

# Postdoc position on the theory of ultracold molecules

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A postdoctoral position is available to work on the theory of cold and ultracold molecules, starting as soon as convenient after January 2020. 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), Imperial College London (Ed Hinds, Mike Tarbutt and Ben Sauer), and the theory group of Dieter Jaksch at Oxford.

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 Innsbruck, Boulder, 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  $\mu$ K in an optical trap. The molecules are formed from ultracold 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

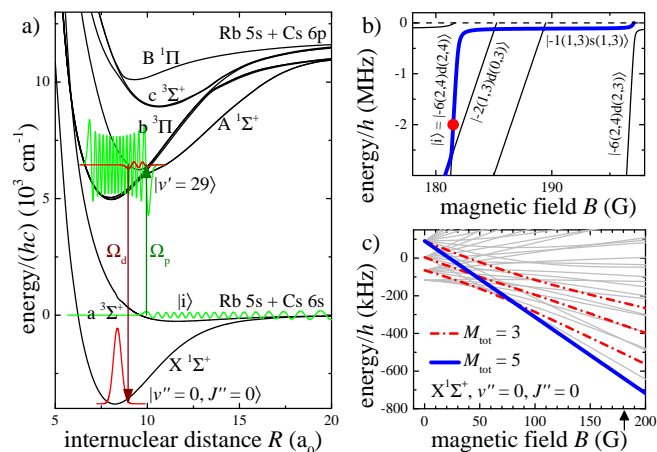


FIG. 1: Production of ground-state RbCs from ultracold Rb and Cs atoms. Top right: the way that magnetic fields are used to form “Feshbach” molecules very near dissociation and then navigate to a state suitable for ground-state transfer. Left: the 2-photon STIRAP scheme used to transfer Feshbach molecules 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.

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 have proposed ways to prevent these losses using shielding with microwave radiation [10].

In parallel with this, the group in London has developed ways to cool CaF to temperatures around  $5 \mu\text{K}$  and confine it in a magnetic trap [11, 12]. We have collaborated with them to understand the hyperfine and Zeeman structure in magnetic fields [13], and shown how very long coherence times can be achieved for microwave transitions in magnetic traps [14]. We have also shown how molecules such as CaF and RbCs can be used to implement qudits (multidimensional analogues of qubits) [15].

We have also done extensive work on precise interaction potentials for atomic interactions [16–22] and on fundamental aspects of magnetically tunable Feshbach resonances [23–25].

### 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: Extending molecule formation to other species: KCs and CsYb*

Our gas of ultracold RbCs opens up many new possibilities, but it has fairly low density. Its density is limited by an unlucky coincidence: the interspecies scattering length for  $^{87}\text{Rb} + \text{Cs}$  is large and positive, so that clouds of the two atoms are hard to overlap (and a mixed BEC phase-separates). We are therefore working to extend molecule formation to KCs, which does not have this problem. In an initial theoretical study, we predicted Feshbach resonances in all three isotopic combinations ( $^{39}\text{KCs}$ ,  $^{40}\text{KCs}$  and  $^{41}\text{KCs}$ ) and studied the miscibility of the atomic mixtures [26]. More recently, the Innsbruck group measured the first Feshbach resonances in  $^{39}\text{KCs}$ , and we adjusted the KCs interaction potentials to make improved predictions of other resonances and miscibility [27]. The new predictions for resonance positions and bound-state energy levels of  $^{41}\text{KCs}$  are shown in Figure 2. Simon Cornish’s experimental group in Durham is

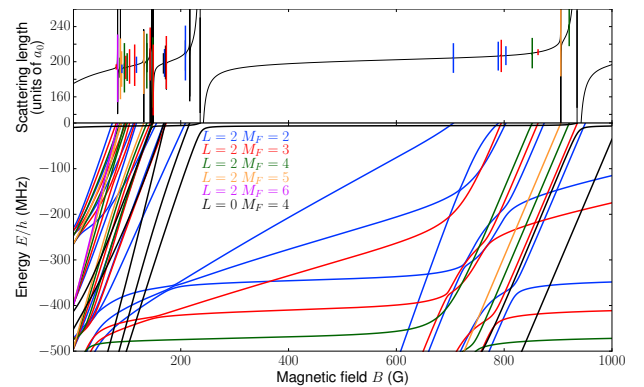


FIG. 2: Scattering length and energies of near-threshold bound states for  $^{41}\text{KCs}$ . Resonance widths greater than  $1 \mu\text{G}$  are shown as vertical bars with lengths proportional to  $\log(\Delta/\mu\text{G})$

currently constructing a KCs apparatus; we will collaborate with them and with the Innsbruck group to form ultracold KCs molecules, transfer them to their absolute ground state, and explore their properties.  $^{40}\text{KCs}$  has the particular advantage that the molecules are *fermionic*, and gases of dipolar fermions have many potential applications.

Molecules formed from pairs of alkali-metal atoms have singlet ground states, with no net electron spin and no significant magnetic moment. We would like to form molecules with both an electric and a magnetic dipole moment, which offer important possibilities for quantum simulation and quantum computing. We are therefore working to form CsYb molecules, which have a  $^2\Sigma$  ground state (with electron spin  $S = \frac{1}{2}$ ). We predicted some years ago that such systems will have magnetically tunable Feshbach resonances [28], and recently collaborated with the Amsterdam group in the first demonstration that the resonances are experimentally observable Rb+Sr [29].

We have now succeeded in making mixtures of ultracold Cs and Yb in Durham. We have measured 1-photon and 2-photon photoassociation spectra and interpreted them to learn about the interaction potentials and scattering lengths [21, 22]. We have now used the interaction potentials to make detailed predictions of the positions and properties of the Feshbach resonances [30]. We are now searching for the Feshbach resonances experimentally; once they are found, it will open up a new set of challenges for both experiment and theory.

#### *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 are approaching this in two different ways. The experimental group in Durham is developing an experiment to form RbCs molecules in tweezers, and the group in London is working to extract CaF molecules from a magneto-optical trap into tweezers. Both these experiments should produce their first results soon.

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 crossing between them that will 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 [15], 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 [31, 32], 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 [33]. 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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- [1] R. V. Krems, W. C. Stwalley, and B. Friedrich. *Cold Molecules: Theory, Experiment, Applications*. (Taylor & Francis, London, 2009).
  - [2] T. Takekoshi, M. Debatin, R. Rameshan, F. Ferlaino, R. Grimm, H.-C. Nägerl, C. R. Le Sueur, J. M. Hutson, P. S. Julienne, S. Kotochigova, and E. Tiemann. ‘Towards the production of ultracold ground-state RbCs molecules: Feshbach resonances, weakly bound states, and coupled-channel models.’ *Phys. Rev. A* **85**, 032506 (2012).
  - [3] M. P. Köppinger, D. J. McCarron, D. L. Jenkin, P. K. Molony, H.-W. Cho, S. L. Cornish, C. R. Le Sueur, C. L. Blackley, and J. M. Hutson. ‘Production of optically trapped  $^{87}\text{Rb}^{133}\text{Cs}$  Feshbach molecules.’ *Phys. Rev. A* **89**, 033604 (2014).
  - [4] P. K. Molony, P. D. Gregory, Z. Ji, B. Lu, M. P. Köppinger, C. R. Le Sueur, C. L. Blackley, J. M. Hutson, and S. L. Cornish. ‘Creation of ultracold  $^{87}\text{Rb}^{133}\text{Cs}$  molecules in the rovibrational ground state.’ *Phys. Rev. Lett.* **113**, 255301 (2014).
  - [5] T. Takekoshi, L. Reichsöllner, A. Schindewolf, J. M. Hutson, C. R. Le Sueur, O. Dulieu, F. Ferlaino, R. Grimm, and H.-C. Nägerl. ‘Ultracold dense samples of dipolar RbCs molecules in the rovibrational and hyperfine ground state.’ *Phys. Rev. Lett.* **113**, 205301 (2014).
  - [6] P. D. Gregory, J. Aldegunde, J. M. Hutson, and S. L. Cornish. ‘Controlling the rotational and hyperfine state of ultracold  $^{87}\text{Rb}^{133}\text{Cs}$  molecules.’ *Phys. Rev. A* **94**, 041403(R) (2016).
  - [7] P. D. Gregory, J. A. Blackmore, J. Aldegunde, J. M.

- Hutson, and S. L. Cornish. ‘ac Stark effect in ultracold polar  $^{87}\text{Rb}^{133}\text{Cs}$  molecules.’ *Phys. Rev. A* **96**, 021402(R) (2017).
- [8] M. D. Frye, P. S. Julienne, and J. M. Hutson. ‘Cold atomic and molecular collisions: approaching the universal loss regime.’ *New J. Phys.* **17**, 045019 (2015).
- [9] P. D. Gregory, M. D. Frye, J. A. Blackmore, E. M. Bridge, R. Sawant, J. M. Hutson, and S. L. Cornish. ‘Are ultracold molecular collisions sticky?’ *Nature Comm.* **10**, 3104 (2019).
- [10] T. Karman and J. M. Hutson. ‘Microwave shielding of ultracold polar molecules.’ *Phys. Rev. Lett.* **121**, 163401 (2018).
- [11] S. Truppe, H. J. Williams, M. Hambach, L. Caldwell, N. J. Fitch, E. A. Hinds, B. E. Sauer, and M. R. Tarbutt. ‘Molecules cooled below the Doppler limit.’ *Nature Physics* **13**, 1173 (2017).
- [12] H. J. Williams, L. Caldwell, N. J. Fitch, S. Truppe, J. Rodewald, E. A. Hinds, B. E. Sauer, and M. R. Tarbutt. ‘Magnetic trapping and coherent control of laser-cooled molecules.’ *Phys. Rev. Lett.* **120**, 163201 (2018).
- [13] J. A. Blackmore, L. Caldwell, P. D. Gregory, E. M. Bridge, R. Sawant, J. Aldegunde, J. Mur-Petit, D. Jaksch, J. M. Hutson, B. E. Sauer, M. R. Tarbutt, and S. L. Cornish. ‘Ultracold molecules: a platform for quantum simulation.’ *Quantum Sci. Technol.* **4**, 014010 (2019).
- [14] L. Caldwell, H. J. Williams, N. J. Fitch, J. Aldegunde, J. M. Hutson, B. E. Sauer, and M. R. Tarbutt. ‘Long rotational coherence times of molecules in a magnetic trap.’ *arXiv:1908.11839* (2019).
- [15] R. Sawant, J. A. Blackmore, P. D. Gregory, J. Mur-Petit, D. Jaksch, J. Aldegunde, J. M. Hutson, M. R. Tarbutt, and S. L. Cornish. ‘Ultracold molecules as qudits.’ *arXiv:1909.07484* (2019).
- [16] M. Berninger, A. Zenesini, B. Huang, W. Harm, H.-C. Nägerl, F. Ferlaino, R. Grimm, P. S. Julienne, and J. M. Hutson. ‘Feshbach resonances, weakly bound molecular states and coupled-channel potentials for cesium at high magnetic field.’ *Phys. Rev. A* **87**, 032517 (2013).
- [17] G. Zürn, T. Lompe, A. N. Wenz, S. Jochim, P. S. Julienne, and J. M. Hutson. ‘Precise characterization of  $^6\text{Li}$  Feshbach resonances using trap-sideband-resolved rf spectroscopy of weakly bound molecules.’ *Phys. Rev. Lett.* **110**, 135301 (2013).
- [18] P. S. Julienne and J. M. Hutson. ‘Contrasting the wide Feshbach resonances in  $^6\text{Li}$  and  $^7\text{Li}$ .’ *Phys. Rev. A* **89**, 052715 (2014).
- [19] J. J. Lutz and J. M. Hutson. ‘Deviations from Born-Oppenheimer mass scaling in spectroscopy and ultracold molecular physics.’ *J. Mol. Spectrosc.* **330**, 43 (2016).
- [20] A. Guttridge, S. A. Hopkins, S. L. Kemp, M. D. Frye, J. M. Hutson, and S. L. Cornish. ‘Interspecies thermalization in an ultracold mixture of Cs and Yb in an optical trap.’ *Phys. Rev. A* **96**, 012704 (2017).
- [21] A. Guttridge, S. A. Hopkins, M. D. Frye, J. J. McFerran, J. M. Hutson, and S. L. Cornish. ‘Production of ultracold Cs\*Yb molecules by photoassociation.’ *Phys. Rev. A* **97**, 063414 (2018).
- [22] A. Guttridge, M. D. Frye, B. C. Yang, J. M. Hutson, and S. L. Cornish. ‘Two-photon photoassociation spectroscopy of CsYb: ground-state interaction potential and interspecies scattering lengths.’ *Phys. Rev. A* **98**, 022707 (2018).
- [23] J. M. Hutson. ‘Feshbach resonances in the presence of inelastic scattering: threshold behavior and suppression of poles in scattering lengths.’ *New J. Phys.* **9**, 152 (2007).
- [24] M. D. Frye and J. M. Hutson. ‘Characterizing Feshbach resonances in ultracold scattering calculations.’ *Phys. Rev. A* **96**, 042705 (2017).
- [25] M. D. Frye and J. M. Hutson. ‘Time delays in ultracold atomic and molecular collisions.’ *arXiv:1907.10653* (2019).
- [26] H. J. Patel, C. L. Blackley, S. L. Cornish, and J. M. Hutson. ‘Feshbach resonances, molecular bound states, and prospects of ultracold-molecule formation in mixtures of ultracold K and Cs.’ *Phys. Rev. A* **90**, 032716 (2014).
- [27] M. Gröbner, P. Weinmann, E. Kirilov, H.-C. Nägerl, P. S. Julienne, C. R. Le Sueur, and J. M. Hutson. ‘Observation of interspecies Feshbach resonances in an ultracold  $^{39}\text{K}$ - $^{133}\text{Cs}$  mixture and refinement of interaction potentials.’ *Phys. Rev. A* **95**, 022715 (2017).
- [28] P. S. Żuchowski, J. Aldegunde, and J. M. Hutson. ‘Ultracold RbSr molecules can be formed by magnetoassociation.’ *Phys. Rev. Lett.* **105**, 153201 (2010).
- [29] V. Barbé, A. Ciamei, B. Pasquiou, L. Reichsöllner, F. Schreck, P. S. Żuchowski, and J. M. Hutson. ‘Observation of Feshbach resonances between alkali and closed-shell atoms.’ *Nature Physics* **14**, 881 (2018).
- [30] B. C. Yang, M. D. Frye, A. Guttridge, J. Aldegunde, P. S. Żuchowski, S. L. Cornish, and J. M. Hutson. ‘Magnetic Feshbach resonances in ultracold collisions between Cs and Yb atoms.’ *Phys. Rev. A* **100**, 022704 (2019).
- [31] J. M. Hutson and C. R. Le Sueur. ‘MOLSCAT: a program for non-reactive quantum scattering calculations on atomic and molecular collisions.’ *Comp. Phys. Comm.* **241**, 9 (2019).
- [32] J. M. Hutson and C. R. Le Sueur. ‘BOUND and FIELD: programs for calculating bound states of interacting pairs of atoms and molecules.’ *Comp. Phys. Comm.* **241**, 1 (2019).
- [33] J. M. Hutson and C. R. Le Sueur. ‘MOLSCAT, BOUND and FIELD, version 2019.0.’ <https://github.com/molscat/molscat> (2019).