

Creating ultracold H₂ by sympathetic cooling with rare gas atoms

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The ability to create cool dilute atomic gases has revolutionized physics over the last twenty years. Considerable attention is now turned to the creation of and study of trapped cold ($T < 1$ K) and ultra-cold ($T < 1$ mK) molecular samples. Cold molecules offer the possibility of investigating in great detail chemical reactions, as well as high-resolution vibration-rotation spectroscopy, and to test fundamental physics beyond the standard model or parity violation at the molecular level.

Molecular hydrogen (H₂) represents an ideal candidate for its simplicity, but also for its relevance to astrophysics. Complexes made of H₂ and a Rare Gas atom have been used for many years as benchmark systems to test various theoretical models as well as computational methods. In particular Ar-H₂ and He-H₂ have attracted a considerable attention.

In this talk I will discuss the sympathetic cooling of H₂ with Rg atoms (Rg=He, Ne, Ar, Kr, Xe) from a theoretical perspective. The first step will be to introduce the experimental conditions that we are interested in simulating [1]. In particular, unlike other similar works, we are interested in investigating cold collisions between Rg atoms and H₂ in its vibrational-rotational ground state.

The first (key) ingredient is the determination of the Potential Energy Surface which parametrizes the Rg-H₂ interaction. Due to their van der Waals character, Rg-H₂ complexes are weakly bound and their physical properties are extremely sensitive to the details of the PES used to model their interaction [2]. I will discuss the state-of-the-art of Rg-H₂ PES and introduce a number of them which were used in the calculations.

The next ingredient is the evaluation of the cross sections for Rg-H₂ scattering. As a consequence of the particular experimental conditions considered the only open channel is the elastic one. Due to the weak character of the Rg-H₂ interaction, the scattering Rg-H₂, which in principle is a three-body problem can be effectively modeled assuming a rigid H₂ diatom, which greatly reduces the computational burden of such calculations [3]. A comparative analysis of the cross sections for all Rg atoms will be presented, and discussed also in terms of the halo features of those complexes [4].

A direct Monte Carlo simulation of the dynamics of the cooling process can be made by means of the Bird method [5]. This simulation will enable the optimization of the experimental apparatus, and to test the cooling capability of the different Rg gases.

The final part of the talk will be devoted to the conclusions and to discuss future perspectives.

References

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