REPORT OF THE ESF SCIENCE MEETING #805

COMOL'06 TRAINING SCHOOL ON ACHIEVEMENTS AND PERSPECTIVES OF COLD MOLECULES

February 26- March 3, 2006, Centre de Physique, Les Houches (France)

I- Summary

Research on cold molecules is evolving rapidly and several approaches to create and manipulate cold molecules have been demonstrated: photoassociation, magnetoassociation via Feshbach resonances (which lead to the first observation of molecular Bose-Einstein condensates), buffer gas cooling and trapping of paramagnetic molecules, Stark deceleration and trapping of dipolar molecules, deceleration of Rydberg systems, and creation of molecules on cold helium clusters.

Applications of cold molecules are promising in several fields, and new perspectives are still being identified. The photoassociation technique already established a new variant of high resolution molecular spectroscopy. The creation of molecular quantum degenerate gases revealed new states of matter, opening ways to investigate the cross-over between Bose condensates and degenerate Fermi gases. Chemical reactivity, assisted by light fields, is predicted to show a different quality in ultracold and quantum degenerate molecular gases. Control of external and internal degrees of freedom of cold molecules will promote this novel field of ultracold physical chemistry. Deceleration of heavy polar molecules is expected to provide good conditions for the search of the electron electric dipole moment. Furthermore, dipolar molecules have been proposed for the realization of a quantum information device.

Since 2002, the groups participating in the COMOL network of the EU are at the forefront of the development of cold molecule research, both on the experimental and the theoretical side. A number of other very active groups have joined this field, supported for instance through the CATS network of the ESF.

In the present document, we report on Training School organized by the COMOL network in its final year of activity. The COMOL Training School is devoted to the perspectives of the rapidly evolving research domain of cold molecules and cold chemistry. The objective is to deliver a solid background to young researchers entering the field through lectures given by scientists at the fore-front of cold molecule research. In addition the training school will foster contacts among students and young researchers working on related problems in international research groups. We mention that a joint workshop organized by both the COMOL and the CATS networks has been held during the week following the school at the same place, which has been attended by about 70 participants.

The training school benefited from the generous financial contribution of the QUDEDIS network. The entire amount has been used to support eleven students for their local accommodation (5 days, full-board) in Les Houches.

II- Description of the scientific content of and discussion at the event

As stated explicitly by the title of the school, the scientific program focussed on recent experimental achievements and breakthroughs in the preparation of samples of cold molecules with well-established techniques, on the expected evolution of these techniques, and on the perspectives offered by new approaches. In parallel, several exploratory theoretical developments were presented, suggesting new possible ways for experimental developments.

The general goal of this research field is the ultimate control of both internal and external degrees of freedom of molecules, in order to prepare them in well-defined states for further use.

The scientific program, displayed in the last section of this report, was composed of eight lectures, four sessions devoted to discussions in small groups, and a series of short contributed talks presented by the young researchers themselves.

A) Lectures

The program included four experimental and four theoretical lectures (of two hours each) delivered by rather young well-established scientists as well as young scientists in the process of starting their own group (e.g. C. Koch, M. Mudrich). For each day we scheduled one experimental lecture and one theoretical lecture, both being related in some way. The covered scientific topics were among the currently most active and promising directions of the cold molecule researches.

1) Monday

- The first experimental lecture was given by **J. Hecker Denschlag** (University of Innsbruck), coming from one of the most active groups in the world, who recently achieved several significant breakthroughs like the Bose-Einstein condensation (BEC) of Cesium, the first realization of a molecular Bose-Einstein condensate, or the observation of Efimov states predicted long time ago for an ensemble of three particles. Dr Denschlag presented an overview of *recent experiments where ultracold molecules* were produced out of degenerate gases of alkali atoms with the help of optical light fields or Feshbach resonances. He emphasized the crucial role of quantum statistics on the observation of BEC of molecules, and on the existence or suppression of inelastic collisions between atoms and molecules.
- Most of the advances described in the first lecture have been achieved by relying on the tuning of the so-called Feshbach resonances by external magnetic fields, which has been one of the topics of the first theoretical lecture given by E. Tiesinga (Gaithersburg). He first presented a general introduction on scattering resonances, which have played an important role in physics as they give information about the internal structure of the target. In the scattering of ultra-cold atoms resonances are known as Feshbach resonances, and Dr Tiesinga discussed their uses in controlling the properties of atomic and molecular Bose-Einstein condensates as well as of atoms trapped in optical lattices. Dr Tiesinga is a member of the group of P. Julienne a NIST, and is an internationally recognized expert in the field.

2) Tuesday

- The second day was devoted to the dynamics of atomic systems in ultracold environment, emphasizing on two emerging directions. **Dr R. Wester** (University of Freiburg) concentrated on the *emerging field of ultracold chemistry* which is investigating molecular collisions at ultracold temperatures. Particularly interesting for controlling cold chemistry is to understand the role of resonance phenomena and

the influence of external electromagnetic fields. Dr Wester discussed the concepts used to describe reaction dynamics at low temperatures and presented the status of experiments in the field. He first focussed on the photoassociation technique which has been successfully used to prepare translationally cold molecular samples in the laboratory. Then he discussed various magnetic and optical trapping experiments and presented first experiments on molecular collisions at low temperatures.

- In her theoretical lecture, **Dr C. Koch** (University of Jerusalem, now at Free University in Berlin) delivered a brief overview over the *methods necessary to model time-dependent processes of ultracold molecules*, i.e. the representation of a wavefunction and its time propagation. She focussed on the understanding of the accuracy as well as on the limitations of the methods, and then discussed the two extreme limiting cases for time-dependent processes, i.e. the sudden approximation and the adiabatic limit. She illustrated her lecture with a number of examples demonstrating the versatility of time-dependent processes in the manipulation of ultracold gases. Dr Koch is currently a member of Pr Kosloff's group at the Fritz Haber Institute in Jerusalem.

3) Thursday

- Manipulation and control of ultracold molecule formation and interactions with external electric fields are expected to be a powerful tool in the coming years. Many spectacular achievements have already been demonstrated in the group of G. Meijer (Fritz Haber Institute, Berlin), in which **Dr H. Bethlem** is involved. His experimental lecture concentrated on *the manipulation of polar molecules using inhomogeneous electric fields*, discussing electrode geometries suited to focus, decelerate, cool, trap, and reflect beams of polar molecules, and the prospects for using these manipulation elements in collision experiments and precision tests. Dr Bethlem also presented the techniques used to calculate the trajectories of the molecules through these elements, and how an intuitive understanding can be obtained by plotting these trajectories in phase space.
- The next theoretical lecture was presented by **Dr J. Bohn** (NIST, Boulder) who is working for several years on *the prospects for influencing the interactions between polar molecules at ultralow temperatures, by applying electrostatic and magnetostatic fields*. His lecture was built upon the basic principles underlying this influence. First the fields can alter the internal structure of the molecules, and he first discussed the dipole moments of individual molecules, where they come from and how they change in a field. Second, the resulting dipole-dipole interaction is strong at low temperatures, and the second part considered pairs of molecules, and how quantum mechanics strongly influences the behaviour of molecule-molecule interactions. In particular, avoided crossings in the adiabatic dipole-dipole potentials are expected to play a dominant role. Finally, Dr Bohn provided examples of control, including the variation of cross sections by orders of magnitude upon the application of electric of magnetic fields; the creation of novel long-range dimer states of polar molecules; and the electric-field-dependent collapse of dipolar Bose-Einstein condensates.

4) Friday

- The last session of the school was devoted to two promising developments related to cold molecule researches. An experimental review lecture about *the field of helium nanodroplets* (He_N) was presented by **Dr M. Mudrich**, recently established in the group of F. Stienckemeier (University of Freiburg). He particularly focused on *the interactions of molecules attached to He_N clusters*, which provide a very cold environment so that the internal degrees of freedom (vibration, rotation) of those molecules are frozen to their ground state. Analogies and fundamental differences to cold

molecules produced by other means, in particular from ultracold atoms, were analysed. Dr Mudrich then considered He_N as ideal "nano-cryostats" and "nanoreactors" for experiments on the spectroscopy and chemical reactions of molecules and complexes. He selected key experiments on the spectroscopy of cold molecules in He_N using microwave up to synchrotron radiation, and emphasized on recent advances in studying the dynamics of He_N-molecule complexes using femtosecond lasers and ion imaging techniques.

- In his lecture, **Dr R. Côté** (University of Connecticut) reviewed recent *theoretical and experimental work on Rydberg molecules*. Indeed, experiments involving Rydberg gases and plasmas have studied translationally cold systems with large amount of internal energy like highly-excited Rydberg, characterized by their exaggerated properties like long radiative lifetimes and strong long-range interactions. Molecular resonances caused by Rydberg-Rydberg excitations have been already detected, while theory predicts several types of Rydberg molecules. Dr Côté first treated *the long-range interactions between Rydberg atoms*, and the properties which can be expected for such molecules. Then he discussed the *experimental evidence for molecular resonances*, modelling the results in the context of the photoassociation of cold atoms as a two-photon process. Finally, he explored the behaviour of macroscopic samples where the excitation of high-lying Rydberg states is strongly suppressed due to long-range forces. Dr Côté is involved in the theory group of the Department of Physics headed by W. Stwalley.

B) Discussion sessions

The Training school featured two lectures per day. The organizers asked to every speaker to propose two topics or questions related to their presentation to be discussed in small groups in the afternoon, after the two lectures. Then all groups merged again together in the lecture room for a round table all groups to confront their approaches and possible controversy about the specific topic. The scientific committee represented by Dr Van der Straten acted as a moderator. The students actually discussed their ideas with all lecturers in a very open and creative way. For most questions they obtained the right answer, they emphasized either a controversy or alternative interpretation, or they even proposed new prospects with a lot of imagination.

B) Contributed talks

All participants were encouraged to present a poster during two dedicated evening sessions. Sixteen contributions submitted by young researchers out of a total of 28 abstracts were selected to present a 15 minute talk about their current work. They were divided in eight theoretical and eight experimental topics, covering most of the current areas of the cold molecule field, including the well-established photoassociation technique, ion cooling and trapping, cold atom/molecules collisions, degenerate molecular gases, or new techniques for molecule deceleration and trapping. We emphasize here the training aspect of these presentations, as it was for most of the students their first oral presentation in front of an international audience. They indeed presented high quality talks accessible for such a broad community mixing people with various backgrounds (like in optics, molecular physics …).

III- Assessment of the results and impact of the event on the future direction of the field

We believe that this training school provided to the participants the opportunity to discover a new field of research, to create new contacts with perspectives of exchange. The discussion sessions were particularly illustrative from this point of view, with a strong enthusiasm of the young researchers to answer to the questions proposed by the lecturers, to confront their thoughts – sometimes with a lot of energy! - within the groups, and to explore other hypothesis. It is important to emphasize on the involvement of the lecturers, who really presented pedagogical talks adapted to the broad audience. In particular, the balance between theory and experiment in the schedule was very instructive for the participants.

We received a very positive feedback from the students at the end of the school, either from private conversations, or from the form we distributed at the end of the school. We distributed to all participants a CD-ROM with the slides of all lectures.

About 40 young researchers attended the training school, coming from various European groups, either already strongly involved in research on cold molecules (like in Innsbruck, Austria, in Berlin, Düsseldorf, Freiburg, Germany, in Roma, Italy, or in Orsay, France), or from groups just entering the field. A few participants also came to enlarge their scientific perspectives. This confirmed that such a Training School was indeed timely, as a conclusion of a series of events which took place during the four years of the COMOL network. The training school was followed by an international workshop at the time where the network finishes, and other projects are in progress (like for instance the ESF program EUROQUAM). These initiatives contributed to the identification of a growing scientific community, which is evolving along two main directions: (i) the study of degenerate gases and their relation with condensed matter physics; (ii) the definition of a new ultracold chemistry, possibly involving photons, with the perspective of controlling the dynamical evolution of ultracold systems.

As already mentioned earlier, the date for both the training school and the workshop coincided with the deadline for submission of papers for a special issue on Cold Molecules edited by Journal of Physics B to be published by Fall 2006, with Olivier Dulieu and Eberhard Tiemann as guest editors. Up o now, 32 papers have been submitted, most of them coming form groups who attended one of these events. As a guest editor, I (O.D.) can certify that several papers have been completed and submitted for this special issue after these events.

IV- Final program

Monday, 27th Feb.

08:45 - 09:00	Opening remarks
09:00 - 11:00	**Johannes Hecker Denschlag** „Ultracold degenerate gases of molecules and atoms“
11:15 - 11:30	Arne-Christian Voigt “Simultaneous magneto-optical trapping of three atomic species”
11:30 - 11:45	Tobias Kraemer “Ultracold Cs: Dimers and Trimers”
11:45 - 12:00	Stefan Riedl “Collective Excitations in the BEC-BCS crossover”
12:00 - 12:15	Ivan Liu “Rydberg atoms in an ultracold atomic gas”
	Lunch
15:00 - 17:00	**Eite Tiesinga** „Feshbach resonances in ultra-cold atom gases“
17:15 - 18:15	**Group sessions**
18:30 - 19:30	**Discussions**
	Dinner

Tuesday, 28th Feb.

09:00 - 11:00	**Christiane Koch** „Ultracold & Ultrafast: Time-dependent processes“
11:15 - 11:30	Florian Lang “The creation of ultracold molecules via the use of magnetic”
11:30 - 11:45	Svetlana Kotochigova “Creating and Controlling Polar Molecules in Optical Lattices”
11:45 - 12:00	Klaus Hoejbjerre “Rotational cooling of molecular ions”
12:00 - 12:15	Chaobo Zhang “Molecular dynamics simulations of sympathetic cooling of ion species in a linear Paul trap”
	Lunch
15:00 - 17:00	**Roland Wester** „Reaction dynamics at low temperatures“

17:15 - 18:15	**Group sessions**
18:30 - 19:30	**Discussions**
	Dinner
21:00 - ...	**Poster Session**

Wednesday, 1st Mar.

18:30 - 18:45	Goulven Quéméner "Ultracold alkali dialkali collisions: a quantum mechanical study"
18:45 - 19:00	Haikel Jelassi "Photoassociation spectroscopy of long range molecular states ^{87}Rb"
19:00 - 19:15	Philippe Pellegrini "Theoretical analysis of the photoassociative spectrocopy of ultracold strontium atoms"
19:15 - 19:30	Slawomir Telega "Rovibrational cooling of molecular gases by electron impact at vanishing collision energies

Thursday, 2nd Mar.

09:00 - 11:00	**John Bohn** „Controlling cold collisions of polar molecules"
11:15 - 11:30	Emanuelle Scifoni "He droplets as cryoreactors of ionic reactions: He + LiH^+ -> HeH^+ + Li"
11:30 - 11:45	Peter Luetzow "A microwave trap for molecules in their absolute ground-state"
11:45 - 12:00	Samuel Meek "A microdecelerator for polar molecules"
12:00 - 12:15	Mourad Telmini "The halfium model: ab initio calculations of highly excited H_2 phaseshifts"
	Lunch
15:00 - 17:00	**Hendrick L. Bethlem** „Manipulating polar molecules using inhomogeneous electric fields"
17:15 - 18:15	**Group sessions**
18:30 - 19:30	**Discussions**

	Dinner
21:00 - ...	**Poster Session**
	Friday, 3rd Feb.
09:00 - 11:00	**Marcel Mudrich** „Cold molecules attached to helium nanodroplets“
11:15 - 13:15	**Robin Coté** „Rydberg systems“
	Lunch
14:30 - 15:30	**Group sessions**
16:00 - 17:00	**Discussions**