEDMs) have already been employed to realize first ultracold controlled chemical reactions, precision measurements, and quantum simulations of many-body dynamics, while prospects for use in quantum computing have driven the recent developments of single-molecule control with optical tweezers. Fast progress motivates an increasing number of research groups worldwide to start investigating polar molecules at ultralow temperatures. Most of the mentioned exciting applications are based on PEDMs resulting in long-range intermolecular dipolar interactions and possibilities for control with an external electric field.

Recently, we have discovered that ground-state diatomic molecules consisting of a silver atom interacting with an alkali-metal atom, such as KAg and CsAg, have PEDMs reaching 10 Debye, while the most polar ultracold molecules considered previously have had PEDMs at least twice smaller. Effectively, characteristic lengths of dipolar interaction in ultracold gases of KAg and CsAg molecules can be more than an order of magnitude larger than those of the most polar ultracold molecules studied until now.

II. RESEARCH PROJECT GOAL

Building on the above discovery of molecules possessing unprecedentedly large PEDMs in their ground states, we will establish a unique national theoretical-experimental consortium at the University of Warsaw and the Institute of Physics of the Polish Academy of Sciences to propose, study, and probe KAg and CsAg molecules for a new generation of ultracold physics and chemistry experiments. We will combine state-of-the-art *ab initio* theory with cutting-edge hot vapor molecular spectroscopy and advanced ultracold photoassociation spectroscopy to investigate and understand their molecular structure, intermolecular interactions, control, dynamics, and formation schemes. The realization of the project will pave the way towards the production of ultracold gases of highly polar ground-state KAg and CsAg molecules in the future.

III. WORK PLAN

In the theory path, we will first employ state-of-the-art *ab initio* techniques of quantum chemistry and molecular physics to accurately investigate the electronic structure of excited states of the KAg and CsAg molecules. We will calculate potential energy curves, transition electric dipole moments, and spin-orbit couplings. These data will be used to study rovibrational structures and predict photoassociation and stimulated Raman adiabatic passage (STIRAP) formation paths of ground-state molecules. Prospect for magnetic Feshbach resonances and magnetoassociation will also be examined. Next, potential applications of ultracold highly polar molecules will be investigated in detail, including quantum-controlled collisions and chemical reactions and quantum many-body simulations.

In parallel, in the hot experimental path, we will construct new spectroscopic cells for the hot vapor spectroscopy of the KAg and CsAg molecules. Because of the extremely high temperature needed for the adequate vapor pressure of Ag atoms generation, cutting-edge materials and techniques will be used. High-resolution molecular spectra will be recorded using laser-induced fluorescence and polarization labeling spectroscopy methods. These data will be used to refine theoretical molecular potential energy curves and photoassociation and STIRAP schemes.

Finally, in the ultracold experimental path, we will build a new high-vacuum apparatus with a laser setup to form a magneto-optical trap with ultracold Ag atoms and next dual-species magneto-optical traps with ultracold K+Ag and Cs+Ag mixtures. We will optimize and characterize in detail both single and mixed species configurations. Finally, we will perform photoassociation spectroscopy of ultracold KAg and CsAg molecules in excited electronic states using transitions below the D_2 line of alkali-metal atoms. The observed vibrational levels will allow us to refine molecular potentials and the STIRAP scheme further.