RESEARCH CONFERENCES

ESF Conference in Partnership with LFUI

Cold and Ultracold Molecules

18-23 November 2012
Universitätszentrum Obergurgl, Austria

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SFB FoQuS Foundations and Applications of Quantum Science

Conference Highlights

Please provide a brief summary of the conference and its highlights in non-specialist terms (especially for highly technical subjects) for communication and publicity purposes. (ca. 400-500 words)

During the last 15 years spectacular advances have been made in controlling quantum systems composed of atomic constituents, revolutionizing the field of traditional atomic, molecular, and optical physics and opening up new and spectacular avenues in such diverse areas as precision spectroscopy, quantum information, quantum many-body and condensed matter physics. The challenge is now to reach the same level of control in molecular systems, for which the presence of additional microscopic degrees of freedom promises a new era for quantum physics and chemistry. In this emerging, strongly multi-disciplinary field, challenges range from the production of cold and ultracold molecules to the application of these cold and ultracold molecules to precision spectroscopy, few-body and many-body quantum physics, chemical physics, and quantum chemistry. The conference “Cold and Ultracold Molecules” (COLUM2012) has brought together top scientists and young researchers from these diverse fields, who are now contributing to an increasing extent to developing new ideas and approaches for the realization of cold and ultracold molecular gases and to identifying new research directions and applications of these novel systems.

Progress in the field of cold molecular physics in the last few years has been astounding. The very high level of the talks at COLUMN2012, the vivacity of the ensuing discussions and of those at the poster sessions are all witnesses of the enthusiasm and talent of researchers in the field, and a clear sign of the success for the conference. Several breakthroughs in experiments and theory have been presented at COLUMN2012, sometimes for the first time in Europe and internationally. Highlights have been numerous, including the presentation of novel cooling techniques for complex, multi-atomic molecules, such as CH_3F molecules, at the Max Planck Institute in Munich, and of very recent results on evaporative cooling of OH radicals and KRb molecules at JILA in the US. These results for very different systems are key steps towards the realization of a quantum degenerate gas of polar molecules, one of the Holy Grails in the field. Exchanges of ideas between theorists and experimentalists have led to proposals for novel cooling techniques based on superradiance in molecules or sympathethic cooling in mixtures of hot molecules and cold Rydberg atoms. Cutting edge ideas included proposals for the realization of exotic phases of matter with dipolar quantum gases, the control of few- and many-body dynamics in these systems, including the first steps towards control of chemical reactions in the ultracold regime – a new and exciting field of research in its own. At low and ultralow temperatures, molecules are being prepared in specific quantum states for their internal degrees of freedom and their external motion. Thus, molecular interactions and reactions involving single quantum states can now be studied and controlled, and the goal is thus to “quantum engineer” chemical processes. The conference COLUMN2012 has been structured to initiate and foster intensive collaborations, in particular between theory and experiment. These collaborations will be an essential ingredient for the overall progress of all of these novel highly interdisciplinary fields.

X I hereby authorize ESF – and the conference partners to use the information contained in the above section on ‘Conference Highlights’ in their communication on the scheme.

Scientific Report

Executive Summary

(2 pages max)

The production of ultracold ensembles of atoms has revolutionized the field of atomic and optical physics and condensed matter physics. The impact of creating ultracold molecules is expected to be at least as large and profound as that made by ultracold atoms. In fact, molecules offer microscopic degrees of freedom absent in atomic gases. This gives ultracold molecular gases unique properties that may allow for the study of new physical phenomena reaching far beyond the focus of traditional molecular science.

In the zero-temperature limit, molecular systems promise the realization of complex but controllable quantum many-body systems, the engineering of novel few-body and many-body quantum states, the implementation of quantum-controlled, state-selective chemistry, and the realization of scalable quantum information schemes with high potential for future technologies in a knowledge-based society. With a large number of recent publications in journals such as Nature, Science, Physical Review Letters and Physical Review Focus, this area of research is well recognized by the scientific community.

The conference “Cold and Ultracold Molecules“ has provided talks from some of the world’s leading experts, as well as from young very promising scientists. The high quality of the involved scientists was reflected in a very high quality of the talks. The latter have all been very well attended during the conference, and have been followed by intense (and friendly) scientific debates at the end of almost each talk. Thanks to the high level of research presented at talks and at the poster sessions, the atmosphere of the conference was extremely stimulating. We got feedback from many participants, expressing their appreciation for the quality of the presentations and the general format of the conference, which included long lunch breaks - perfect for discussions. Poster sessions have been very successful, lasting long after the allocated hours. The long lunch breaks have been ideal times for people to do networking and start collaborations. We are aware of at least a few collaborative research initiatives which have started at the conference among participants with the aim to apply to collaborative grant initiatives, such as FP7 STREPs.

There have been several scientific highlights worthy of notice. Examples are the development of new techniques to cool molecules to cold and ultracold temperatures, via direct and indirect (e.g., STIRAP mediated) techniques. In this respect the results from the JILA group for evaporative cooling of magnetically trapped OH radicals have been particularly surprising. This potentially opens a path all the way to Bose-Einstein condensation of dipolar radicals, as well as allowing cold- and ultracold-chemistry studies of fundamental reaction mechanisms. State-of-the-art experiments are currently under way to produce a quantum gas of strongly dipolar bosonic RbCs molecules, while another team at JILA is already observing evaporative cooling of fermionic KRb polar molecules. Sisyphus-like techniques to cool polyatomic molecules from the Munich MPQ group are paving the way towards cooling comparatively complex molecules such as CH3F, an achievement which was unthinkable just few years ago. Theoretical work on new cooling techniques such as super-radiance-based technology, cooling of hot molecules in mixtures with cold Rydberg-excited atoms may provide new avenues to cool to sub-millikelvin temperatures new species of molecules.

Theoretical ideas for quantum simulations and the realization of exotic many-body phenomena with cold molecules trapped in optical lattices are at the cutting edge of AMO theory, as well as

condensed matter. Further on the theoretical side, the few body physics of Efimov-type resonances is providing surprisingly precious insights to understand novel experiments from the Innsbruck group on few-body physics. These works, both theoretical and experimental, have very broad implications for fields as diverse as cold atomics and molecular physics and high-energy nuclear physics.

Due to the relative novelty and importance of this field of research, several of the topics touched in this conference are bound to provide exciting, fundamental, breakthroughs in the next 5 to 10 years. In addition to the research subjects mentioned above, the growing field of quantum chemistry is bound to play a key role in opening new and exciting areas of research. At low and ultralow temperatures, molecules are being prepared in specific quantum states for their internal degrees of freedom and their external motion. Thus, molecular interactions and reactions involving single quantum states can now be studied and controlled. The goal is thus to “quantum engineer” chemical processes. A large multimillion / multi-university MURI initiative sponsored by the Air Force is currently under way in the US to study ultracold chemistry. Nothing like that is currently being planned in Europe, which is a strategic error. Nevertheless, at the COLUM2012 conference, exciting, state-of-the-art experimental results towards the realization of controlled chemical reactions have been put forward by European groups and in Israel. Examples are cold collisions of molecular ions in Switzerland, as well as the realization of merged neutral supersonic beams and the ensuing manifestation of clear non-classical effects in the resulting reactions, reported by a group at Weizmann (IL).

Very exciting new research directions may come from combining control techniques based on ultrafast lasers with the ultracold temperatures of current experiments. In these experiments at exceedingly low temperatures, particles hardly move on the timescale dictated by ultrafast (e.g., femtosecond) laser. Using ultrafast laser probes, scientists are now exploring novel ways to monitor and manipulate dynamics of molecular processes and chemical reactions in ways previously thought impossible.

Overall, the conference “Cold and Ultracold Molecules” was a resounding success. It is the impression of most of the participants that coordinated actions towards further strengthening ties within this remarkably innovative, diverse, productive community would be highly desirable, both at the international and European levels. If at all possible, these actions should encompass the organization of further conferences in the field, COST actions, and the organization of large- and medium- scale collaborative grant initiatives, equivalent to EUROCORES and STREP-type initiatives.

Scientific Content of the Conference

(1 page min.)

- *Summary of the conference sessions focusing on the scientific highlights*
- *Assessment of the results and their potential impact on future research or applications*

The conference sessions have been characterized by the remarkably high quality of talks, which mirrors the remarkably high quality of the speakers.

Here is a breakdown of the conference, session by session, focusing on a few (of the many) highlights:

Session I :

This session was devoted to presentations from the groups which are leading research in the field of dipolar *atomic* quantum gases. This topics is very important, since a few groups in Europe and one group in the US (Lev, Stanford) have already developed techniques to cool complex magnetic atoms with comparatively large magnetic dipole moments towards quantum degeneracy both with bosonic and fermionic systems, and are already performing groundbreaking measurements of many-body properties.

In detail, Benjamin Lev (Stanford US) has presented recent results concerning the realization of the first degenerate quantum gas of fermionic particles, using Dy atoms with a large dipole moment. His group is also very close to realize bose-fermi mixtures. His group is also moving towards the realization of a quantum gas of Dy particles on a chip, as a novel platform to perform microscopy.

Bruno Laburthe-Tolra (Paris) has presented exciting results about magnetic effects in a dipolar quantum gas of Cr atoms. In particular, he has observed spontaneous magnetization of a Bose-Einstein Condensate to a ferromagnetic state above a critical field of about 100 microGauss, and spontaneous de-magnetization below that. This is in contrast to theoretical predictions. In addition, they have observed magnetic changing collisions for particles trapped in an optical lattice.

The Innsbruck group of Francesca Ferlaino (Innsbruck) has reported the breakthrough observations of Feshbach resonances in fermionic systems of Er atoms as well as the formation of weakly-bound molecules of $Er_{2,}$ with very large magnetic dipole moments. This should enable her group to address key questions of many-body dipolar physics using their current setup.

Session II :

The Zurich group of Prof. Merkt has presented recent results for Stark decelerators of atoms and molecules excited to a Rydberg state *on a chip*. This will of potential use to study interactions of atoms and molecules with surfaces.

Alexander Glätzle from the theory group of Prof. Zoller in Innsbruck has proposed a new technique to cool polar molecules during collisions with cold atoms excited to a Rydberg state. This technique is a combination of sympathetic cooling of the molecules with very large elastic cross sections (and thus potentially very efficient) and Sisyphus-type *collisional* cooling, where spontaneous emission of a photon on the atomic side takes away collision energy.

In the key-note talk, the JILA group (US) with Jun Ye has presented breakthrough experimental results concerning prospects for evaporative cooling of non-bialkali OH molecules (an absolute prime), as well as of KRb molecules. These results possibly pave the way to the realization of the first quantum gas of polar molecules.

Session III:

This session was entirely devoted to the key problem of developing new ways to cool different kind of molecules to cold (sub-millikelvin) and ultracold (sub-microkelvin) temperatures.

Prof. Rempe from MPI in Munich has reported on experiments based on Sisyphus-type ideas to cool electrically trapped complex multi-atomic molecules, such as CH_3F molecules. These breakthrough experiments, which were unthinkable just few years ago, pave the way towards cooling polyatomic molecules to sub-millikelvin temperatures, a Holy-Grail in the field.

Prof. Susanne Yelin from Univ. Connecticut (US) has presented theoretical ideas to cool molecules by exploiting the superradiant effect.

J. Barry, from DeMille's group in Yale (US) has reported on recent experiments with direct laser cooling of SrF molecules. This is a very interesting (and potentially seminal) result, since laser cooling seemed impossible to perform on molecules, due to the large number of internal states compared to atoms. It is an interesting question to understand how general the scheme used by the Yale team is.

Session IV:

Highlights in this session were:

1) the detailed presentation of recent results from the Jin/Ye group in JILA regarding the experiments with cold KRb molecules prepared in the absolute groundstate. The exciting news are that a new setup is now ready, where molecules are trapped in an optical lattice in a two dimensional geometry (in order to minimize losses induced by *attractive* dipolar collisions). Repulsive dipolar interactions between the molecules are now observed, and will be soon used to perform evaporative cooling. This is expected to be a viable path the reach quantum degeneracy in this system.

2) the recent results from Nägerl's group in Innsbruck (AT), regarding the preparation of a cold gas of RbCS molecules in the absolute ground state. These molecules, with a large dipole moment of 1.25 Debye, have been recently prepared in the ground state. Nägerl's group is now implementing a new scheme to produce a collisionally stable gas where particles are trapped in an optical lattice. This should allow for the realization of a bosonic quantum gas of dipolar molecules.
3) Prof. Zwierlein (MIT, US) has reported his group's achievement of ultracold fermionic Feshbach molecules of NaK. This is an ideal starting point to try to realize a gas of groundstate molecules, using so-called STIRAP techniques, which one of the main goals of this new experiment.

Session IV:

This session was mainly dedicated to few-body physics

Prof. Salomon (ENS Paris) has reported about recent measurements of beyond-mean-field effects in a strongly interacting bosonic quantum gas, a long-standing problem in condensed matter and atomic physics.

Prof. Greene (Purdue Univ. US) has presented state-of-the-art calculations for Efimov effects in heteronuclear systems. In particular, he has explained the universal behavior of 3-body collisions based on the properties of 2-body scattering alone – a remarkable observation from the

experimental Innsbruck group with Ferlaino and Nägerl. These results have great value in the conceptual understanding of few-bod effects in cold collisions, in the interpretation of experimental data from various groups, as well as for suggesting new experiments.

Session VI:

This session presented several theory talks and one experimental one. Highlights included:

1) The presentation of novel basic Hamiltonians by Prof. Lewenstein (ICFO, Spain) to describe the physics of dipolar particles in optical lattices. This will have important consequences for the realization of quantum simulations in experiments with polar molecules.

2) Dr. Bohn (JILA; US) has introduced a novel method based on a statistical approach to describe the properties of collisions, possibly relevant to the study of complex molecules, beyond bi-alkali ones. Compared to purely atomic collisions, ultracold molecular collisions potentially support a much larger number of Fano-Feshbach resonances due to the enormous number of ro-vibrational states.

3) Dr. Narevicius's group (Weizmann Institute, IL) has observed experimentally *quantum effects in cold reactions with merged beams.* Indeed, experiments have lagged theory in exploring chemical interactions at temperatures so low that translational degrees of freedom can no longer be treated classically. The difficulty has been to realize in the laboratory low-enough collisional velocities between neutral reactants to access this regime. Narevicius has reported the realization of merged neutral supersonic beams and the manifestation of clear non-classical effects in the resulting reactions.

Session VII:

This session was focused on new ideas and experiments to control atoms and molecules. Highlights included:

1) Prof. Ohmori (IMS, Japan) has reported on first experiments to control interactions in a cold gas of Rydberg-excited atoms using ultrafast laser techniques.

2) Prof. Corkum (Univ. Ottawa, CA) has reported on his groundbreaking experiments on aligning and orienting molecules with intense light pulses

Session VIII:

1) Prof. Hinds (Imperial College, London) has reported on his latest results on precision measurements of the electric dipole moment of electrons, using YbF molecules. The current record that was set by his group is of precision of one part in 10^{-28}. These experiments are enormously contributing to rule out (supersymmetric) theories beyond the standard model of high-energy physics.

2) Profs. Softley and Willitsch have presented exciting results for cold ion-molecular collisions. These are first groundbreaking steps towards the realization of cold controlled chemistry in these systems.

Forward Look

(1 page min.)

- *Assessment of the results*
- *Contribution to the future direction of the field – identification of issues in the 5-10 years & timeframe*
- *Identification of emerging topics*

The field of cold and ultracold molecules is on the verge of a quantum revolution. The excitement in the community is palpable, due to a series of recent theoretical and experimental breakthroughs and several prospected ones coming on the way. Particularly exciting are all the results concerning the development of new techniques to cool molecules to cold and ultracold temperatures, via direct and indirect (e.g., STIRAP mediated) techniques. In this respect the results from the JILA group with radical OH molecules have been particularly surprising. In very recent experiments, evaporative cooling has been observed in magnetically trapped OH radicals, which potentially opens a path all the way to Bose-Einstein condensation of dipolar radicals, as well as allowing cold- and ultracold-chemistry studies of fundamental reaction mechanisms. Through the combination of an extremely high gradient magnetic quadrupole trap and the use of the OH Λ-doublet transition to enable highly selective forced evaporation, cooling by an order of magnitude in temperature was achieved and yielded a final temperature of the order of mK. This is unexpected (and wonderful) news for the whole community. Another team in the same group is now observing evaporative cooling of polar fermionic KRb molecules, which would pave the way towards quantum degeneracy with a gas of fermionic groundstate polar molecules. Sisyphus-like techniques to cool polyatomic molecules from the Munich MPQ group are paving the way towards cooling comparatively complex molecules such as CH_3F, an achievement which was unthinkable just few years ago (results published in Nature 2012).

Theoretical work on new cooling techniques such as super-radiance-based technology, cooling of hot molecules in mixtures with cold Rydberg-excited atoms may provide new avenues to cool to sub-millikelvin temperatures new species of molecules. Theoretical ideas for quantum simulations and the realization of exotic many-body phenomena with cold molecules trapped in optical lattices are at the cutting edge of AMO theory, as well as condensed matter. Further on the theoretical side, the few body physics of Efimov-type resonances is providing surprisingly precious insight to understand key novel experiments from the Innsbruck group on few-body physics. These works, both theoretical and experimental, have very broad implications for fields as diverse as cold atomics and molecular physics and high-energy nuclear physics.

Due to the relative novelty and importance of this field of research, several of the topics touched in this conference are bound to provide exciting, fundamental, breakthroughs in the next 5 to 10 years. In addition to the research subjects mentioned above, the growing field of *quantum chemistry* is bound to play a key role in opening new and exciting areas of research. At low and ultralow temperatures, molecules are being prepared in specific quantum states for their internal degrees of freedom and their external motion. Thus, molecular interactions and reactions involving single quantum states can now be studied and controlled. The goal is to “quantum engineer” chemical processes. In the zero-temperature limit, quantum effects will control the chemical reactivity, and external fields will allow full coherent control over a molecular collision process. New theoretical approaches need to be developed to track a molecular reaction process, taking into

account all quantum degrees of freedom. In the US there is currently an important new MURI research effort under way in this direction, combining expertise in cold and ultracold collisions of atoms and molecules with theories and techniques developed in the chemistry community. The latter are particularly apt at describing short-ranged interactions and chemical reactions between comparatively complex systems, however are often phenomenological in nature. In AMO physics, parameters in the theories are often microscopically justified and derived. Thus, the combination of theories and experiments from the cold atom community and the cold chemistry may end up fostering new breakthroughs in both fields. A large multimillion / multi-university MURI initiative sponsored by the Air Force is currently under way in this direction in the US. Nothing like that is currently being planned in Europe, which is a strategic error.

Very exciting new research directions may come from combining control techniques based on ultrafast lasers with the ultracold temperatures of current experiments. In these experiments at exceedingly low temperatures, particles hardly move on the timescale dictated by ultrafast (e.g., femtosecond) laser. Thus, using ultrafast laser probes, scientists are now exploring novel ways to monitor and manipulate dynamics of molecular processes and chemical reactions in ways previously thought impossible.

- Is there a need for a foresight-type initiative?

Yes! This is clearly an up-and-coming field, with breakthroughs happening every day more frequently. Currently, there are no large scale networking programs on ultracold molecules in Europe, which is a misstep, given the strength of scientific activity in this field in Europe. A EUROCORES initiative would have been highly stimulating for the community.

Atmosphere and Infrastructure

- *The reaction of the participants to the location and the organization, including networking, and any other relevant comments*

The atmosphere of the conference was extremely stimulating, thanks to the very high level of the talks and of research presented at the poster sessions. We had feedback from many participants, who have confirmed their appreciation of the quality of the presentations and the general format of the conference, which included long lunch breaks (perfect for discussions). The atmosphere was also very informal, so that many discussions which were generated at the talks continued during the long lunch breaks and at/after poster sessions. Poster sessions have been very successful, lasting long after the allocated hours. The long lunch breaks have been ideal times for people to do networking and start collaborations. We are aware of at least a few collaborative research initiative which have started at the conference among participants (some of them with the intent to apply to collaborative grant initiatives, such as FP7 STREPs).

The Infrastructure in Obergurgl was very good, with a very helpful staff. Participants have appreciated the possibility to choose between seated lunch at the venue, or a simple box.

As a remark, the overall cost per participant at this ESF conference was rather high, compared to those of conferences of similar size and at similar locations.

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Date & Author: 17/12/2012 Guido Pupillo