Postdoc position on the theory of ultracold molecules

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A postdoctoral position will be advertised in late 2025 to work on the theory of cold and ultracold molecules. The starting date will be as soon as convenient after March 2026.
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). Current grants include

1. Cooling molecules to quantum degeneracy (2022-26)
2. Developing Molecular Quantum Technologies (2022-26)
3. Controlling collisions between laser-cooled molecules and atoms (2025-28)
4. Leveraging Yb clock states to form lattices of $^2\Sigma$ CsYb molecules (2025-29)
5. Quantum many-body physics with ultracold polar molecules (2025-30)

These grants are joint with a variety of leading experimental and theoretical groups in the field, including the groups of Simon Cornish (Durham), Mike Tarbutt (Imperial College London) and colleagues at Harvard and JILA (Boulder, Colorado). We also have a wide network of collaborative links to experimental and theoretical groups around the world, including Birmingham, King's College London, Hannover, Innsbruck, Paris, Warsaw, Rice, Maryland and elsewhere.
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 the Quantum Light and Matter grouping in the Physics Department and the Joint Quantum Centre (JQC) Durham-Newcastle.

Ultracold Molecules

The study of ultracold molecules (below a few μK and recently as low as 6 nK) is a "hot topic" in modern physics and chemistry [2]. The potential applications of such molecules include

- 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")
- precision measurement (for 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)
- 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 provide a fascinating playground for exploring quantum ideas. Quantum devices based on them are starting to emerge, and we expect to use them for many applications in quantum science.

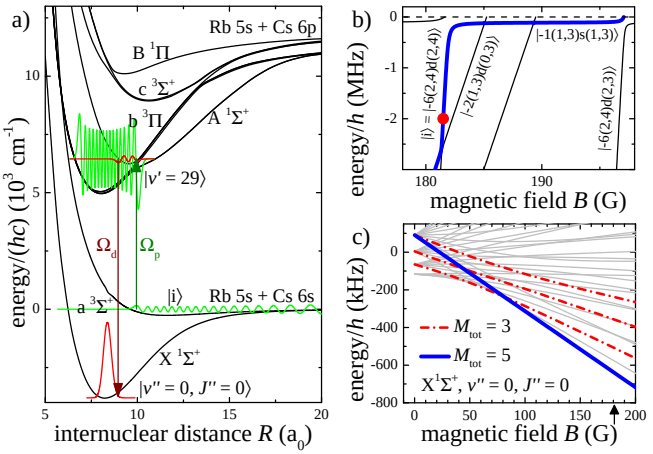

FIG. 1: Production of ground-state RbCs from ultracold Rb and Cs atoms. Top right: the way that magnetic fields are used to form "Feshbach" molecules very near dissociation and then navigate to a state suitable for ground-state transfer. Left: the 2-photon STIRAP scheme used to transfer Feshbach molecules to the absolute ground state. Bottom right: the pattern of hyperfine levels for RbCs in its rovibrational 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. [1] for more details.

Recent achievements

We have collaborated with many experimental groups to help them produce ultracold molecules. Our longest-running collaboration has been with the experimental groups in Durham and Innsbruck: we have produced ultracold RbCs molecules at temperatures around 1 μK in an optical trap [1, 3] and transferred them to their absolute ground state by Stimulated Raman Adiabatic Passage (STIRAP) [4, 5]. The procedure is illustrated schematically in Figure 1. We have used the molecules for microwave spectroscopy, understood the hyperfine structure, and demonstrated coherent control of the rotational, hyperfine and Zeeman levels [6–8]. We have achieved long coherence times needed for quantum operations, and we have obtained new insights into "sticky collisions" between molecules and their effects on loss rates from traps [9, 10].

We have a long-standing interest in producing precise interaction potentials for atomic interactions [11–20]. A recent publication that takes a tutorial approach is our paper on Na+Cs [19] on Na+Cs. We have also worked on fundamental aspects of magnetically tunable Feshbach resonances [21] and ways to characterise them theoretically [22, 23].

Mike Tarbutt's group at Imperial College can now cool CaF to temperatures around 5 μK and confine it in a magnetic trap [24, 25]. We have collaborated with them to understand the hyperfine and Zeeman structure in magnetic fields [26], and shown how very long coherence times can be achieved for microwave transitions in magnetic traps [27]. We have investigated the collisions of these molecules with atoms in both magnetic [28] and magneto-optical [29] traps. We have also shown how molecules such as CaF and RbCs can be used to implement qudits (multidimensional analogues of qubits) [30]. Most recently, we have theoretically explored resonances in collisions between CaF molecules and Rb atoms [31]. This theoretical work provided the basis for a new research grant (#3 above), which plans to implement the proposals experimentally. The newly appointed post-doc is expected to contribute to this project.

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.

Project 1: Cooling molecules to quantum degeneracy

Our current samples of RbCs and CaF are at temperatures in the microkelvin regine, but not yet 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 sympathetic 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.

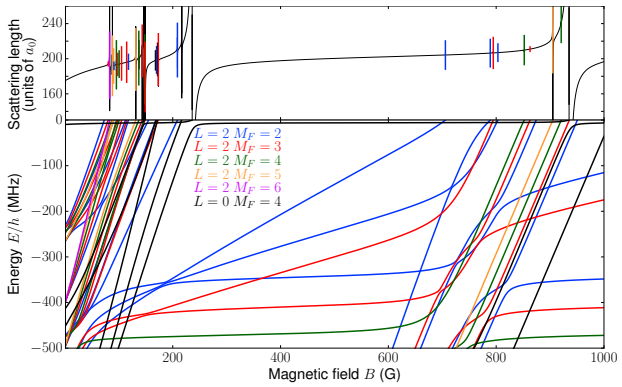

FIG. 2: Scattering length and energies of near-threshold bound states for ^{41}KCs. Resonance widths greater than 1 μG are shown as vertical bars with lengths proportional to $\log(\Delta/\mu\mathrm{G})$

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Some years ago, we proposed that these losses might be prevented by *shielding* the molecules with microwave radiation [32]. 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 recently been used to make both Fermi-degenerate gases of $Na^{40}K$ [33] and Bose-Einstein condensates of NaCs [34]. We have demonstrated that microwave shielding is in principle universal for polar molecules [35], but there are nevertheless problems in achieving the microwave frequencies and intensities needed for important molecules, including RbCs.

An alternative approach, which may avoid the difficulties, is to engineer repulsive potentials with static electric fields by bringing different rotational states of pairs of molecules into degeneracy with one another. We have shown that this approach should be very effective for CaF [36] and most of the alkali dimers [37]. We have also shown that static-field shielding offers exciting possibilities in quantum science: it works very similarly for different spin states of the molecules, so offers opportunities to implement quantum magnetism with SU(N) symmetry [38, 39]

Shielding methods are likely to be very important to future developments with ultracold molecules, so we are working intensively on extensions of them. These include

- variants of microwave shielding that can be applied to molecules such as RbCs;

- the role of spin in microwave shielding;
- the advantages of two-field shielding, combining either microwave and static fields or two different microwave fields.

Project 2: Extending magnetoassociation to new diatomic molecules
We are currently 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 opportunities for quantum simulation and quantum computing. We predicted some years ago that such systems will have magnetically tunable Feshbach resonances [40, 41], and subsequently collaborated with the Amsterdam group in the first demonstration that the resonances are experimentally observable in Rb+Sr [42]. 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 [16, 17]. We have used the interaction potentials to make detailed predictions of the positions and properties of the Feshbach resonances [43], and we have recently succeeded in locating the first resonances, in Cs+^{173}Yb [44].
Unfortunately the resonances involving ground-state Sr and Yb are extremely narrow, and it has not yet been possible to use them to make molecules by magnetoassociation. We have therefore recently investigated collisions of alkali-metal atoms with Yb atoms in their ^{3}P states, and shown that they offer new possibilities for resonances and molecule formation [45, 46]. This theoretical work provided the basis for a new research grant (#4 above), in which Simon Cornish's group will implement the proposals experimentally for Cs+Yb. We will collaborate them to model the interaction potentials, predict and interpret Feshbach resonances, and understand the spectroscopy.

Project 3: Mixtures of ultracold molecules and atoms
Mike Tarbutt's group at Imperial College London has cotrapped ultracold CaF with Rb and measured rates of inelastic loss in both magnetic and magneto-optical traps [28, 29]. We collaborated with them to interpret the results theoretically. We have also investigated the prospects of Feshbach resonances in CaF+Rb theoretically, and shown that they should exist [31]. The predicted resonances are suitable both for sympathetic cooling of CaF by Rb and for magnetoassociation to form triatomic CaFRb molecules. We have recently started a new project in which Mike Tarbutt's group will locate the resonances experimentally and use them to carry out magnetoassociation to form CaFRb. We will collaborate with them to understand the interaction potentials, Feshbach resonances and near-threshold bound states. Later in the grant, we will work to understand the electronic spectroscopy, in order to transfer the ultracold triatomic molecules to their absolute ground state.
Other Projects
We have a new EPSRC Programme Grant on *Quantum many-body physics with ultracold polar molecules*. This is a wide-ranging project with experiments in Durham and at Imperial College London and theory in Durham and Birmingham (Hannah Price's group) and King's College London (Joe Bhaseen's group). Our work on shielding (Project 1 above) fits in this Programme, but there will also be opportunities for work on other aspects of quantum science across quantum magnetism, quantum simulation, and quantum measurement.
The newly appointed post-doc(s) will be appointed with funding from the grants on CaF+Rb, CsYb and many-body physics described above, and will work principally on those. However, there will be opportunities to contribute to the other projects in the group, and new directions often emerge.

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. Our packages MOLSCAT, BOUND and FIELD [47, 48] are powerful general-purpose programs for carrying out quantum-mechanical bound-state and scattering calculations using coupled-channel methods. We have made them available as open source on github [49], with the full documentation also on arXiv [50]. 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. Most recently we have adapted them to handle collisions shielded by microwave and static electric fields.
We have a long-standing interest in *interaction potentials* for atom-atom and atom-molecule systems. We often start with interaction potentials from the literature, or calculate our own using advanced 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. 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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