

# EuroQUAM Satellite Meeting on Cold and Ultracold Molecules

Durham University  
17-18 April, 2009



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## Programme

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### *Friday 17 April*

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|---------------|-------------------------------------|
| 13:30 – 15:00 | Scientific committee meeting        |
| 15:00 – 17:00 | Laboratory tours                    |
| 18:30 – 20:00 | Tour of Durham Cathedral            |
| 20:00 – 22:00 | Dinner at the Undercroft Restaurant |
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### *Saturday 18 April*

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|--------------|-------------------------------|
| 9:15 – 17:45 | Conference talks              |
| 19:30 –      | Dinner at Collingwood College |
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## Schedule of talks - Saturday 18 April

9:15	<b>Cold and ultracold polar molecules.</b> Jun Ye JILA, National Institute of Standards and Technology and University of Colorado.	<i>Keynote Talk</i>
10:00	<b>Hyperfine-changing collisions of cold molecules.</b> Jesus Aldegunde Department of Chemistry, Durham University, UK.	<i>ColPolMol</i>
10:30	Morning Coffee	
11:00	<b>Observation of an Efimov spectrum in an atomic system.</b> Matteo Zaccanti LENS and Physics Department, Università di Firenze, Italy.	<i>QuDipMol</i>
11:30	<b>Cavity cooling of the internal and external motion of molecules.</b> Regina de Vivie-Riedle Ludwig-Maximilians-Universität München, Germany.	<i>CMMC</i>
12:00	<b>Towards sympathetic cooling of molecules with ultracold atoms.</b> Adela Marian Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.	<i>ColPolMol</i>
12:30	Lunch	
2:00	<b>Understanding Feshbach molecules with long range quantum defect theory.</b> Paul Julienne National Institute of Standards and Technology, Gaithersburg, USA.	<i>Keynote Talk</i>
2:45	<b>Interacting Bosonic and Fermionic atoms in 3D optical lattice potentials.</b> Sebastian Will Johannes Gutenberg-Universität Mainz, Mainz, Germany.	<i>DQS</i>
3:15	<b>Collisional properties of heteronuclear mixtures with resonant interspecies interaction.</b> Jesper Levinsen Université Paris Sud, Orsay, France.	<i>Fermix</i>
3:45	Afternoon Tea	
4:15	<b>Critical fluctuations of an attractive Bose gas in a double well potential.</b> Marek Trippenbach Institute of Theoretical Physics, Warsaw University, Warsaw, Poland.	<i>CIGMA</i>
4:45	<b>Cold guided beams of polar molecules.</b> Laurens van Buuren Max-Planck-Institut für Quantenoptik, Garching, Germany	<i>CMMC</i>
5:15	<b>What do you care about what molecules are?</b> Olivier Dulieu Laboratoire Aimé Cotton (LAC), Orsay, France.	<i>QuDipMol</i>
5:45	Close	

## Abstracts (in alphabetical order)

### **Hyperfine-Changing Collisions of Cold Molecules**

*J. Aldegunde and Jeremy M. Hutson*

Department of Chemistry, Durham University, Science Laboratories, South Road, Durham DH1 3LE, UK.

What are the hyperfine energy levels of alkali dimers and how stable are they to collisions are questions of great interest for the ultracold community. Their relevance lies in the fact that, if we wish to produce a molecular quantum gas from a handful of ultracold dimers, all the molecules must be in the same hyperfine state and be stable to collisions. The results we present, consisting of a description of the hyperfine structure of the alkali molecules and on preliminary results about their scattering behaviour, will help to answer these questions.

### **Cold guided beams of polar molecules.**

*L.D. van Buuren, M. Motsch, C. Sommer, M. Zeppenfeld, S. Pohle, M. Schenk, J. Bayerl, P.W.H. Pinkse, G. Rempe*

Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany.

Cold molecules offer new perspectives for fields of research ranging from chemistry, spectroscopy to astrophysics. To this end many methods have been developed to produce cold samples of natural polar molecules. Of these, the electrostatic velocity filtering and guiding method by means of a quadrupole electrostatic guide [1], stands out by the relative simplicity of the technique, the continuous character of the produced beams and the relatively high fluxes that can be obtained.

Recently, we have significantly increased our understanding of the guiding and filtering technique by studying the parameter dependence of the guided molecule flux [2]. The data, measured at various source pressures, are in good agreement with our model which takes into account collisions between guidable slow and non-guidable fast molecules in the vicinity of the source exit. These studies therefore allow for optimization of the source depending on the requirements of the application.

Apart from its dependence on collisions during the beam formation, the detector signal exhibits a characteristic dependence on the strength of the applied guiding fields for different classes of molecules. This is demonstrated strikingly by the comparison between the three water isotopologs  $\text{H}_2\text{O}$ ,  $\text{D}_2\text{O}$ , and  $\text{HDO}$  [3]. In contrast to  $\text{HDO}$ , whose permanent electric dipole moment is not parallel to the molecule principal axis, the Stark shifts of  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  are purely quadratic and hence weaker than that of  $\text{HDO}$ . The observed signals are in excellent agreement with our theoretical predictions. For the water isotopologs, the beams consist of molecules in only a few rotational states.

To be able to increase the population in the lowest guidable states of molecules, we have combined the electrostatic velocity filtering and guiding technique with buffer-gas cooling. In this set up, the molecules are cooled by collisions with a cryogenic helium gas before they enter the guide [4]. A strong increase in state purity is demonstrated in a laser depletion experiment with formaldehyde. With this technique we measure the rotational state distribution by sequentially depleting individual rotational states in a guided beam with a UV laser beam tuned to selected transitions [5].

In the future, our continuous beams of cold molecules can be employed to perform high-precision experiments, to study state-specific cold collisions, and to load traps in which novel cooling techniques might bring them to the ultracold regime.

[1] T. Junglen, T. Rieger, S.A. Rangwala, P.W.H. Pinkse, G. Rempe, *Eur. Phys. J. D*, 2004, 31, 365

[2] M. Motsch, C. Sommer, M. Zeppenfeld, L.D. van Buuren, P.W.H. Pinkse, G. Rempe, accepted for publication in *New Journal of Physics*; arXiv: 0812.2850

[3] M. Motsch, L.D. van Buuren, C. Sommer, M. Zeppenfeld, G. Rempe, P.W.H. Pinkse, *Phys. Rev. A*, 2009, 79, 013405

[4] C. Sommer, L.D. van Buuren, M. Motsch, S. Pohle, J. Bayerl, P.W.H. Pinkse, G. Rempe, *Faraday Discussions* 142: Cold and Ultracold Molecules; arXiv: 0812.1923

[5] L.D. van Buuren, C. Sommer, M. Motsch, S. Pohle, M. Schenk, J. Bayerl, P.W.H. Pinkse, G. Rempe, *Phys. Rev. Lett.*, 2009, 102, 033001

## **What do you care about what molecules are?**

**Olivier Dulieu**

Laboratoire Aimé Cotton (LAC), Orsay, France.

The field of cold and ultracold molecules has recently witnessed a number of spectacular advances reliant upon the high quality of our knowledge of molecular structure at a very fundamental level. This talk will illustrate this premise in the context of the current meeting, highlighting the characteristics of molecules that we all care about.

## **Understanding Feshbach molecules with long range quantum defect theory**

**Paul S. Julienne**, *Thomas Hanna and Eite Tiesinga*

National Institute of Standards and Technology (NIST), 100 Bureau Drive, Gaithersburg, Maryland, USA.

Understanding the interactions of two ultracold species requires understanding the states in the long-range potentials associated with the species. In particular, van der Waals quantum defect theory offers a very powerful and simple tool to characterize the near-threshold bound and scattering states of two atoms, including weakly bound Feshbach molecules. Such molecules serve as a gateway to forming more deeply bound polar molecules. In addition to allowing a classification of Feshbach molecules, the theory allows an approximate calculation of all the resonances in all collision channels using a knowledge of only three parameters, namely, the van der Waals coefficient and singlet and triplet scattering lengths, plus the known atomic hyperfine splittings and the analytic frame transformation between the atomic and molecular basis sets. The quantum defect results will be compared to full coupled channels calculations.

## **Towards sympathetic cooling of molecules with ultracold atoms.**

**Adela Marian**, *Henrik Haak, Sophie Schlunk, Wieland Schöllkopf, and Gerard Meijer*

Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6, 14195 Berlin, Germany.

We are aiming to combine an existing cold-atom apparatus with a molecular beam machine in order to pursue sympathetic cooling of molecules with ultracold atoms using spatially overlapped traps. To this end, we have recently demonstrated that a magnetic trap for atoms can be spatially overlapped with an AC electric trap. Moreover, we have experimentally verified that the magnetically trapped atoms are not perturbed by the AC electric fields needed for trapping molecules.

In this talk, I will briefly present our results on AC electric trapping. Then, I will describe a new design for a Stark decelerator that we have developed especially for the sympathetic cooling experiment, in conjunction with a compact ultrahigh vacuum molecular beam apparatus. The new decelerator can accommodate all the spatial and vacuum requirements imposed by the atom apparatus.

## **Collisional properties of heteronuclear mixtures with resonant interspecies interaction.**

**Dmitry Petrov**

Laboratoire LPTMS, Université Paris-Sud, Bat. 100, 91405 Orsay Cedex, France.

We consider a heteronuclear Fermi-Fermi mixture close to an interspecies Feshbach resonance and discuss atom-dimer scattering properties in the presence of an external confining potential, restricting the system to a quasi-2D geometry. We find that there is a peculiar atom-dimer p-wave resonance which can be tuned by changing the frequency of the confinement. Our results have implications for the ongoing experiments on Li-K mixtures, where this mechanism can be used to switch the p-wave interaction between a K atom and a Li-K dimer from attractive to repulsive.

## Critical fluctuations of an attractive Bose gas in a double well potential

*M. Trippenbach, P. Zin, J. Chwedenczuk, B. Oles and K. Sacha*

Institute of Theoretical Physics, Physics Department, Warsaw University, Hoza 69, PL-00-681 Warsaw, Poland.

We consider a Bose gas with an attractive interaction in a symmetric double well potential. In the mean field approximation, the ground state solution spontaneously breaks the symmetry of the trapping potential above certain value of the interaction strength. We demonstrate how the Landau-Ginzburg scheme of the second order phase transition emerges from the quantum model and show the link to the spontaneous symmetry breaking mentioned above. We identify the order parameter, the critical point and analyze quantum fluctuations around it.

## Cavity cooling of the internal and external motion of molecules

*R. de Vivie-Riedle<sup>1</sup>, M. Kowalewski<sup>1</sup>, G. Morigi<sup>2</sup>, P.W.H. Pinkse<sup>3</sup>*

<sup>1</sup>Department für Chemie und Biochemie, Ludwig-Maximilians-Universität München, Germany.

<sup>2</sup>Departament de Física, Universitat Autònoma de Barcelona, Spain.

<sup>3</sup>Max-Planck Institut für Quantenoptik, Garching, Germany.

Ultracold molecules play an important role in quantum information processing, astrochemistry, high-resolution spectroscopy, cold collisions and cold chemistry. Major quantum effects and new quantum phases are expected in the ultracold regime. The preparation of cold molecules, however, is still challenging. Due to the absence of closed transitions in molecules, classical laser cooling schemes successful for atoms are not suitable for molecules. Beyond the well established nonoptical cooling methods [1,2], only few laser cooling methods have been proposed taking into account the details of the internal molecular structure [3, 4]. First we present our theoretical approach for the cooling of the internal molecular degrees of freedom in a cavity using far off-resonant Raman transitions [3]. Excited rovibrational levels are depopulated by vacuum-stimulated anti-Stokes Raman scattering into the mode of a high-finesse cavity. We take into account the competing effects of spontaneous and coherent Raman processes amplified by the cavity. The scheme provides a flexible cooling method concerning the laser wavelength. It works for rotational as well as for vibrational levels and allows simultaneous cooling of the external degrees of freedom [5]. In the second part we introduce a new alternative approach for cavity mediated cooling of molecules confined in harmonic traps. The idea is to use vibrational transitions in the infrared regime for sideband cooling of translational motion. The scheme introduced in [6], in essence a cavity-enhanced version of side-band cooling in the Lamb-Dicke regime, is applied to vibrational levels of a molecule to form an almost closed cooling cycle. The equations are evaluated for a set of polar polyatomic molecules and a realistic optical cavity in the infrared. Ab initio methods are used to determine transition dipole moments of the rovibrational modes, their lifetimes and their polarizabilities. Based on these data, we select a set of suitable molecules for the cooling process. We simulate the scheme in two different types of traps. First neutral molecules trapped by an optical potential are considered. Possible trap depths for a given set of laser parameters are evaluated. Secondly the scheme is used for optical cooling of charged molecules in ion traps. The theoretical results predict cooling of molecular ions into the ground state of the trap on a sub-millisecond time scale.

[1] J. Doyle, B. Friedrich, R.V. Krems, and F. Masnou-Seeuws, "Editorial: Quo vadis, cold molecules?" *Eur. Phys. J. D* **31**, 149–164 (2004).

[2] O. Dulieu, M. Raoult, and E. Tiemann, *J. Phys. B* **39**, 19 (2006).

[3] G. Morigi, P. W. H. Pinkse, M. Kowalewski, R. de Vivie-Riedle, *Phys. Rev. Lett.* **99**, 073001 (2007).

[4] J. T. Bahns, W. C. Stwalley, and P. L. Gould, *J. Chem. Phys.* **104**, 9689 (1996).

[5] V. Vuletić, S. Chu, *Phys. Rev. Lett.* **84**, 3787 (2000).

[6] S. Zippilli, G. Morigi, *Phys. Rev. Lett.* **95**, 143001 (2005).

## **Interacting Bosonic and Fermionic Atoms in 3D Optical Lattice Potentials**

*Sebastian Will, Thorsten Best, Simon Braun, Ulrich Schneider, Kin Chung Fong, Lucia Hackermüller, and Immanuel Bloch*

Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany.

In recent years, ultracold atoms in optical lattices have begun to reveal their potential to simulate condensed matter systems with the exceptional control offered by atomic physics. With our apparatus we perform experiments directed towards quantum simulation using ultracold bosonic  $^{87}\text{Rb}$  and fermionic  $^{40}\text{K}$  atoms loaded to a 3D optical lattice, that features tunability of the underlying harmonic confinement. Additionally harnessing intra- and interspecies Feshbach resonances as a direct control knob for interactions, we investigate strongly interacting quantum systems along several routes: Using repulsively interacting  $^{40}\text{K}$  Fermi-Fermi mixtures we have been able to realize an implementation of the Fermi Hubbard model. A direct measurement of compressibility allowed us to identify metallic, Fermi liquid and band insulating phases as well as an emergent Mott insulating phase in the strongly interacting regime. In  $^{87}\text{Rb}$ - $^{40}\text{K}$  Bose-Fermi mixtures with tunable interspecies interactions we have characterized the previously observed shift of the bosonic superfluid to Mott insulating transition and found interaction-induced self-trapping to be the dominant cause. Recently, we have been able to peek beyond the single-band Hubbard model in a purely bosonic  $^{87}\text{Rb}$  system: The investigation of quantum phase diffusion in a deep lattice made interaction-induced multi-band physics directly observable and allowed us to visualize number-squeezed many-body states upon approaching the bosonic Mott insulator. These results and the current status of our efforts will be presented.

## **Cold and ultracold polar molecules**

*Jun Ye*

JILA, National Institute of Standards and Technology and University of Colorado, Boulder, Colorado 80309-0440, USA.

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Study of ultracold molecules promises important prospects such as novel control of chemical reactions and molecular collisions, precision measurement of fundamental physical properties, and new methods for quantum information processing and simulations of quantum states of matter. A variety of chemically interesting molecular species can be prepared in a single internal state at temperatures of a few milliKelvins. Located in a magnetic trap and polarized under a uniform electric field, these molecules now allow explorations of low-energy scatterings near the quantum threshold and they will be subject to studies of collision and reaction dynamics that are dominated by long-range, anisotropic dipolar interactions.

A quantum degenerate gas of polar molecules will greatly facilitate these activities. Towards this goal, we start with an ultracold dual-species atomic gas mixture near quantum degeneracy. Combining Feshbach resonance and optical Raman transfer, we achieve highly efficient, fully coherent conversion of the ultracold Rb-K atom pairs to polar molecules in their absolute ro-vibrational ground state. The resultant molecular gas has basically the same phase space density as the original dual-species atomic gases, with a trapped density of  $10^{12} \text{ cm}^{-3}$  at a temperature of 300 nK and a measured permanent electric dipole moment of 0.5 Debye. These molecules can also be prepared in a single nuclear spin state and preliminary ultracold collisions will be discussed.

## **Observation of an Efimov spectrum in an atomic system.**

***Matteo Zaccanti***

LENS and Physics Department, Università di Firenze, and INFN-CNR, Via Nello Carrara 1, 50019 Sesto Fiorentino, Italy.

In 1970 the Russian physicist V. Efimov predicted a puzzling quantum-mechanical effect that is still of great interest today. He found that three particles subjected to a resonant pairwise interaction can join into an infinite number of loosely bound states even though each particle pair cannot bind. Interestingly, the properties of these aggregates, such as the peculiar geometric scaling of their energy spectrum, are universal, i.e. independent of the microscopic details of their components. Despite an extensive search in many different physical systems, including nuclei, atoms and molecules, Efimov spectra still elude observation. Here we report on the discovery of two bound trimer states of potassium atoms very close to the Efimov scenario, which we reveal by studying three-particle collisions in an ultracold gas. Our observation provides the first evidence of an Efimov spectrum and allows a direct test of its scaling behaviour, shedding new light onto the physics of few-body universal systems.

## List of Participants

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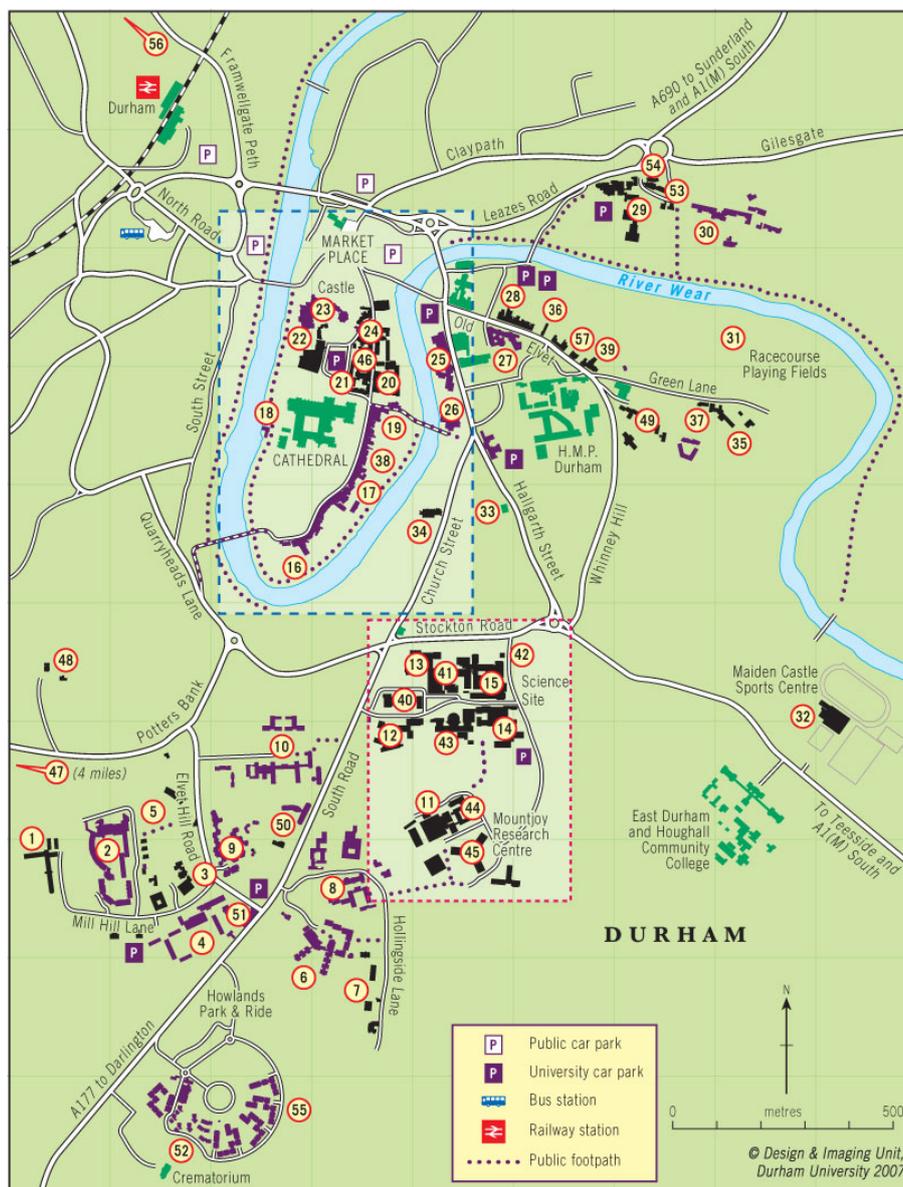
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## Local and Travel Information

- Laboratory tours: meet in the entrance to the physics department (40 on map) at 15:00.  
Contact: David Carty (david.carty@durham.ac.uk)
- Tour of Durham Cathedral: we will walk to the Cathedral from the Science site leaving from the entrance to physics department (12 on map) at 18:00 sharp!
- Talks: all presentations will be held in lecture theatre Ph8 in the physics department (12 on map)
- Accommodation: all attendees will be housed in Collingwood College (6 on map).



### Useful travel links:

- Travelling to Durham with links to further maps: <http://www.dur.ac.uk/travel/todurham/>
- Newcastle airport: <http://www.newcastleairport.com/>
- Metro link from Newcastle airport to city centre: <http://www.nexus.org.uk/wps/wcm/connect/Nexus/Metro/>
- National rail enquiries: <http://www.nationalrail.co.uk/>