ANNUAL CONVENTION 2019

IRTG CoCo

Cold Controlled Ensembles in Physics and Chemistry

BOOK OF ABSTRACTS

5th CoCo Annual Convention

August 5 – 9, 2019

University of British Columbia
Vancouver, Canada

Imprint

IRTG 2079 / Cold Controlled Ensembles in Physics and Chemistry

Institute of Physics
University of Freiburg
Hermann-Herder-Straße 3
D - 79104 Freiburg

UBC Faculty of Science
Vancouver Campus
2036 Main Mall
Vancouver, BC Canada V6T 1Z1.

Organisation

IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“

Organizers

Takamasa Momose, University of British Columbia

Email: momose@chem.ubc.ca

Frank Stienkemeier, University of Freiburg

Email: stienkemeier@uni-freiburg.de

Simone Ortolf, University of Freiburg

Email: irtg-coco-coordination@physik.uni-freiburg.de

Katharina Pessel, University of Freiburg

Email: katharina.pessel@physik.uni-freiburg.de

Financial Support

General Information

Duration

Monday, August 5, 2019, 8:00 a.m. – Friday, August 9, 2019, 6:00 p.m.

Accommodation

Conferences & Accommodation UBC Vancouver
Ponderosa Commons Front Desk
2075 West Mall
Vancouver, BC, Canada V6T 1Z2
Tel: 604.822.2708

Travel information

BY TAXI
From the Vancouver International Airport, a taxi will take around 20 minutes to the Ponderosa Commons.

BY PUBLIC TRANSPORT
Please note that there is no direct bus service from Vancouver International Airport (YVR):
From YVR, take the Canada Line SkyTrain (all routes head north)
Transfer at one of the following stations

- Oakridge Station (41 Ave. & Cambie St.): Take bus #41 or #43
- Broadway City Hall Station (Broadway & Cambie St.): Take bus #99 (B-Line)
- Olympic Village Station (4 Ave. & Cambie St.): Take bus #84

Arrive at UBC. (UBC is final stop; all buses stop within a 15-minute walk of the Ponderosa Studios.

Locations

The IRTG Annual Convention 2019 takes place at UBC Vancouver Campus:

Walter Gage Residence
5959 Student Union Blvd., Vancouver, B.C. V6T 1K2

Michael Smith Laboratories
#301-2185 East Mall, Vancouver, BC V6T 1Z4

Department of Chemistry, UBC Faculty of Science
2036 Main Mall, Vancouver, BC Canada V6T 1Z1

1: Ponderosa Commons
2: Walter Gage Residence
3: Michael Smith Laboratories
4: Chemistry Buildings
4 A: Kirk Madison Group / Lab
4 B: Dinner on August 6
5: Sage Restaurant (PI Dinner)
6: Soccer field
7: New Bus loop
8: MOA – Museum of Anthropology


8
MOA
5
University Centre
2
Gage Residence
7
SRC
Aquatic Centre
4B
4A
1
Oak House
Ponderosa Commons
3
6
Cecil Green Park House
Green College
Chan Centre
Wood Belkin Theatre Art Gallery
Music
Nitobe Garden
Old Aud
Brock Commons
Chancellor Place
Place Vanier Residence
Somerset Studios
AMS Nest
Alumni Centre
War Memorial
Bookstore
St. John's College
Marine Drive Residence
EOS
Beaty Biodiversity Museum
Hospital
Orchard Commons
Totem Park Residence
Thunderbird Residence
Hawthorn Place
UBC Tennis Centre
Doug Mitchell Centre
Thunderbird Park
Thunderbird Stadium
UBC Botanical Garden and Centre for Plant Research
Wesbrook Village
Hampton Place
Acadia Park Residence
Fairview Crescent Residence
East Campus
University Endowment Lands (UEL)
Pacific Spirit Regional Park
Wreck Beach
CHANCELLOR BLVD
NW MARINE DR
CRESCENT RD
MEMORIAL RD
AGRICULTURAL RD
STUDENT UNION BLVD
WALTER GAGE RD
UNIVERSITY BLVD
LOWER MALL
WEST MALL
MAIN MALL
EAST MALL
HEALTH SCIENCES MALL
WESBROOK MALL
AGRONOMY RD
THUNDERBIRD BLVD
STADIUM RD
WEST 16th AVE
ACADIA RD
Tech
6500
6400
6300
6200
6100
6000
5900
5700
5600
5500
E-W
STREET BLOCK #'s
N-S
1700
1800
1900
2000
2100
2200
2300
2400
2500
2600
3200
3300
3400

Meals & Drinks

Meals and drinks during the scientific program are included in the conference fee. Dinner on Sunday, Aug 4, as well as breakfast and lunch on Monday, Aug 5, will be self-organized. Remember Monday is a holiday in British Columbia! Please find the information on where the meals will take place in the program below (p.11-15).

Final Dinner, Aug 8

As our IRTG will end this year, the final dinner will be a special farewell event. We booked a "Sunset Dinner Cruise": a round trip through the Vancouver harbor with a beautiful view of the city and a west coast buffet dinner.

Excursion

Monday the 5th of August is a holiday in British Columbia. Since the university is closed on this day, we use the day for excursions.

In the morning, we do a **whale watching tour** of several hours (duration 3-6 hours, depends on weather conditions and success in whale watching). Please bring suitable clothing, the organizers recommend several layers, sun protection, camera, snacks and drinks. We have booked an open-air vessel only for the IRTG group.
More information you will find here: https://www.whalesvancouver.com/

In the afternoon, we will visit the famous **MOA – the Museum of Anthropology**, which is one of the leading museums of First Nations culture in the Pacific Northwest. It is located on Marine Drive in the University Endowment Lands.

The museum is closely linked to the UBC. The extensive collection is housed in a concrete building whose architectural style is reminiscent of the half-timbered houses of the local native people. The museum has numerous large sculptures, totem poles and cultural objects. Although the museum specializes in the indigenous peoples of the Pacific Northwest Coast, the collection of approximately 38,000 ethnographic and 535,000 archaeological objects also includes objects from all other continents. There is currently a special exhibition on the subject: “*Shadows, Strings and other Things – The Enchanting Theatre of Puppets*”.

More information you will find here: https://moa.ubc.ca/

Free time activities

On Friday night, no dinner or event is planned. After the end of the Annual Convention’s program, there is free time.

WiFi

There is WiFi access throughout the accommodation area and the campus.

Program of the IRTG Annual Convention 2019

Monday, August 5, 2019

6:45 a.m.	**Ponderosa Commons** Meeting with Manish at the Front Desk
7:00 a.m.	**Depart** at the Bus loop (7)
8:15 a.m.	**Arrival Granville Island**
8:30 a.m. - 1:00 p.m.	**Whale Watching Tour** Granville Island, Vancouver Bay
4:00 p.m. - 6:00 p.m.	**Museum of Anthropology (MOA)** Guided tour
7:00 p.m. – 9:00 p.m.	**Dinner** Gage Residence, Fort Camp Lounge (2)

Breakfast and Lunch on Monday will be self-organized!

Program of the IRTG Annual Convention 2019

Tuesday, August 6, 2019

7:30 a.m.	**Breakfast** Gage Residence, Fort Camp Lounge (2)
9:00 a.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
10:30 a.m.	**Coffee Break 1** Michael Smith Lab (MSL) 101 (3)
11:00 a.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
12:30 p.m.	**Lunch** Michael Smith Lab (MSL) 101 (3)
3:30 p.m.	**PI Meeting** Michael Smith Lab (MSL) 102 (3)
4:30 p.m.	**PAC Meeting 1** Chem / Phys (4)
5:30 p.m.	**Lab Tour Madison research group** Chem / Phys Basement (4A)
6:30 p.m.	**PI Dinner** Sage Restaurant (5), Ideals Lounge
7:00 p.m.	**Dinner** Chem (4B) D213

Program of the IRTG Annual Convention 2019

Wednesday, August 7, 2019

7:30 a.m.	**Breakfast** Gage Residence, Fort Camp Lounge (2)
9:00 a.m.	**Lectures** Gage Residence, Isabel MacInnes Ballroom (2)
10:30 a.m.	**Coffee Break** Gage Residence, Fort Camp Lounge (2)
11:00 a.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
12:30 p.m.	**Lunch** Gage Residence, Fort Camp Lounge (2)
1:30 p.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
3:00 p.m.	**Coffee Break** Gage Residence, Fort Camp Lounge (2)
3:15 p.m.	**PAC Meetings 2** Chem / Phys (4)
3:30 p.m.	**Poster Session** Gage Residence, Fireplace Lounge (2)
4:30 p.m.	**Soccer Game** South Field (6)
7:00 p.m.	**Dinner** Gage Residence, Fireplace Lounge (2)
8:00 p.m.	**After Dinner Talk by Edward Grant** Gage Residence, Isabel MacInnes Ballroom (2)

Program of the IRTG Annual Convention 2019

Thursday, August 8, 2019

7:30 a.m.	**Breakfast** Gage Residence, Fort Camp Lounge (2)
9:00 a.m.	**Lectures** Gage Residence, Isabel MacInnes Ballroom (2)
10:30 a.m.	**Coffee Break 1** Gage Residence, Fort Camp Lounge (2)
11:00 a.m.	**Lectures** Gage Residence, Isabel MacInnes Ballroom (2)
12:30 p.m.	**Lunch** Gage Residence, Fort Camp Lounge (2)
1:30 p.m.	**Lectures** Gage Residence, Isabel MacInnes Ballroom (2)
3:00 p.m.	**Coffee Break 2** Gage Residence, Fort Camp Lounge (2)
3:15 p.m.	**PAC Meetings 3 + 4** Chem / Phys (map 4)
3:30 p.m.	**Poster Session** Gage Residence, Fireplace Lounge (2)
5:40 p.m.	**Bus to Vancouver Harbour** Bus leaves at the bookstore
6:30 p.m.	**Final Dinner “Sunset Dinner Cruise”** Gage Residence, Fireplace Lounge (2)
9:30 p-m.	**Bus to Ponderosa Commons** Return bus to campus

Program of the IRTG Annual Convention 2019

Friday, August 9, 2019

7:30 a.m.	**Breakfast** Gage Residence, Fort Camp Lounge (2)
9:00 a.m.	**PhD personal meetings** Michael Smith Lab (MSL) 101 & 102 (3)
10:30 a.m.	**Coffee Break 1** Michael Smith Lab (MSL) 101 (3)
11:00 a.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
12:30 p.m.	**Lunch** Michael Smith Lab (MSL) 101 (3)
1:30 p.m.	**Lectures** Michael Smith Lab (MSL) 102 (3)
2:00 p.m.	**Closing Session** Michael Smith Lab (MSL) 102 (3)
3:00 p.m.	**Coffee Break 2** Gage Residence, Fort Camp Lounge (2)
3:00 p.m.	**PAC Meetings 5** Chem / Phys (4)
4:00 p.m.	**Lab Tour – Jones research group** Lobby of QMI, Stewart Blusson Quantum Matter Institute
	Free evening

PAC Meetings

The PAC meetings serve to discuss the status of your projects with both supervisors and to prepare the annual report. They will take place in the offices of the UBC supervisors (4). For the Annual Convention we have organized meetings for PhD students with supervisors from UF and UBC. The doctoral students with supervisors from only one side or in the case that one of your supervisors is not present: Please schedule an appointment as soon as possible.

Tuesday, August 6, 2019 (4:30 – 5:15 pm)

PAC 1

Moritz Michelbach, Frank Stienkemeier, Takamasa Momose

Simon Dold, Bernd v. Issendorff, Edward Grant

Wednesday, August 7, 2019 (3:30 – 4:15 pm)

PAC 2

Janine Franz, Stefan Buhmann, Edward Grant

Denis Uhland, Kirk Madison, Tobias Schätz

Marcel Binz, Frank Stienkemeier, Valery Milner

Thursday, August 8, 2019 (3:15 – 4:45 pm)

PAC 3

3:15 – 4:00 pm

Audrey Scognamiglio, Frank Stienkemeier, Valery Milner

Pascal Weckesser, Tobias Schätz, Kirk Madison

Manish Vashishta, Takamasa Momose, Katrin Dulitz

PAC 3

4:00 – 4:45 pm

Jordan Fordyce, Valery Milner, Frank Stienkemeier

Erik Frieling, Kirk Madison, Tobias Schätz

PAC 4

4:45 – 5:15 pm

Daniel Uhl, Frank Stienkemeier, Roman Krems

Friday, August 9, 2019 (3:00 – 4:30 pm)

PAC 5

3:00 – 3:45

Ulrich Bangert, Frank Stienkemeier, Takamasa Momose

3:45 – 4:30

Brendan Moore, Takamasa Momose, Frank Stienkemeier

Personal Meetings

The doctoral students of the UF have elected two PI's, Stefan Buhmann and Michael Walter, as 'persons of trust'. In addition to the supervisors, they are contact persons for any topics where a further dialogue is helpful.

Friday, August 9, 2019

	Stefan Buhmann		**Michael Walter**
9:00	Dominik Ertel	9:00	Friedemann Landmesser
9:10	Uli Bangert	9:10	Moritz Michelbach
9:20	Sebastian Wenderoth	9:20	Andreas Wituschek
9:30	Selmane Ferchane	9:30	Tobias Sixt
9:40	Audrey Scognamiglio	9:40	Simon Dold
9:50	Matthias Bohlen	9:50	Janine Franz
10:00	Pascal Weckesser	10:00	Fabian Thielemann
10:10	Marcel Binz	10:10	Daniel Uhl

Abstracts

-

PI lectures & After Dinner Talk

Chiral Molecules in Laser Fields with Twisted Polarization

I. Tutunnikov[1], E. Gershnabel[1], J. Floß[2], P. Brumer[2], and **I. Sh. Averbukh**[1]

1Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot 7610001, Israel

2Chemical Physics Theory Group, Department of Chemistry, and Center for Quantum Information and Quantum Control, University of Toronto, Toronto, Ontario M5S 3H6, Canada

We present a novel pure optical method for enantioselective orientation of chiral molecules by means of laser fields with twisted polarization [1, 2]. Several field implementations are considered, including a pair of delayed cross-polarized laser pulses, polarization-shaped pulses, and an optical centrifuge. We show that the twisted light selectively orients two enantiomers along or against the propagation direction of the laser beam, which leads to the out-of-phase time-dependent dipole signals for different enantiomers. We discuss the underlying orientation mechanism both classically and quantum-mechanically, and theoretically explore its operation for a range of chiral molecules of various complexity: hydrogen thioperoxide (HSOH), propylene oxide (CH_3CHCH_2O, or PPO) and ethyl oxirane ($CH_3CH_2CHCH_2O$). Most recently, the orientation of chiral PPO molecules by means of an optical centrifuge was experimentally achieved at UBC [3], thus providing the first demonstration of enantioselective laser control over molecular rotation. Moreover, we report here a principally novel phenomenon – persistent field-free molecular orientation lasting orders of magnitude longer than the duration of the exciting laser pulses [2,4]. This effect is unique for chiral molecules driven by laser fields with twisted polarization, and it is in sharp contrast with all the previously known techniques for laser molecular orientation, in which the post-pulse orientation rapidly disappears shortly after the end of the laser pulse. We provide plausible classical arguments for the appearance of this phenomenon, and support them

by the results of full quantum mechanical treatment. The experimental test of our predictions is currently underway. The presented results demonstrate generality, versatility and robustness of our optical method for manipulating molecular enantiomers in the gas phase. This approach opens new avenues for detecting molecular chirality, measuring enantiomeric excess and separating enantiomers with the help of inhomogeneous external fields.

References

[1] E. Gershnabel and I. Sh. Averbukh. Orienting asymmetric molecules by laser fields with twisted polarization. Phys. Rev. Lett., **120**:083204, 2018.

[2] Ilia Tutunnikov, Erez Gershnabel, Shachar Gold, and Ilya Sh. Averbukh. Selective orientation of chiral molecules by laser fields with twisted polarization. The Journal of Physical Chemistry Letters, **9**(5):1105-1111, 2018.

[3] Alexander A. Milner, Jordan A.M. Fordyce, Ian MacPhail-Bartley, Walter Wasserman, Valery Milner, Ilia Tutunnikov, and Ilya Sh. Averbukh, “Controlled Enantioselective Orientation of Chiral Molecules with an Optical Centrifuge”, Phys. Rev. Lett. **122**, 223201, (2019)

[4] Ilia Tutunnikov, Johannes Floss, Erez Gershnabel, Paul Brumer, and Ilya Sh. Averbukh, “Laser induced persistent orientation of chiral molecules”,arXiv:1905.12609, (2019)

Controlled enantioselective orientation of chiral molecules with an optical centrifuge

A. A. Milner[1], J. A. M. Fordyce[1], I. MacPhail-Bartley[1], W. Wasserman[1], I. Tutunnikov[2], I. Sh. Averbukh[2], and **V. Milner[1]**

1Department of Physics & Astronomy, The University of British Columbia, Vancouver, Canada

2Department of Chemical and Biological Physics, The Weizmann Institute of Science, Rehovot, Israel

We initiate unidirectional rotation of chiral molecules with an optical centrifuge and detect their spatial orientation by means of Coulomb explosion imaging. We show that the centrifuge-induced orientation of one of the molecular axes in the laboratory frame depends on the relationship between the chiral handedness of the enantiomer and the direction of the laser-induced molecular rotation. The effect is reproduced in the numerical simulations of the centrifuge excitation followed by Coulomb explosion of the centrifuged molecule. The demonstrated technique offers not only an alternative way of differentiating between molecular enantiomers, but also a new approach to enantioselective manipulation of chiral molecules with light.

Computational Studies of *Extreme* Bonding: Fringe Bonds, σ Conductance, and Unconventional Aromaticity

Yan Alexander Wang* & Jian-Xiong Yang

Department of Chemistry, University of British Columbia, Vancouver, Canada
yawang@chem.ubc.ca

This talk will provide answers to the following seven questions theoretically:

1) How long a C–C σ single bond can be?
2) Can two sp^2 C atoms form only σ bonds?
3) Are antibonding orbitals always more stable than bonding orbitals?
4) Can a saturated organic material have good electric conductivity through a σ network?
5) Can a H atom participate in an aromatic π bond?
6) Is the transition state (activated complex) always unobservable?
7) What can such crazy ideas have anything to do with the real world?

Historical Background of the Aforementioned Seven Questions

Several years ago, my group studied the intramolecular hydrogen-bond (IHB) systems in acetylacetone and its α-halo derivatives [*PCCP* **18**, 344 (2016)]. We found that the IHB proton transfer is an early, sudden quantum tunneling process without going through the classical C_{2v} transition state whereas virtually all textbooks have been claiming the opposite on this subject. More amazingly, the classical C_{2v} transition state of the IHB proton transfer is aromatic! What is its significance? It is the first ever identified aromatic π system (albeit only a transition state) involving a H atom! Since then, we have designed several new ground-state aromatic H-π systems.

Inspired by our expedition in unconventional aromaticity, we have been wondering how extremely we can push the length limit of a common chemical bond without breaking it. For instance, the longest C−C single *σ* bond that has been realized experimentally is slightly above 1.80 Å long [*Chem.* **4**, 795 (2018)] whereas the predicted longest C−C bond is about 2.33 Å in drum-shaped propellanes [*JACS* **119**, 1449 (1997)]. Very recently, we have successfully designed several new *saturated* organic molecules, in which two C atoms can form an extremely long C−C *σ* bond with a world-record *ca*. 2.8 Å bond length. Preliminary calculations have predicted the band gaps of corresponding saturated organic polymers (made from the monomers with the long C−C *σ* bond) to be around 1.68~2.26 eV, which is already nearly the same as those unsaturated conducting organic polymers currently in use.

Quantum-state-controlled reactive atom-atom collisions

Tobias Sixt[1], Jonas Grzesiak[1], Jiwen Guan[1], Markus Debatin[1], Vivien Behrendt[1], Simon Hofsäass[1], Pinrui Shen[2], Thilina Muthu-Arachchige[1], Frank Stienkemeier[1], Marcel Mudrich[3], Katrin Dulitz[1]

1. Institute of Physics, University of Freiburg, Hermann-Herder-Str.3, 79104 Freiburg i. Br., Germany
2. Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, V6T 1Z1, Canada
3. Department of Physics and Astronomy, Ny Munkegade 120, 8000 Aarhus C, Denmark

With a total of only five electrons involved, He-Li represents a collision system especially suitable for fundamental studies of chemical reactivity. In our scattering experiments, we observe Li+ and LiHe+ ions produced during the autoionization of Li(22P) by metastable He in the 21;3S states. The lithium atoms are confined in a magneto-optical trap (MOT) which offers the advantage of a high-density, ultracold and stationary scattering target, whose properties can be easily monitored and controlled using external fields. In combination with a high-density, supersonic beam source for metastable He, it is possible to observe high signal count rates.

The efficient suppression of autoionizing collisions is a stringent requirement to achieve quantum degeneracy in metastable rare gases. Thus far, such loss processes have been avoided by electron-spin polarizing the collision partners. In this contribution, I will report on the efficient suppression of Penning ionization in collisions between metastable He and laser-excited Li atoms. Our results can only be explained by both electron-spin conservation and the conservation of total molecular orbital angular momentum along the internuclear axis. The latter has hitherto not been exploited for reaction control.

I will also provide details about the experimental setup including an original optical quenching scheme [2] which allows us to distinguish between the relative rates of Li with He(21S0) and He(23S1), respectively. The influence of elastic He-Li collisions on the steady-state Li atom number in the MOT is described, and it is shown how the collision data is used to estimate the excitation efficiency of the discharge source. I will also show that reactive collisions can be used to directly probe the temperature of the Li cloud without the need for an additional time-resolved absorption or fluorescence detection system.

References

[1] Jonas Grzesiak, Takamasa Momose, Frank Stienkemeier, Marcel Mudrich and Katrin Dulitz, J. Chem. Phys. 150(3), 034201, 2019.

[2] Jiwen Guan, Vivien Behrendt, Pinrui Shen, Simon Hofsäass, Thilina Muthu-Arachchige, Jonas Grzesiak, Frank Stienkemeier, and Katrin Dulitz, Phys. Rev. Appl. 11(5), 054073, 2019.

What makes scientific communication so important?

Edward Grant

Department of Chemistry, Department of Physics & Astronomy, University of British Columbia

Professional scientists, one and all, spend at least half of their working lives communicating. Why? What makes scientific communication so important for the individual scientist? So important for science as a whole? This after-dinner talk will take a light-hearted look at scientific communication in an effort to address these questions. Recognizing the *Why* will lead us naturally to an examination of the *How* - in a realm of audience participation.

Abstracts

–

Presentations of doctoral students and PostDoc’s

Tracking Attosecond Electronic Coherences Using Phase-Manipulated Extreme Ultraviolet Pulses

Andreas Wituschek[1], Lukas Bruder[1], Daniel Uhl[1], Marcel Binz[1], Ulrich Bangert[1], Rupert Michiels[1], Giuseppe Sansone[1], Carlo Callegari[2], Michele di Fraia[2], Oksana Plekan[2], Miltcho Danailov[2], Alexander Demidovich[2], Kevin C. Prince[2], Paolo Cinquegrana[2], Paolo Sigalotti[2], Ivaylo Nikolov[2], Enrico Allaria[2], Luca Gianessi[2], Giuseppe Penco[2], Primož Rebernik Ribič[2], Najmeh S. Mirian[2], Carlo Spezzani[2], Finn H. O'Shea[2], Simone Spampinati[2], Tim Laarman[3], Andreas Przystawik[3], Marcel Drabbels[4], Marcel Mudrich[5], Richard James Squibb[6], Raimund Feifel[6], Stefano Stranges[7], Paolo Piseri[8], Giulio Cerullo[9] and Frank Stienkemeier[1]

[1]Physikalisches Institut, Universität Freiburg, Germany. [2]Elettra-Sincrotrone, Trieste, Italy. [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. [4]Laboratory of Molecular Nanodynamics, Ecole Polytechnique Lausanne, Switzerland. [5]Department of Physics and Astronomy, Aarhus University, Denmark. [6]Department of Physics, University of Gothenburg, Sweden.[7]University of Rome "La Sapienza", Italy. [8]Universita` degli Studi di Milano, Italy. [9]IFN-CNR and Dipartimento di Fisica, Politecnico di Milano, Italy

Experiments utilising advanced coherent control and nonlinear spectroscopy schemes are powerful tools that allow the study and control of the dynamics of atomic and molecular systems. The advent of novel light sources in the extreme ultraviolet (XUV) region paved the way for the extension of these tools to the XUV, potentially allowing similar experiments with an unprecedented spatial and temporal resolution. However, this promise has not yet been honoured due to the experimental difficulty of creating XUV pulse trains with precisely controlled timing and phase properties.

In this work we use an XUV pulse pair to measure directly in the time domain the coherent evolution and dephasing of electronic XUV wave packets. We demonstrate this in helium and for an autoionizing resonance in argon (Fig. 1). Two collinear XUV pulses were created at the FERMI free-electron laser (FEL) operated in double seed-pulse mode [1]. We controlled the relative phase and delay of the pulse pair independently by acting only on the fundamental ultraviolet seed pulse [2]. Imparting a shot-to-shot phase modulation lead to modulated photoion/electron yields [3]. Subsequent lock-in demodulation shows a particularly high sensitivity and allows the isolation of different harmonic contributions in the total signal. This phase manipulation technique facilitates a wide range of nonlinear spectroscopy as well as coherent control schemes, and is universally applicable to the whole wavelength range accessible with seeded FELs. In addition, it can be combined with tabletop High Harmonic Generation sources.

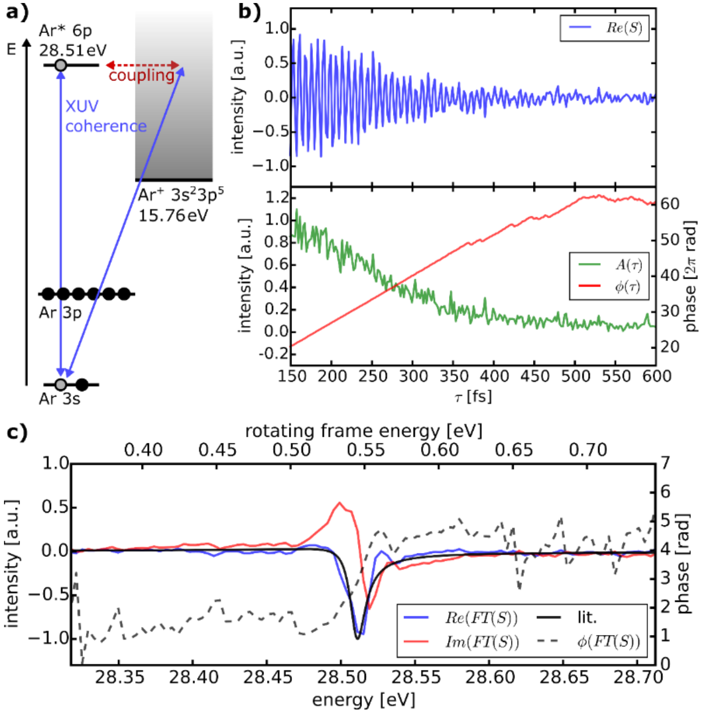


Fig. 1 a) Excitation scheme for preparation and probing of the Ar 3s-6p inner subshell-valence coherence **b)** Demodulated ion signal (real part, amplitude, phase) measured in the rotating frame. **c)** Fourier transform. The characteristic Fano line shape is recovered due to phase sensitive detection

References

[1] A. Wituschek et al., arXiv:1906.07112 (2019)

[2] A. Wituschek et al., Opt. Lett. **44**, 943 (2019)

[3] L. Bruder, U. Bangert, and F. Stienkemeier, Optics Express **25**, 5302 (2017)

Preparing and probing an ultracold fermi gas for atom-ion experiments

Pascal Weckesser, Fabian Thielemann, Isabelle Lindemann, Florian Hasse
Leon Karpa and Tobias Schaetz

Institute of Physics, University of Freiburg, Germany

The interplay of ultracold atoms and ions has gained interest in the atomic physics community [1,2], due to its wide applications in quantum simulations of solid state systems [3] as well as in quantum computing [4]. In order to implement a reliable atom-ion platform, it is necessary to prepare the mixture at ultracold temperatures, where only few partial-waves contribute to the scattering process. Choosing a proper atom-ion mixture with high mass imbalance (as ^{6}Li and ^{138}Ba$^+$) has recently been proposed to be a promising candidate for reaching the quantum limit [5] .

In this talk our setup creating 10^4 ^{6}Li-atoms at a temperature of 50µK will be presented. This cold fermi gas is realized by evaporatively cooling a thermal gas in a crossed optical dipole trap at high magnetic fields. The implementation of these magnetic fields as well as our detection scheme, high field absorption imaging, will be introduced.

As an outlook we discuss our first measurements between a single ^{138}Ba$^+$ ion immersed in a cold cloud of Li atoms. Hereby we observe sympathetic cooling into the few partial-wave regime.

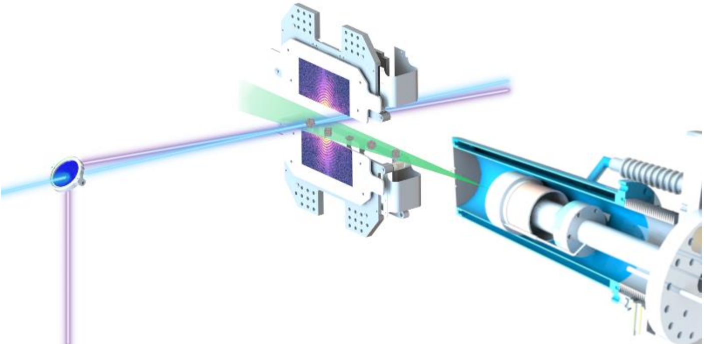
References

[1] A. Haerter et al., Contemporary Physics, volume 55, issue 1, pages 33-45 (2014).
[2] M. Tomza et al. "Cold hybrid ion-atom systems." *arXiv:1708.07832* (2017).
[3] U. Bissbort et al., Phys.Rev.Lett. 111.8 (2013): 080501.
[4] Doerk et al., Phys. Rev. A 81.1 (2010): 012708
[5] M. Cetina et al., Phys.Rev.Lett. 109,253201 (2012).

Time-resolved imaging of the dynamics of free metal clusters and nanocrystals

Simon Dold

Institute of Physics, University of Freiburg, Germany



X-Ray diffraction has been proven a viable tool to determine the 3D structure of metal clusters [1]. The temporal resolution of this technique is only limited by the duration of the FEL x-ray puls (≈100fs) which enables imaging ultrafast processes. Such diffraction experiments on metal clusters in gas-phase are highly demanding as they require high intensities of both, clusters and X-ray beam to vanquish low cross-sections for scattering processes. To overcome this difficulties a carefully taylored source for clusters was set up.
I will report on the results of our efforts to utilize ultrashort X-Ray pulses as a tool to resolve ultrafast processes in nanoscale systems by imaging structure in a time-dependent manner.

References

[1] Ingo Barke, et al. The 3d-architecture of individual free silver nanoparticles captured by x-ray scattering. *Nature communications*, 6, 2015.

Spectroscopy of oligoacene molecules attached to argon clusters

Matthias Bohlen [1], Moritz Michelbach [1], Rupert Michiels [1], Corey Allen Rice [1], Aaron LaForge [1,2], Frank Stienkemeier [1]

[1] Institute of Physics, University of Freiburg, Freiburg, Germany
[2] University of Connecticut, Department of Physics, Storrs, CT, USA

The energy conversion efficiency of solar cells is generally limited by the Shockley-Queisser limit [1]. One way to circumvent this limit is through the use of organic photovoltaics (OPV), where specific charge and energy transfer processes can lead to higher conversion efficiencies. Polyaromatic hydrocarbons such as oligoacene molecules exhibit interesting quantum effects such as singlet fission, triplet-triplet annihilation, or superradiance and make promising candidates for OPV applications. Recently, anthracene, tetracene and pentacene molecules attached to the surface of neon clusters have been shown to provide interesting model systems for detailed studies of such effects [2]. We have extended these measurements to the spectroscopy of oligoacenes deposited to the surface of argon clusters. For this purpose, we developed a liquid-nitrogen-source to cover a wide temperature range for the production of argon clusters. First results show tremendous disturbances of the fluorescence signals due to Rayleigh-scattering from argon clusters, which necessitates an extensive single-shot analysis to extract fluorescence information. First results indicate collective lifetime reducing effects for pentacene attached to argon clusters, exhibiting clear similarities to previous investigations on neon matrices.

[1] W. Shockley and H. J. Queisser, J Appl Phys **32**, 510 (1961)
[2] S. Izadnia et al., J. Phys. Chem. Lett. **8**, 2068 (2017)

Spectroscopy of pentacene dimers in rare gas matrices

M. Michelbach[1], M. Bohlen[1] and F. Stienkemeier[1]

[1]*Institute of Physics, University of Freiburg, Freiburg, Germany*

Oligoacene molecules such as pentacene are promising candidates for organic solar cells which can achieve photon-to-current conversion efficiencies beyond the 30% Shockley-Queisser[1] limit. The underlying process to create multiple charge carriers from a single photon is called singlet fission where an excited molecule can partially transfer energy to a neighboring ground state molecule, and thereby create a correlated triplet pair[2]. This conversion process influences the excitation lifetime of the excited molecule and can be measured via time resolved laser induced fluorescence[3].

A detailed study of this process needs high temporal resolution and a well-known intermolecular distance. To use the advantages of rare gas spectroscopy we need to specify the doping conditions and the size distribution of the cluster beam. Thus, we investigated the cluster sizes with various methods such as the so-called titration method or Rayleigh-scattering to aid a better understanding of collective effects of chromophores attached to these clusters.

A different approach is the deposition of bis-TIPS-pentacene as a „macro-molecule “, accommodating two pentacene molecules in a well-defined distance as a model system[5]. With this we want to investigate an intramolecular singlet fission process in a spectral and time resolved manner.

[1] W. Shockley and H. J. Queisser, J Appl Phys 32, 510 (1961)

[2] M. B. Smith, J. Michl, Chem. Rev. 110, 6891-6936, (2010)

[3] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017)

[4] L. F. Gomez et al.; J. Chem. Phys. **135**, 154201 (2011)

[5] S. R. Reddy, J. Phys. Chem. Lett., 9, 5979-5986, (2018)

Towards Cold Chiral Radicals

Brendan Moore

Department of Chemistry, UBC Faculty of Science, Vancouver, CA

The origins of homochirality, the existence of biological molecules as specifically one enantiomer in living systems, have been a subject of debate in recent years. It has been shown that the presence of enantiomeric excess can be amplified through fundamental chemical processes, leading to a homochiral system. One theory that can explain this enantiomeric excess is the difference in energy between enantiomers of chiral molecules due to parity violation. For most chiral molecules, this energy difference is on the order of mHz to Hz. A recent study by Suzuki *et al.* has shown that chiral radicals have enhanced parity violation energy differences up to kHz. In combination with molecular slowing techniques, this energy difference is feasible to measure experimentally. Zeeman deceleration has been proven effective for slowing and trapping of radicals, and is therefore a suitable technique for the trapping of chiral radicals. We will characterize the chiral radical production by photolysis and electric discharge in combination with matrix isolation spectroscopy in solid parahydrogen. Our initial radical production studies as well as matrix-isolated spectroscopic studies of the parent molecule used for radical production will be presented.

Photoisomerization of azobenzene and its substituted derivatives: the effect of Protonation

M. Ari[1], S. Kalthoum[1], and M. Walter[1,2]

1Institute of Physics, University of Freiburg, Freiburg, Germany

2Fraunhofer IWM, MikroTribologie Centrum TC, Freiburg, Germany

One of the most used organic chromophores for optical switching applications are azobenzenes. Azobenzenes exhibit a reversible isomerisation process between its trans and cis isomers of different stability. After a photochemical conversion, the spontaneous thermal back reaction occurs. While the photoinduced trans-to-cis isomerisation reaction can be performed in a few femtoseconds, the rate of the thermal cis-to-trans back reaction depends greatly on the chemical architecture of the system and the environment [1]. While slow thermally back-isomerising azoderivatives are valuable photoactive basic materials for information storage purposes, transmitting at the molecular scale with response times within the nanosecond or picosecond range will enable the potential application of azobenzene-based materials in micropumps and autonomous valves. Novel absorption spectroscopy experiments have shown that the rate of thermal back-isomerization is strongly dependent on pH [2].

With the purpose of understanding the mechanism underlying the isomerization and the changes in reaction paths and energy barriers due to protonation, in collaboration with the group of Andreas Walther from the Institute of Macromolecular Chemistry in Freiburg, we investigated the protonation sites of an azo-derivative (Arylazopyrazole structure (AAP)). Large effects on back reaction rates were observed experimentally. We computationally explored the relative energy profiles for the isomerization along the CNNC-dihedral angle of unprotonated and protonated AAP. We've found out that protons clearly prefer to be placed at the azo-bridge and while unprotonated form prefers rotation path for the back-isomerization, the protonated form prefers inversion. The effect of different substitution patterns is investigated also by substitution of a methoxy group. Methoxy substitution change the basic character from cis isomer to trans.

[1] Beilstein J. Org. Chem. 2012, 8, 1003.
[2] J. Phys. Chem. A 2009, 113, 13144.

Two-dimensional electronic spectroscopy of molecules in helium nanodroplet isolation

U. Bangert, L. Bruder, M. Binz, D. Uhl, and F. Stienkemeier

Institute of Physics, University of Freiburg, Germany

We present the first two-dimensional electronic spectroscopy (2DES) study of cold molecules (sub Kelvin internal temperature) prepared by helium nanodroplet isolation (HENDI) [1]. In contrast to conventional pump-probe spectroscopy, 2DES reveals coherent and incoherent dynamics in molecular systems, giving detailed insight into system-bath interactions, charge/energy transfer and structural changes [2]. Until now, most 2DES studies were conducted with liquid/solid phase samples, due to their high target density. However, with the recent development of highly sensitive methods, dilute gas phase samples like molecular beams have become accessible. The HENDI technique is of special interest, since it provides internally cold molecules and flexible doping capabilities. The latter is used to synthesize arbitrary molecular complexes.

As a first benchmark system, we studied weakly bound Rb molecules attached to helium nanodroplets. Our results, including dynamics due to molecule-matrix interaction, show the applicability of 2DES to samples with extreme low target densities ($\leq 10^7 \mathrm{cm}^{-3}$).

The final goal of the project is to study charge transfer in organic complexes. We currently take the next step by investigating our first organic molecule, Phthalocyanine, embedded in helium nanodroplets.

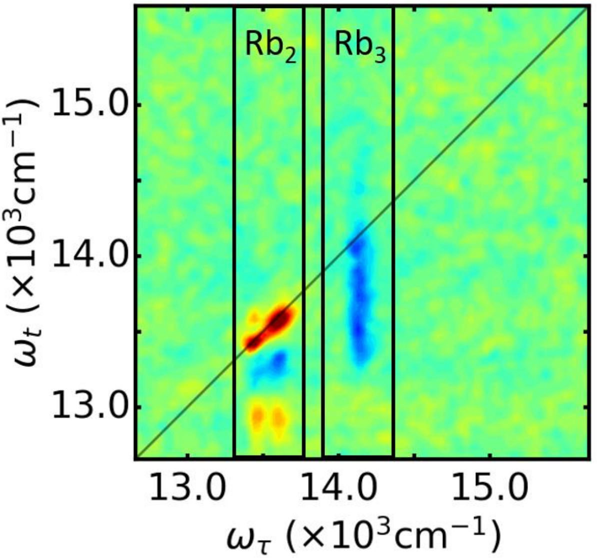


Figure 1

2D-spectrum of Rb_2 *and* Rb_3 *attached to helium nanodroplets at a pump probe delay of 200fs.* ω_τ *and* ω_t *are the pump and probe frequency respectively. The* Rb_2/Rb_3 *features are assigned by comparison of the spectral profile along the pump axis to high-resolution absorption spectra.*

References

[1] L. Bruder et al., *Nature Communications* 9: 4823, (2018).

[2] F. D. Fuller & J. P. Ogilvie, *Annual Review of Physical Chemistry* 66, 667–690 (2015).

High intensity effects in two-dimensional electronic spectroscopy

M. Binz[1], U. Bangert[1], L. Bruder[1], F. Landmesser[1], D. Uhl[1], L. Chen[2], M. F. Gelin[2], W. Domcke[2], and F. Stienkemeier[1]

[1] *Institute of Physics, University of Freiburg, Germany*
[2] *Chemistry Department, Technical University of Munich, Germany*

Usually, two-dimensional electronic spectroscopy (2DES) experiments are performed in the regime where perturbation theory holds and the signal can be described by the third-order polarization. However, to measure nonlinear signals, higher laser intensities are generally of advantage as the signal scales with higher order of the incident light fields. Furthermore, new 2DES schemes have been implemented [1,2] where tight focusing is crucial and thus laser intensities beyond the weak-perturbation limit may be reached. Recently, a theoretical description for 2DES experiments beyond the weak perturbation limit has been reported [3] showing peak shape distortions and phase shifts, which may be exploited to gain additional information but can also lead to artifacts. In collinear 2DES experiments, we explore these high intensity effects in our lab by studying a simple, clean model system comprising of a rubidium atom vapor. By comparing these experiments with simulations, we hope to get a direct intuition of intensity effects in 2D spectroscopy.

References

[1] V. Tiwari, Y. A. Matutes, A. T. Gardiner, T. L. C. Jansen, R. J. Cogdell, and J. P. Ogilvie, Nat Commun **9**, 4219 (2018)

[2] S. Goetz, D. Li, V. Kolb, J. Pflaum, and T. Brixner, Opt. Express **26**, 3915-3925 (2018)

[3] L. Chen, E. Palacino-González, M. F. Gelin, and W. Domcke, J. Chem. Phys. **147**, 234104 (2017)

Many-body effects in cold molecules using phase-modulated two-dimensional coherent spectroscopy

Friedemann Landmesser, Ulrich Bangert, Lukas Bruder, Marcel Binz, Daniel Uhl and Frank Stienkemeier

Institute of Physics, University of Freiburg, Germany

Many-body quantum states are considered to play a crucial role in atomic and molecular systems with respect to dissipation as well as excitation and energy transfer processes (cf. quantum efficiencies of biological light harvesting complexes [1]). We aim to investigate collective effects in organic molecules by multiple-quantum coherence experiments where multiphoton processes can be separated from one-photon transitions and can be assigned to specific particle numbers [2,3]. In a first step, we will adapt a detection scheme based on phase-modulated two-dimensional coherent spectroscopy which was already used to investigate multi-atom Dicke states in potassium vapor [2,4]. Measurements on a rubidium vapor will serve as a benchmark. To apply the detection scheme to organic molecular systems, we will adapt our helium nanodroplet source to produce solid rare gas clusters, that can be doped with hundreds of organic molecules. The cluster surface acts as a well-defined, cold environment [5]. In lifetime measurements, collective effects of weakly interacting organic molecules have already been identified at increasing doping densities [5].

[1] F. Fassioli, R. Dinshaw, P. C. Arpin, and G. D. Scholes, J. Royal Soc. Interface 11, 20130901 (2014).
[2] S. Yu et al., Opt. Lett. 44, 2795 (2019).
[3] L. Bruder, M. Binz, and F. Stienkemeier, Phys. Rev. A 92, 053412 (2015).
[4] L. Bruder et al., Phys. Chem. Chem. Phys. 21, 2276 (2019).
[5] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).

Production of Ultracold Lithium Triplet Dimers by STIRAP

Denis Uhland, Erik Frieling, Gene Polovy, Kirk Madison

University of British Columbia

Ultra-cold atomic ensembles have enabled experimental studies of few and many-body quantum phenomena including topological insulators, many-body pairing phenomena, and superfluidity. The use of ultra-cold molecular ensembles is expected to provide access to even richer phenomena than atoms due to their complex internal structure. Cold molecules are also key to studying and understanding chemistry near T=0 where reactions are dominated by quantum effects. Motivated by this, we have developed an experimental apparatus that can produce Li dimers from laser-cooled Li atoms and, eventually, LiRb molecules from Li+Rb atomic ensembles. Beginning with a gas of Li atoms, we form loosely bound Feshbach dimers by evaporation near a Feshbach resonance. We then manipulate the internal state of these molecules, transferring them into deeply bound ro-vibrational levels of the $a(1^3\sum^{+}{}_{\mathrm{u}})$ triplet potential using stimulated Raman adiabatic passage (STIRAP). Having the possibility to transfer an ultra-cold molecular ensemble to different quantum states immediately opens the window for studies in ultra-cold chemistry.

Initial-state dependence of the long-time dynamics in a spin-boson system

Sebastian Wenderoth and Michael Thoss

Institute of Physics, University of Freiburg, Germany

Thermalization of a system refers to the process of approaching a unique steady state that depends only on a few macroscopic observables. Triggered by the development of new experimental tools, for example in cold atom or trapped ion experiments, the question how an isolated quantum system can equilibrate to such a state under its own dynamics has recently received renewed interest. Various numerical studies suggest that subsystems of isolated quantum systems can equilibrate under unitary time evolution. This relaxation is caused by the remainder of the system acting as an effective bath. However, as the hybridization between the subsystem and the remainder increases this simple picture breaks down and the influence of the remainder on the subsystem can change qualitatively.

Inspired by a recent experiment with trapped-ions [1], we investigate a special type of a spin-boson model. Employing the multilayer multiconfiguration time dependent Hartree method [2], we simulate the dynamics of the system in a numerically exact way. As a function of the spin-boson coupling, we observe a qualitative change of the dynamics of the spin, induced by the coupling to the bosonic modes, ranging from the usual relaxation dynamics for small couplings to non-stationary long-time states of the spin that depend on its initial state.

References

[1] G.Glos et al., Phys. Rev. Lett. 117, 170401 (2016)
[2] H. Wang et al., J. Chem. Phys. 119, 1289 (2003)

Development of a software based lock-in amplifier for phase-modulated spectroscopy

D. Uhl[1], M. Binz[1], U. Bangert[1], F. Landmesser[1] and F. Stienkemeier[1]

[1]*Institute of Physics, University of Freiburg, Germany*

Two-dimensional electronic spectroscopy (2DES) is a powerful tool to study coherences and correlations on ultrafast time scales. We implemented a 2DES setup combined with a doped helium droplet beam in our lab. However, the target density in doped helium droplet beams is several orders of magnitudes lower than in bulk condensed phase samples. We adapted a phase modulation technique [1] that introduces a lock-in detection to overcome this issue.

To further improve our detection scheme, we developed a software based lock-in amplifier. This offers the possibility to demodulate our signal at different harmonics and thus gives us the advantage to observe any desired separate multiphoton processes in the pre-analysis. The algorithm is mainly based on a digital phase locked loop to detect the phase and frequency of the incoming reference signal. Hence, it is possible to demodulate the signal for different harmonics by conserving the phase information. It also provides a much higher flexibility with our measurements such as simultaneous detection with custom demodulator and filters algorithms or individually optimized acquisition times for specific applications.

References

[1] P. F. Tekavec, G. A. Lott and A. H. Marcus, J. Chem. Phys. 127, 214307 (2007)

The Auger Effect in Dispersing and Absorbing Environments

J. Franz[1], R. Bennett[1,2], and S. Y. Buhmann[1,2]

[1]*University of Freiburg, Germany*
[2]*Freiburg Institute for Advanced Studies, Germany*

The Auger effect is the radiationless decay of an inner-shell ionised atom. In this process, the atom relaxes by filling the inner vacancy with an outer shell electron, but instead of releasing the excess energy in form of a photon (spontaneous decay) the energy is reabsorbed by another electron belonging to the same atom. This effect finds many applications: for example in Auger electron spectroscopy, it is used to study material properties of surfaces. It is well established that dielectric environments can have a significant impact on spontaneous decay (Purcell effect) [1] as well as interatomic energy transfer rates [2]. We present a general expression for the intra-atomic Auger process in the presence of dielectric environments that can be used both as a new starting point for ab initio quantum chemistry, or within the quantum-optical formalism of macroscopic quantum electrodynamics in order to circumvent complex numerics. Within our description, the decay rate can be given in analytical form for some simple environments. We compare Auger decay with a competing process known as interatomic Coulombic decay, focussing on their behaviour in the presence of surfaces.

REFERENCES

1. Purcell, E. M., *Proc. Am. Phys. Soc.*, Vol. 69, 674, 1946.
2. Hemmerich, J. L., R. Bennett, and S. Y. Buhmann, *Nature Commun.*, Vol. 9, 2934, 2018.

Rotational motion of carbon disulfide in helium nanodroplets

Jordan Fordyce, Ian MacPhail-Bartley, Frank Stienkemeier*, and Valery Milner

Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada
**Physikalisches Institut, Universität Freiburg, Freiburg, Germany*

Nanodroplets ideally capture single carbon disulfide molecules and are then exposed to two laser beams to study the behaviour of fast rotating molecules immersed in superfluid helium. The first beam excites the molecule to some rotational state and the second beam, a femtosecond “probe”, ionizes the molecules. The first “pump” beam can be a femtosecond “kick” pulse or a laser pulse whose linear polarization undergoes accelerated rotation around the direction of the laser beam , called an “optical centrifuge”, that excites molecules to extreme rotational states. The recorded velocity map ion image is analyzed to study the dynamics of the rotational state by quantifying the degree of confinement of the molecules to the rotational plane.

Driving a rigid rotor to an extreme rotational state confines the molecules to the plane almost perfectly, but the bonds are actually soft and can stretch. Molecules like nitrogen spin like rigid rotors, but molecules like carbon disulfide have their rotational motion strongly affected by centrifugal distortion. For carbon disulfide this type of behaviour occurs at high rotational frequencies; around 5.5 THz 1 , even though the optical centrifuge can spin up to 10 THz. A helium droplet may couple to a superrotor and prevent rotational motion by amplifying the centrifugal distortion experienced by the molecule 2, lowering the final rotational frequency.

It has been demonstrated that for some molecules the rotational dynamics in helium are the same when excited by a kick pulse but others are impacted by the centrifugal distortion. This new development could explain some of the challenges exciting molecules with the optical centrifuge. Moving forward, a kick pulse can be used as an indication of the expected degree of planar confinement for candidate molecules to be driven by the centrifuge. The first step in doing this is to benchmark our operating point using carbon disulfide.

1: A. Milner, et al., J. Chem. Phys., **147** , 124202 (2017)
2: I. Cherepanov, et al., arXiv:1906.12238 (2019)

Energy difference between chiral enantiomers induced by weak interactions

Fumika Suzuki

Department of Physics / Chemistry, University of British Columbia, Vancouver, CA

Many molecules are chiral which can exist in left- and right-handed forms. There is an important scientific mystery relating to chiral molecules. It is known that living cells are homochiral, namely they are normally consist exclusively of left-handed amino acids. It has been proposed that the electroweak force affects left- and right-handed chiral molecules differently and that enantiomers do not have the same electronic energies due to the parity violating weak neutral current interaction mediated by Z bosons. It is then suggested that the discrimination of enantiomers by the electroweak force may be related to the symmetry breaking that caused the emergence of homochirality in the early universe. In this talk, I will discuss the energy difference of four-atom chiral molecules arising from the electroweak interactions and its dependence on geometry of the molecule.

Quantum state dependent chemistry of ultra-cold 6Li2 dimers

Erik Frieling

Department of Physics and Astronomy, The University of British Columbia,
Vancouver, CA

Reactive and inelastic collisions of ultra-cold molecules has generally been observed to follow a universal rate law described by the quantum Langevin model. The salient feature of this law is an independence of the reaction probability from the short-range physics of the interaction. We report on reactive and inelastic collisions of 6Li2 dimers in several ro-vibrational states of the a(13Σ+u) potential. While the v = 0, 5, 8 are observed to decay at the universal limit, decay of the |v = 9, N = 0⟩ state exhibits a deviation from universality, opening up the possibility of using external magnetic fields to tune the reaction rate.

Fragmentation channels of pentacene and pentacene embedded in helium nanodroplets upon electron impact ionization

A. Scognamiglio, N. Rendler, R. Michiels, B. von Issendorff, K. Dulitz and F. Stienkemeier

Institute of Physics, University of Freiburg, Freiburg, Germany

The isolation of atoms, molecules and molecular complexes in rare-gas cluster beams, and particularly in helium nanodroplets, offers a versatile method for the study of energetic and dynamical properties of these systems, because the cluster environment provides low temperature conditions with minimal perturbation by the environment[1]. The interaction of the molecule with the cold He environment leads to a strong cooling of the molecular degrees of freedom. In that case, He nanodroplets may freeze some of the fragmentation channels observed in an effusive beam, especially those which appear after subsequent fragmentation of short-lived decomposition intermediates[2], [3], [4]. Moreover, depending on whether the helium nanodroplets are formed in the subcritical or supercritical regime, it is expected that the charge-transfer mechanism to the dopant competes with the fragmentation of the helium clusters [5], [6]. In addition to charge-transfer ionization, Penning ionization is also playing a role in the observation of multiply-ionized parent ions [7].

In this contribution, preliminary results of pentacene fragmentation pathways in the absence and in the presence of He nanodroplets are presented. In addition to that, first characterization measurements of the He droplet source will be discussed.

[1] F. Stienkemeier and K. K. Lehmann, “Spectroscopy and dynamics in helium nanodroplets,” *J. Phys. B At. Mol. Opt. Phys.*, vol. 39, no. 8, pp. R127–R166, Apr. 2006.

[2] W. K. Lewis *et al.*, “Electron Impact Ionization in Helium Nanodroplets: Controlling Fragmentation by Active Cooling of Molecular Ions,” *J. Am. Chem. Soc.*, vol. 126, no. 36, pp. 11283–11292, Sep. 2004.

[3] S. Yang, S. M. Brereton, M. D. Wheeler, and A. M. Ellis, “Electron Impact Ionization of Haloalkanes in Helium Nanodroplets,” *J. Phys. Chem. A*, vol. 110, no. 5, pp. 1791–1797, Feb. 2006.

[4] S. Denifl, “Formation of cations and anions upon electron interaction with (doped) helium droplets,” *Eur. Phys. J. Spec. Top.*, vol. 222, no. 9, pp. 2017–2033, Oct. 2013.

[5] T. Ruchti, B. E. Callicoatt, and K. C. Janda, “Charge transfer and fragmentation of liquid helium droplets doped with xenon,” *Phys. Chem. Chem. Phys.*, vol. 2, no. 18, pp. 4075–4080, 2000.

[6] W. K. Lewis, C. M. Lindsay, R. J. Bemish, and R. E. Miller, “Probing Charge-Transfer Processes in Helium Nanodroplets by Optically Selected Mass Spectrometry (OSMS): Charge Steering by Long-Range Interactions,” *J. Am. Chem. Soc.*, vol. 127, no. 19, pp. 7235–7242, May 2005.

[7] H. Schöbel *et al.*, “Sequential Penning Ionization: Harvesting Energy with Ions,” *Phys. Rev. Lett.*, vol. 105, no. 24, Dec. 2010.

Trapping polyatomic molecules using Microwaves inside a superconducting cavity

Manish Vashishta[1], Katsunari Enomoto[2],Pavle Djuricanin[1],Takamasa Momose[1]

University of British Columbia[1], Vancouver, Canada
University of Tayoma[2], Japan

The trapping of molecules in microwave fields was proposed many years ago [1], but it has not been realized so far. In the last several years we have been investigating the manipulation and trapping of polyatomic molecules using strong microwave field created in superconducting microwave cavity [2]. Here we report our latest progress on the possibility of trapping molecules in a microwave trap we are developing.

Here, microwave radiations close to the inversion doublet splitting in para-ammonia with quantum numbers, |J,K >= |1, 1 > are applied to a superconducting cavity at a temperature of 3 K. A superconducting cavity with a high-quality factor will provide a deep potential to manipulate motions of polar molecules. We will discuss the characterization of the cavity by measuring the quality factor at various temperature from 298 K to 3 K. We will also discuss the AC stark shifts of NH3 molecules under the fields, which we are currently working on.

Our discussion is based on using this cavity for trapping stark decelerated NH3 molecules. The successful demonstration of trapping NH3 molecules inside a microwave trap will open new pathways to cool polyatomic molecules below 1 mK via sympathetic cooling. Development of microwave trap will enable us to trap the ground state of polar polyatomic molecules. These ground state molecules are best suited for sympathetic cooling with ultra-cold atomic gases due to their low losses during the thermalization process.

References:

1. . DeMille, D. R. Glenn, J. Petricka. The European Physical Journal D - Atomic, Molecular, Optical and Plasma Physics, 2004, Volume 31, Number 2, Page 375,D

2. -Katsunari Enomoto, Pavle Djuricanin, Ilja Gerhardt, Omid Nourbakhsh, Yoshiki Moriwaki, Walter Hardy, Takamasa Momose. Applied Physics B, 2012, Volume 109, Number 1, Page 149

Thermometry of a single trapped ion immersed in an ultracold atomic gas

Fabian Thielemann, Pascal Weckesser, Isabelle Lindemann, Florian Hasse
Leon Karpa and Tobias Schaetz

Institute of Physics, University of Freiburg, Germany

Atom-ion mixtures at ultracold temperatures could provide an interesting system to investigate quantum phenomena of long-range attractive potentials [1,2]. Reaching temperatures below the s-wave threshold, at which only a single partial wave contributes to the scattering process, is of special interest for experimental control of the interaction. This regime could be reached by sympathetic cooling of a heavy ion ($^{138}Ba^+$), trapped in a radio-frequency trap, with a light coolant (^6Li) [3].

In this talk we will present and characterize our method to measure the temperature of a single trapped ion. As the intended application, we will show first results that demonstrate sympathetic cooling of a barium ion in a cloud of lithium at a temperature of approximately 50µK.

References

[1] A. Haerter et al., Contemporary Physics, volume 55, issue 1, pages 33-45 (2014).

[2] M. Tomza et al. "Cold hybrid ion-atom systems." *arXiv:1708.07832* (2017).

[3] M. Cetina et al., Phys.Rev.Lett. 109,253201 (2012).

100 kHz Attosecond Pulse Source for Coincidence Spectroscopy

Dominik Ertel[1*], Anna-Lena Jäger[1], Samuel Kellerer[1], Matteo Moioli[1], Hamed Ahmadi[1], Fabio Frassetto[2], Luca Poletto[2] and Giuseppe Sansone[1]

[1]Institute of Physics, University of Freiburg, Freiburg, Germany
[2]CNR-Institute of Photonics and Nanotechnologies (CNR-IFN), Padova, Italy
**dominik.ertel@physik.uni-freiburg.de*

Attosecond coincidence spectroscopy builds a powerful tool to study ultrafast phenomena in atoms and molecules [1, 2, 3]. Here, we present an attosecond extreme ultraviolet (XUV) pulse source with high repetition rates up to 100 kHz, developed for photoelectron/-ion coincidence spectroscopy. Near-infrared (NIR) laser pulses with up to 400 µJ pulse energy and a pulse duration of around 300 fs are temporally compressed using a gas-filled hollow-core fiber [4, 5]. Afterwards, we use these pulses to generate trains of attosecond pulses via high-order harmonic generation in noble gases. RABITT (Reconstruction of Attosecond Beating by Interference of Two-photon Transitions) based coincidence pump-probe spectroscopy is performed using a reaction microscope. The long acquisition measurements require an ultrastable control of the delay between pump (XUV) and probe (NIR). A novel non-interferometric delay line enables intrinsic delay synchronization within a few attoseconds over several hours. Our coincidence spectroscopy setup will enable the investigation of electronic and coupled electronic-nuclear dynamics. This could shed new light on the first instants of photoionization and subsequent nuclear dynamics in small-sized molecules.

References

[1] F. Krausz et al., Rev. Mod. Phys. **81**, 163 (2009).
[2] J. Vos et al., Science, **360**, 1326 (2018).
[3] L. Cattaneo et al., Nature Physics, **14**, 733 (2018).
[4] M. Nisoli et al., Appl. Phys. Lett. **68**, 2793 (1996).
[5] J. Beetar et al., J. Opt. Soc. Am. B **36**, A33 (2019).

Singlet fission in Pentacene dimers on top of Argon cluster surfaces

Selmane Ferchane

Institute of Physics, University of Freiburg, Germany

Singlet fission (SF) is a spontaneous photoexcited splitting phenomenon in which an organic chromophore in an excited singlet state shares its energy with a neighboring chromophore in ground-state converting into a pair of triplet excited states. Singlet fission is a process that holds a potential to supplant the traditional solar energy conversion scheme (Shockley–Queisser limit) as a great promise for future photon-to-current conversion solar energy organic materials with high efficiencies. Although, the singlet fission process has been known since decades, as the phenomena remains relatively obscure about how the mechanism is undergoing to this day.

In order to get more insight into these processes, we investigate pentacene dimer chromophores on top of Argon cluster within density functional theory (DFT). Similar systems are experimentally studied in the Stienkemeier group. In the first step, a number of Pentacene dimers with different spatial configurations are studied in space and on top of the Argon cluster surfaces. We calculate binding energies, most favorable positions with lowest ground state energy and other ground state properties prior to the investigation of singlet fission phenomenon itself.

Using Gaussian processes with composite kernels to interpolate and extrapolate global potential energy surfaces

Jun Dai

University of British Columbia[1], Vancouver, Canada

Gaussian process regression has recently emerged as a powerful, system-agnostic tool for building global potential energy surfaces (PES) of polyatomic molecules. While the accuracy of GP models of PES increases with the number of potential energy points, so does the numerical difficulty of training and evaluating GP models. Here, we demonstrate an approach to improve the accuracy of global PES without increasing the number of energy points. The present work reports four important results. First, we show that the selection of the best kernel function for GP models of PES can be automated using the Bayesian information criterion as a model selection metric. Second, we demonstrate that GP models of PES trained by a small number of energy points can be significantly improved by iteratively increasing the complexity of GP kernels. The composite kernels thus obtained maximize the accuracy of GP models for a given distribution of potential energy points. Third, we show that the accuracy of the GP models of PES with composite kernels can be further improved by varying the training point distributions. Fourth, we show that GP models with composite kernels can be used for physical extrapolation of PES. We illustrate the approach by constructing the six-dimensional PES for H_3O^+. For the interpolation problem, we show that this algorithm produces a global six-dimensional PES for H_3O^+ in the energy range between zero and 21,000 cm^{-1} with the root mean square error 65.8cm^{-1} using only 500 randomly selected {\it ab initio} points as input. To illustrate extrapolation, we produce the PES at high energies using the energy points at low energies as input. We show that one can obtain an accurate global fit of the PES extending to 21,000 cm^{-1} based on 1500 potential energy points at energies below 10,000 cm^{-1}.

Quantum-state-controlled Penning collisions between lithium atoms and metastable helium atoms

Tobias Sixt, Jiwen Guan, Markus Debatin, Frank Stienkemeier, and Katrin Dulitz

Institute of Physics, University of Freiburg, Germany

Our work is aimed at understanding the mechanistic details of reactive collisions and at controlling the outcome of chemical reactions. In our experiment, we study quantum-state-controlled Penning collisions between lithium atoms (Li) and metastable helium atoms (He*) at various collision energies, e.g., to study the influence of electron-spin polarization on the reaction rate. For this, we have combined a supersonic beam source for He* atoms with a magneto-optical trap (MOT) for Li atoms.[1] Our initial investigations have shown that the reaction rate dramatically depends on the initial electronic states of the reaction partners. In order to get full quantum-state control of the reaction partners, the Li atoms are optically pumped into selected electronic hyperfine and magnetic substates. Additionally, we produce a pure beam of He(2^3S_1) by the optical depletion of the He(2^1S_0) state using a novel excitation scheme.[2] In this contribution, I will give an overview over the different methods used to achieve quantum-state control of the reaction partners and I will discuss experimental results that show the dependence of the reaction rate on the initial electronic state of both He* and Li.

References

[1] J. Grzesiak, T. Momose, F. Stienkemeier, M. Mudrich and K. Dulitz, *J. Chem. Phys.* **150**, 034201 (2019).

[2] J. Guan, V. Behrendt, P. Shen, S. Hofsäss, T. Muthu-Arachchige, J. Grzesiak, F. Stienkemeier and K. Dulitz, Phys. Rev. Applied **11**, 054073 (2019).

List of Participants

UBC & UF PI's

Stefan Buhmann, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Katrin Dulitz, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Edward Grant, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Bernd von Issendorff, Institute of Physics, University of Freiburg, Stefan-Meier-Str. 20, 79104 Freiburg, Germany.

Roman Krems, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Kirk Madison, Department of Physics & Astronomy, Vancouver Campus, 325 - 6224 Agricultural Road, Vancouver, BC V6T 1Z1

Valery Milner, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Takamasa Momose, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Giuseppe Sansone, Institute of Physics, University of Freiburg, Stefan-Meier-Str. 19, 79104 Freiburg, Germany.

Michael Walter, Freiburger Materialforschungszentrum (FMF), Stefan-Meier-Str. 19, 79104 Freiburg, Germany.

Tobias Schätz, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Frank Stienkemeier, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Michael Thoss, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Alexander Wang, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

VISITING SCIENTISTS

Ilya Averbukh, Department of Chemical Physics, Weizmann Institute of Science, Rehovot 76100, Israel.

Tatsuhisa Kato, Institute for the Promotion of Excellence in Higher Education, Kyoto University, Yoshida Nihonmatsu-cho, Kyoto 606-8501, Japan.

PARTICIPANTS

Meral Ari, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Ulrich Bangert, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Marcel Binz, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Matthias Bohlen, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Colton Carlson, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Jun Dai, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Simon Dold, Institute of Physics, University of Freiburg, Stefan-Meier-Str. 20, 79104 Freiburg, Germany.

Dominik Ertel, Institute of Physics, University of Freiburg, Stefan-Meier-Str. 19, 79104 Freiburg, Germany.

Selmane Ferchane, Institute of Physics, University of Freiburg, Stefan-Meier-Str. 19, 79104 Freiburg, Germany.

Jordan Fordyce, Department of Physics and Astronomy, 6224 Agricultural Road, Vancouver, BC Canada V6T 1Z1.

Janine Franz, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Erik Frieling, Department of Physics and Astronomy, 6224 Agricultural Road, Vancouver, BC Canada V6T 1Z1.

Jiahong Hu, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Friedemann Landmesser, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Moritz Michelbach, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Brendan Moore, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Audrey Scognamiglio, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Pinrui Shen, Department of Physics and Astronomy, 6224 Agricultural Road, Vancouver, BC Canada V6T 1Z1.

Tobias Sixt, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Fumika Suzuki, Department of Physics / Chemistry, University of British Columbia, 6224 Agricultural Road/2036 Main Mall, Vancouver BC, V6T 1Z1.

Fabian Thielemann, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Daniel Uhl, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Denis Uhland, Department of Physics and Astronomy, 6224 Agricultural Road, Vancouver, BC Canada V6T 1Z1.

Manish Vashishta, Department of Chemistry, UBC Faculty of Science, Vancouver Campus, 2036 Main Mall, Vancouver, BC Canada V6T 1Z1.

Perrin Waldock, Department of Physics and Astronomy, 6224 Agricultural Road, Vancouver, BC Canada V6T 1Z1.

Pascal Weckesser, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Sebastian Wenderoth, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Andreas Wituschek, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

IRTG 2079 Annual Convention 2019

5th to 9th August

UBC Vancouver Campus, Canada

	Monday, August 5th	Tuesday, August 6th	Wednesday, August 7th	Thursday, August 8th	Friday, August 9th
		Welcome			
9:00	Excursion	PI Lecture Ilya Averbukh	PI Lecture Alexander Wang	PI Lecture Katrin Dulitz	PhDs personal Meeting Stefan Buhman Michael Walter
9:30		PI Lecture Valery Milner			
10:00	Whale Watching Tour 7:00 - 2:00		PostDoc Presentation Meral	PhD Presentation Jordan	
10:30		Break	Break	Break	Break
11:00		PhD Presentation Andreas	PhD Presentation Uli	PostDoc Presentation Fumika	PhD Presentation Selmane
11:30		PhD Presentation Pascal	PhD Presentation Marcel	PhD Presentation Erik	PhD Presentation Jun
12:00		PhD Presentation Simon	PhD Presentation Friedemann	PhD Presentation Audrey	PhD Presentation Tobias
12:30		Lunch	Lunch	Lunch	Lunch
01:00					
01:30		PhD Presentation Matthias	PhD Presentation Sebastian	PhD Presentation Manish	Closing Session
02:00		PhD Presentation Moritz	PhD Presentation Daniel	PhD Presentation Fabian	
02:30		PhD Presentation Brendan	PhD Presentation Janine	PhD Presentation Dominik	
03:00		Break	Break	Break	Break
03:30	Museum of Anthropology (MOA) 4:00 - 6:00	PI Meeting	Poster-session PAC 2	Poster-session PAC 3	PAC 5
04:00					Lab Tour
04:30		PAC 1	Soccer Game		
05:00				PAC 4	
05:30		Lab Tour		Final Dinner Sunset Dinner Cruise	
06:00					
06:30		PI Dinner Dinner			
7:00	Dinner		Dinner		
07:30					
8:00			After Dinner Talk Edward Grant		
08:30					Free evening