Postdoc position on the theory of ultracold molecules

Professor Jeremy M. Hutson, FRS
Departments of Chemistry and Physics, University of Durham
https://jmhutson.webspace.durham.ac.uk; email J.M.Hutson@durham.ac.uk

A postdoctoral position is available to work on the theory of cold and ultracold molecules, starting as soon as convenient after February 2023. The main topics we work on are:

1. Collisions of ultracold atoms and molecules
2. Formation of ultracold molecules from atoms
3. Properties of ultracold molecules in electric, magnetic, microwave and laser fields
4. Applications of ultracold molecules to quantum science

The group has substantial funding from the Engineering and Physical Sciences Research Council (EPSRC). This post is funded under the EPSRC Programme Grant *QSUM: Quantum Science with Ultracold Molecules* (2017-22), joint with experimental groups at Durham (Simon Cornish) and Imperial College London (Mike Tarbutt and Ben Sauer) and a second grant on *Cooling Molecules To Quantum Degeneracy* with the same group at Imperial. We also have a grant on *Developing Molecular Quantum Technologies* that funds collaborations with cold-molecule groups at Harvard and University of Colorado, Boulder.
Jeremy Hutson is a member of both the Physics and Chemistry Departments at Durham. This position will be based in the Chemistry Department, but with membership of the Joint Quantum Centre (JQC) Durham/Newcastle and the Quantum Light and Matter grouping in the Physics Department. We also have a wide network of collaborative links to experimental and theoretical groups around the world, including Boulder, Harvard, Innsbruck, Maryland and elsewhere.

General

The study of cold molecules (below 1 K) and ultracold molecules (below 1 mK and as low as 100 nK) is a "hot topic" in modern physics and chemistry [1]. The potential applications of such molecules include

- precision measurement (applications such as detecting the electric dipole of the electron, which is important for physics beyond the Standard Model of particle physics, or detecting the time-variation of fundamental "constants" such as the fine-structure constant or the electron-to-proton mass ratio)
- quantum simulators, in which cold molecules are used to create "designer Hamiltonians" and can be used to solve problems in quantum condensed matter physics that are completely unapproachable with conventional computers
- quantum information manipulation and storage ("quantum computing")
- development of a controlled ultracold chemistry, in which chemical transformations are carried out on a complete ensemble of molecules simultaneously and preserving quantum-mechanically coherence.

Ultracold molecules may turn out to be a transformational technology for the middle of the 21st century. It is not inconceivable that your iPhone will contain arrays of ultracold molecules in 25 years time, and even if it does not we will have learned a great deal of new physics and explored new phases of matter using the quantum playground that ultracold molecules provide.

Recent achievements

In collaboration with experimental groups in Durham and Innsbruck, we have succeeded in producing ultracold RbCs molecules at a temperature around 1 μK in an optical trap. The molecules are formed from ultracold

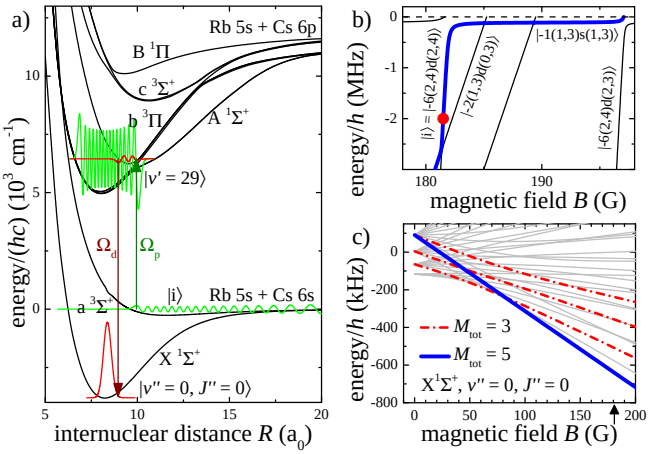

FIG. 1: Production of ground-state RbCs from ultracold Rb and Cs atoms. Top right: the way that magnetic fields are used to form "Feshbach" molecules very near dissociation and then navigate to a state suitable for ground-state transfer. Left: the 2-photon STIRAP scheme used to transfer Feshbach molecules to the ground state. Bottom right: the pattern of hyperfine levels in the ground state, showing that the state formed becomes the absolute ground state at fields above 90 G. None of this would have been possible without guidance from theory: see ref. [2] for more details.

atoms by magnetoassociation [2, 3], and then transferred to their absolute ground state by Stimulated Raman Adiabatic Passage (STIRAP) [4, 5]. The procedure is illustrated schematically in Figure 1. RbCs was only the second polar molecule to be formed in this way, though several groups around the world have now succeeded in producing other ground-state alkali dimers.

We have used our gas of ultracold RbCs for microwave spectroscopy of the hyperfine structure and demonstrated coherent control of the rotational, hyperfine and Zeeman levels [6]. We have understood the crucial interplay between the hyperfine levels and the AC Stark effect due to a trapping laser [7], and we have obtained new insights into "sticky collisions" between molecules and their effects on loss rates from traps [8, 9].

We are also working to extend magnetoassociation to systems beyond the alkali dimers. We are particularly interested in molecules formed from an alkali-metal atom and a closed-shell atom such as Sr or Yb. Such molecules have both an electric and a magnetic dipole moment, and offer important possibilities for quantum simulation and quantum computing. We predicted some years ago that such systems will have magnetically tunable Feshbach resonances [10], and subsequently collaborated with the Amsterdam group in the first demonstration that the resonances are experimentally observable in Rb+Sr [11]. In Durham, we have succeeded in making mixtures of ultracold Cs and Yb, and have measured 1-photon and 2-photon photoassociation spectra to learn about the interaction potentials and scattering lengths [12, 13]. We have used the interaction potentials to make detailed predictions of the positions and properties of the Feshbach resonances [14], and we have recently succeeded in locating the first resonances, in Cs+^{173}Yb [15]. In parallel with this, we have investigated collisions of alkali-metal atoms with Yb atoms in their ^{3}P states, which offer new possibilities for resonances and molecule formation [16, 17].

The experimental group at Imperial College has developed ways to cool CaF to temperatures around 5 μK and confine it in a magnetic trap [18, 19]. We have collaborated with them to understand the hyperfine and Zeeman structure in magnetic fields [20], and shown how very long coherence times can be achieved for microwave transitions in magnetic traps [21]. We have investigated the collisions of these molecules with atoms in both magnetic [22] and magneto-optical [23] traps. We have also shown how molecules such as CaF and RbCs can be used to implement qudits (multidimensional analogues of qubits) [24].

We have done extensive work on precise interaction potentials for atomic interactions [12, 13, 25–30]. A good example of this that takes a tutorial approach is our recent paper on Na+Cs [31]. We have also worked on fundamental aspects of magnetically tunable Feshbach resonances [32–34].

Current Projects

The study of cold molecules is an extremely fast-moving field. We have specialist conferences once or twice a year at which people from the world's leading groups meet to discuss recent progress and future directions. Almost every one of these meetings turns up major new experimental directions that require theoretical input and new theory that proposes new experiments. It is therefore quite hard to predict exactly what will be of most interest in even 6 months' time. The project ideas below are based on the current state of the art, but that will change, and the projects will adapt too.

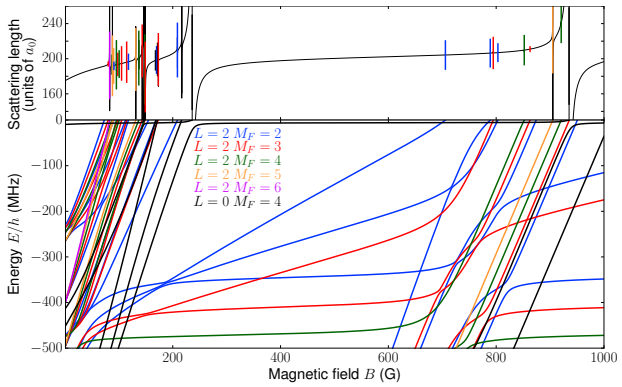

FIG. 2: Scattering length and energies of near-threshold bound states for ^{41}KCs. Resonance widths greater than 1 μG are shown as vertical bars with lengths proportional to $\log(\Delta/\mu\mathrm{G})$

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Project 1: Cooling molecules to quantum degeneracy

Our current samples of RbCs and CaF are at temperatures in the microkelvin regine, but not cold enough or dense enough for Bose-Einstein condensation or Fermi degeneracy. To achieve this, we need ways to cool them further, and the most promising candidates are evaporative cooling (by elastic collisions with other molecules the same) and evaporative cooling (by elastic collisions with other, colder, atoms or molecules). These are standard techniques for atoms, but for molecules there is an obstacle: most molecular pairs are lost from the trap when they collide, because of reactive collisions, 3-body processes, or laser absorption.

We have proposed ways to prevent these losses using shielding with microwave radiation [35]. The idea is to engineer a repulsive interaction between the molecules at long range, which prevents collisions reaching the short-range region where loss takes place. Microwave shielding has now been implemented for CaF and fermionic NaK. An alternative approach, which may be more effective, is to engineer repulsive potentials with static electric fields by bringing different rotational states of pairs of molecules into degeneracy with one another [36]. We are currently investigating this approach theoretically for CaF, with funding from our EPSRC grant on *Cooling Molecules To Quantum Degeneracy*, while an experiment is built at Imperial College.

An important aspect of this work is understanding the processes that occur at short range. Our work on microwave shielding supposed that all collisions that reach short range result in loss. However, it is likely that the short-range loss is really incomplete; rather remarkably, this can either increase or decrease the collisional loss, because of interference between the incoming and reflected waves. We have previously developed a model for handling partial short-range loss for single-channel scattering [37], which we have applied to collisions of both RbCs [8, 9] and CaF [22, 23]. We are currently working to extend these ideas to multichannel scattering, where they will have very powerful applications.

Project 2: Molecules in tweezer traps

A major goal of our Programme grant *QSUM: Quantum Science with Ultracold Molecules* is to trap ultracold molecules in arrays of optical tweezers and to use them for applications in quantum science. Tweezers will allow us to create designer arrays of ultracold molecules with chosen geometries and interactions.

We have done extensive theoretical work to help understand experiments at Harvard on forming NaCs molecules in tweezers [38, 39]. Meanwhile, the experimental group in Durham has developing an experiment to trap atom pairs in tweezers, and we have collaborated with them to investigate inelastic collisions in tweezers [40, 41]. We have very recently succeeded in forming RbCs molecules in tweezers. In parallel the group at Imperial College is working to extract CaF molecules from a magneto-optical trap into tweezers.

Atoms and molecules in tweezers pose a multitude of questions:

1. How does magnetoassociation work for a pair of atoms in a tweezer? The scattering states are converted into bound states by confinement in the potential well of the tweezer light. In addition, the relative and centre-of-mass motions of the pair are coupled. How do we calculate the resulting energy levels and the avoided crossings between them that can be used for magnetoassociation?

2. What are the energy levels of molecules in tweezers? The hyperfine structure is modified by the trapping light, whose intensity and polarization depends on position within the tweezer. This creates coupled anharmonic surfaces for the different internal states. What are the resulting motional states, and how can they be manipulated to transfer molecules to the motional ground state?

3. Once we have created designer arrays of molecules, we will want to understand the interactions between them and control their quantum states. Each molecule can be viewed as a qubit or qudit [24], according to the number of levels that can be manipulated coherently. We will want to develop ways to couple multiple qubits/qudits via the dipole-dipole interaction and manipulate them with applied electric, magnetic, microwave and laser fields.

Tools

We use a wide range of theoretical methods, ranging from molecular electronic structure theory to simulations of atomic and molecular clouds. Our greatest expertise is in *quantum calculations of atomic and molecular collisions* and the weakly bound states that are formed between pairs of atoms and molecules. We have recently published new versions of our MOLSCAT, BOUND and FIELD packages [42, 43], which are powerful general-purpose programs for carrying out quantum-mechanical bound-state and scattering calculations using coupled-channel methods. We have also made them available as open source on github [44]. The packages are very versatile, and we can often fit new types of bound-state and scattering calculations into their framework. In recent years we have adapted them to handle interactions and collisions in electric, magnetic and radiofrequency fields, and to handle atomic and molecular species of many different types.

We have a long-standing interest in *interaction potentials*. We often start with interaction potentials from the literature, or calculate our own using advance molecular electronic structure methods. The systems of interest for ultracold atoms and molecules are particularly challenging for such calculations, because they usually involve multiple electronic states and heavy, highly polarisable collision partners. Nevertheless, once high-precision experimental results become available, we usually need to refine the potentials to fit the experiments and to predict new ones. Such refinement has been crucial in many of the advances described above.

Prospects

We are in a world-leading position in the theory of both ultracold molecule formation and cold molecular collisions, and there are many leading experimental labs around the world who are keen to collaborate with us. There is much to explore in the quantum playground provided by ultracold atoms and molecules.

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