COURTYARD Hotel Berlin – Köpenick
Grünauer Str. 1, 12557 Berlin

21.-23. August 2005

Book of Abstracts
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Preface

Dear Colleagues,

The James Franck Symposium is one of the major highlights of the very active and successful Israeli – German collaboration in chemical physics and physical chemistry. Since 1989 the symposium has established an outstanding platform for the exchange of ideas and resulted in successful joint efforts to explore laser matter interaction with molecules, clusters, nano-structures, ultracold atomic and molecular systems and even biologically relevant molecules. Additional stimulus arose from the so called James-Franck-Programme - a small but very important resource for financial support into cutting edge research through the German Minerva foundation and several universities in Israel.

The symposium is held typically in annual alternation in Germany and Israel, the year 2005 sees this meeting for the first time in Berlin. This is at the place where James Franck and Gustav Hertz performed their pioneering work on electron excitation of atoms which was instrumental in establishing the quantum nature of atomic structure – the work for which they received the Nobel prize in 1925. What an auspicious coincidence to meet exactly 80 years later here in Berlin, during the internationally celebrated Einstein year, in the honour of James Franck!

The present programme summarized in this little book of abstracts, appears quite adequate to honour this occasion. With a focus on spectroscopy, ultrafast dynamics and function of complex systems, ranging from small clusters in the gas phase via nano-systems and bio-molecules in the gas phase, on surfaces and in condensed matter all the way to Bose-Einstein condensates of ultracold molecules. The programme offers a truly exciting and challenging approach to stimulate further progress in this rapidly evolving field of research between physics, chemistry, material- and laser-science.

Following tradition, the culmination of this symposium is the James-Franck-Lecture honouring the contribution of a distinguished scientist to our field. In this year the James-Franck-Lecturer is Moshe Shapiro. His theoretical and experimental work on quantum control belongs to the recent milestones in the whole field of laser chemistry. The lecture will be given in the Leibniz Hall of the Berlin–Brandenburg Academy of Science – located at Berlins most beautiful, historical city-square. Thus we are looking forward to a truly outstanding and memorable occasion.
Such an international meeting cannot be arranged without substantial financial resources. I want to express our profound thanks to the 4 funding institutions, the Max Born Institute, Berlin, the Max Planck Institute for Quantum Optics, Garching, the Hebrew University Jerusalem and the Tel Aviv University for their strong support without which this all would not have happened.

While these organisations provided the major part of the expenses, there are additional things which are nice to have and may -outside the scientific programme- give the symposium its ultimate attractiveness, but cannot be financed through taxpayers moneys. We have, however, been fortunate to find several very generous private sponsors which are listed on the next page. We are very grateful to them for enabling these important aspects of any successful conference and express our deep thanks. More will have to be said about people involved in the preparation and organisation of the meeting. This will be done in due course during the conference.

Welcome thus to Berlin. We wish you three stimulating, personally as well as scientifically rewarding days in Berlin

And of course we hope you will find the time to visit the Max Born Institute next Wednesday morning.

Berlin, 21\textsuperscript{st} August 2005  
Ingolf Hertel
SPONSORS

Schering AG
Müllerstr. 178, Berlin-Mitte
http://www.schering.de

Berliner Glas KGaA
Herbert Kubatz GmbH & Co.
Waldkraiburger Str. 5, 12347 Berlin
http://www.berlinerglas.de

Institute for Scientific Instruments GmbH
Rudower Chaussee 29/31, 12489 Berlin
http://www.ifg-adlershof.de

OpTecBB e. V.
Rudower Chaussee 25, 12489 Berlin
http://www.optecbb.de

Wista Management GmbH
Rudower Chaussee 17, 12489 Berlin
http://www.wista.de
Organisation

Local organization

Chair: Prof. Dr. Ingolf V. Hertel

Conference Secretary: Catrin Lekve
Tel.: ++49 – 30 – 65479 154 (at the conference site), Email: lekve@mbi-berlin.de

Associates: Dr. Claus-Peter Schulz
Dr. Thomas Schultz
Dr. Tim Laarmann

Max Born Institute (MBI), Berlin-Adlershof, Tel.: ++49-30-6392 1201
Fax: ++49-30-6392 1209

Funding Institutions

Max Born Institute (MBI)
for Nonlinear Optics and Short Pulse Spectroscopy im Forschungsverbund Berlin e.V

Max-Planck-Institut für Quantenoptik (MPQ)
Hans-Kopfermann-Straße 1
85748 Garching, Germany

The Hebrew University
91904 Jerusalem, Israel

Tel Aviv University
69978 Tel Aviv, Israel

The James Franck Beirat

Prof. Dr. Wolfgang Demtröder, Fachbereich Physik, Universität Kaiserslautern
Prof. Dr. Gustav Gerber, Institut für Physik, Universität Würzburg
Prof. Dr. Joshua Jortner, School of Chemistry, Tel Aviv University
Prof. Dr. Karl Kompa, MPQ für Quantum Optics, Garching (Chair)
Prof. Dr. Eli Kolodny, Technion, Haifa
Prof. Dr. Raphael Levine, Department of Physical Chemistry, Hebrew University, Israel
Prof. Dr. Moshe Shapiro, Chem. Phys., Weizmann Institute of Science, Rehovot, Israel
Prof. Dr. Zamik Rosenwaks, Chemical Physics, Ben Gurion University, Israel

Conference site: Courtyard Hotel, Grünauer Straße 1, 12557 Berlin,
Phone: 49 30 654790, Fax: 49 30 65479550

Emergency call: 110 (police), 112 (fire) – direct button at the hotel telephones
General Information

Hotel accommodation, meals, drinks

Hotel accommodation is provided free of charge for all registered participants for the conference dates (arrival 21\textsuperscript{st} evening departure 24\textsuperscript{th} morning). This does \textbf{not include} any extra charges such as telephone, Internet access, minibar, extra meals and drinks etc. booked on your room. These costs will be charged to you according to your individual balance.

The following meals are also included in the arrangement for registered participants: breakfast on Mo, Tu and We, buffet lunch on Mo and Tu, buffet dinner Su and Mo. The reception and conference buffet dinner after the James Franck Lecture is also included for registered participants (sponsored).

At registration you will receive vouchers for \textbf{one} alcoholic or non-alcoholic beverage \underline{per meal}. Further drinks can be ordered at the participants expenses. Coffee, tea and light refreshments are offered during coffee breaks free of charge.

The poster session with social get-together on Monday evening features free drinks sponsored by the companies mentioned on page 7.

Accompanying persons do not have to pay extra for the use of double rooms. This includes breakfast is also included. However, their meals will be charged to the registered participant.

Extra nights (including breakfast) and extra meals have to be paid by participants on an individual basis. You do, however, enjoy the specifically negotiated reduced rates at the Courtyard Hotel Köpenick.

No kosher food

In the registration forms sent out none of the participants indicated that she/he would require kosher food. Hence Kosher food is not forseen during the symposium. We would do our best to get it provided in case it should be desired nevertheless. However that might proof difficult on such short notice.

Posters

Only a few (albeit very interesting) posters will be presented, including those of the sponsors. The posters should be up during the whole conference for informal discussion. The official poster session is, however, on Monday evening and will mainly serve as free time for informal discussions in a relaxed atmosphere with some drinks. You should not make different plans for that evening since one of the main benefit of such a conferences is the scientific discussion in small groups which is to be stimulated in such an environment.

Cultural activity

Across the river Dahme at which the Conference Hotel is located there is the historical City-Castle Köpenick. We plan to make a guided tour to the castle on Tuesday afternoon. It is important that you register for this on Sunday evening or Monday morning at the latest at the registration desk.
Internet Access

All hotel rooms are equipped with internet access and the possibility to dial into the WLAN with a laptop.

Vouchers to allow the access of the WLAN via a password can be purchased at the reception for the following cost:

- 30 minutes = 5.00 €
- 120 minutes = 10.00 €
- 1 day = 12.50 €
- 2 days = 23.00 €
- 3 days = 33.60 €

We will hand out flyers with all necessary information at check-in.

- a password will be handed out to you when you purchase the access at the reception
- adapters for GANAG access in the rooms are available at the reception for a deposit of 120.00 €
- the clock for the purchased internet access time starts ticking with the activation by password and can not be interrupted
- in addition, an open, free of charge computer in the lounge may be used for brief periods of internet access

Visit to the Max Born Institute (MBI)

The Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy is located in Berlin-Adlershof, City for Science, Industry and Media - about 20 minutes from the conference hotel. Both, the MBI and Adlershof are worthwhile seeing.

The MBI conducts basic research in the field of nonlinear optics and ultrafast dynamics of the interaction of light with matter and pursues applications that emerge from this research. It develops and uses ultrafast and ultra-intense lasers and laser-driven short-pulse light sources in a broad spectral range in combination with methods of nonlinear spectroscopy. With about 180 scientists the MBI belongs to the strongest laser based research institutes in Germany. It is a member of the Leibniz Association (together with the Max Planck Society, the Fraunhofer Society and the Helmholtz Centres one of the four big non non-university research organisations). The Leibniz institutes are funded jointly by the federal government of Germany and the German states (die Länder).

You are cordially invited to join a guided tour on Wednesday 24th in the morning. To allow us some time for preparing the transfer and the guided visit(s), please let us know until Sunday evening or Monday morning at the latest if you plan to come.
James Franck – Biography

James Franck was born on August 26, 1882, in Hamburg, Germany. After attending the Wilhelm Gymnasium there, he studied mainly chemistry for a year at the University of Heidelberg, and then studied physics at the University of Berlin, where his principal tutors were Emil Warburg and Paul Drude. He received his Ph.D. at Berlin in 1906 under Warburg, and after a short period as an assistant in Frankfurt-am-Main, he returned to Berlin to become assistant to Heinrich Rubens. In 1911, he obtained the "venia legendi" for physics to lecture at the University of Berlin, and remained there until 1918 (with time out for the war in which he was awarded the Iron Cross, first class) as a member of the physics faculty having achieved the rank of associate professor.

After World War I, he was appointed member and Head of the Physics Division in the Kaiser Wilhelm Institute for Physical Chemistry at Berlin-Dahlem, which was at that time under the chairmanship of Fritz Haber. In 1920, Franck became Professor of Experimental Physics and Director of the Second Institute for Experimental Physics at the University of Göttingen. During the period 1920-1933, when Göttingen became an important center for quantum physics, Franck was closely cooperating with Max Born, who then headed the Institute for Theoretical Physics. It was in Göttingen that Franck revealed himself as a highly gifted tutor, gathering around him and inspiring a circle of students and collaborators (among them: Blackett, Condon, Kopfermann, Kroebel, Maier-Leibnitz, Oppenheimer, and Rabinovich, to mention some of them), who in later years were to be renowned in their own fields.

After the Nazi regime assumed power in Germany, Franck and his family moved to Baltimore, U.S.A., where he had been invited to lecture as Speyer Professor at Johns Hopkins University. He then went to Copenhagen, Denmark, as a guest professor for a year. In 1935, he returned to the United States as Professor of Physics at Johns Hopkins University, leaving there in 1938 to accept a professorship in physical chemistry at the University of Chicago. During World War II Franck served as Director of the Chemistry Division of The Metallurgical Laboratory at the University of Chicago, which was the center of the Manhattan District's Project.

In 1947, at the age of 65, Franck was named professor emeritus at the University of Chicago, but he continued to work at the University as Head of the Photosynthesis Research Group until 1956.

While in Berlin Professor Franck's main field of investigation was the kinetics of electrons, atoms, and molecules. His initial researches dealt with the conduction of electricity through gases (the mobility of ions in gases). Later, together with Hertz, he investigated the behaviour of free electrons in various gases - in particular the inelastic impacts of electrons upon atomwork which ultimately led to the experimental proof of some of the basic concepts of Bohr's atomic theory, and for which they were awarded the Nobel Prize, for 1925. Franck's other investigations, many of which were carried out with collaborators and students, were also dedicated to problems of atomic physics - those on the exchange of energy of excited atoms (impacts of the second type, photochemical researches), and optical problems connected with elementary processes during chemical reactions.

During his period at Göttingen most of his studies were dedicated to the fluorescence of gases and vapours. In 1925, he proposed a mechanism to explain his observations of the photochemical dissociation of iodine molecules. Electronic transitions from a normal to a higher vibrational state occur so rapidly, he suggested, that the position and momenta of the nuclei undergo no appreciable change in the process. This proposed mechanism was later expanded by E. U.

Condon to a theory permitting the prediction of mostfavoured vibrational transitions in a band system, and the concept has since been known as the Franck-Condon principle.

Mention should be made of Professor Franck's courage in following what was morally right. He was one of the first who openly demonstrated against the issue of racial laws in Germany, and he resigned from the University of Göttingen in 1933 as a personal protest against the Nazi regime under Adolf Hitler. Later, in his second homeland, his moral courage was again evident when in 1945 (two months before Hiroshima) he joined with a group of atomic scientists in preparing the so-called "Franck Report" to the War Department, urging an open demonstration of the atomic bomb in some uninhabited locality as an alternative to the military decision to use the weapon without warning in the war against Japan. This report, although failing to attain its main objective, still stands as a monument to the rejection by scientists of the use of science in works of destruction.

In addition to the Nobel Prize, Professor Franck received the 1951 Max Planck Medal of the German Physical Society, and he was honoured, in 1953, by the university town of Göttingen, which named him an honorary citizen. In 1955, he received the Rumford Medal of the American Academy of Arts and Sciences for his work on photosynthesis, a subject with which he had become increasingly preoccupied during his years in the United States. In 1964, Professor Franck was elected as a Foreign Member of the Royal Society, London, for his contribution to the understanding of exchanges of energy in electron collisions, to the interpretation of molecular spectra, and to problems of photosynthesis.

Franck was first married (1911) to Ingrid Josefson, of Göteborg, Sweden, and had two daughters, Dagmar and Lisa. Some years after the death of his first wife, he was married (1946) to Hertha Sponer, Professor of Physics at Duke University in Durham, North Carolina (U.S.A.).

Professor Franck died in Germany on May 21, 1964, while visiting in Göttingen.

From Nobel Lectures, Physics 1922-1941, Elsevier Publishing Company, Amsterdam, 1965

This autobiography/biography was written at the time of the award and later published in the book series Les Prix Nobel/Nobel Lectures. The information is sometimes updated with an addendum submitted by the Laureate. To cite this document, always state the source as shown above.
Scientific Programme

Business meeting of the James-Franck-Beirat

Sunday, the 21st August 2004 (15:00 h), at the Courtyard Hotel Berlin Köpenick
Members of the James-Franck-Beirat only.

Time table of scientific programme

<table>
<thead>
<tr>
<th>Sunday 21st</th>
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<tbody>
<tr>
<td>16:00- 19:30 h</td>
<td>arrival, welcome, light buffet dinner</td>
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<tr>
<td>20:00-21:30 h</td>
<td><strong>From clusters to nanodroplets</strong></td>
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<td>Chair: Wolfgang Demtröder, Kaiserslautern</td>
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<tr>
<td>20:00-20:25 h</td>
<td><strong>Uzi Even</strong>, Tel Aviv</td>
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<td>Shaped nozzles in supersonic beams</td>
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<td>20:30-20:55 h</td>
<td><strong>Ori Chesnovsky</strong>, Tel Aviv</td>
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<td></td>
<td>Bivalent metal clusters revisited</td>
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<td>21:00-21:25 h</td>
<td><strong>Frank Stienkemeier</strong>, Freiburg</td>
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<td>Real-time studies of doped helium nanodroplets: coherence and relaxation</td>
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<tr>
<td>8:30-10:30h</td>
<td>Clusters and complexes</td>
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<td>8:30-8:55h</td>
<td>Wolfgang Christen, HU Berlin</td>
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<tr>
<td>9:00-9:25h</td>
<td>Eli Kolodney, Haifa</td>
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<td>9:30-9:55h</td>
<td>Tamotsu Kondow, Toyota, Japan</td>
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<td>10:00-10:25h</td>
<td>Ayelet Gross, Jerusalem</td>
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<td>Coffee break</td>
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<tr>
<td>11:00-12:30h</td>
<td>Clusters and ultrafast dynamics</td>
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<tr>
<td>11:00-11:25h</td>
<td>Andreas Heidenreich, Tel Aviv</td>
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<td>11:30-11:55h</td>
<td>Ludger Wöste, FU Berlin</td>
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<tr>
<td>12:00-12:25h</td>
<td>Roland Mitric, HU Berlin</td>
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<td></td>
<td>Lunch Break</td>
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<tr>
<td>14:30-16:30h</td>
<td>Dynamics of molecules and complexes</td>
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<td>14:30-15:00</td>
<td>Tobias Brixner, Universität Würzburg</td>
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<tr>
<td>15:00-15:25h</td>
<td>Eberhard Riedle, Munich</td>
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<tr>
<td>15:30-15:55h</td>
<td>Haim Levanon, Jerusalem</td>
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<tr>
<td>16:00-16:25h</td>
<td>Haim Diamant, Tel Aviv</td>
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<td></td>
<td>Coffee break</td>
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<tr>
<td>17:00-18:30h</td>
<td>Nanosystems</td>
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<tr>
<td>17:00-17:25h</td>
<td>Yuval Ebenstein, Jerusalem</td>
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<td>Time</td>
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| 17:30-17:55 h | Micha Asscher, Jerusalem  
Metalllic nano-clusters growth and film patterning via weakly bound buffer layer |
| 18:00 -18:25 h | Kai Fauth, Stuttgart  
Interfaces with and within magnetic clusters and nanoparticles |
| 20:30 h - open end | Poster session and social get together |

**Tuesday 23rd**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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</table>
| 8:30-10:30 h | Biomolecules  
Chair: Martina Havenith, Bonn |
| 9:00-9:25 h  | Marcus Motzkus, Marburg  
Quantum control spectroscopy of biomolecules |
| 9:30-9:55 h  | Thomas Schultz, MBI Berlin  
Excited state dynamics of microsolvated DNA bases and base pairs |
| 10:00 -10:25 h | Markus Gerhards, Düsseldorf  
Analysis of isolated extended beta-sheet model systems by combined IR/UV spectroscopy |
|              | Coffee break                                                          |
| 11:00-12:30 h | Biomolecules and ultra cold atoms and molecules  
Chair: Alfred Holzwarth, Mülheim |
| 11:00-11:25 h | Nikolaus Ernsting, HU Berlin  
A molecular IR spectrometer for biopolymers |
| 11:30-11:55 h | Ron Folman, Beer-Sheva  
Recent development in atomchips |
| 12:00 -12:25 h | Ehoud Pazy, Beer-Sheva  
On the Conversion of Ultracold Fermionic Atoms to Bosonic Molecules via Feshbach Resonances |
| 12:30 -14:00 h | Lunch Break                                                           |
| 14:00-16:00 h | Visit to Castle Köpenick or other social activity                   |

Please register at the conference office as early as possible.
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>17:00 h</td>
<td>Bus to Berlin Brandenburg Academy of Science (BBAW)</td>
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<tr>
<td>18:15 h</td>
<td><strong>The James-Franck Lecture</strong></td>
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<td><strong>Moshe Shapiro, Weizmann Institute</strong></td>
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<td></td>
<td>&quot;Coherent Control - from concept to reality&quot;</td>
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<td></td>
<td>Chair and introduction: Ingolf Hertel, MBI Berlin</td>
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<tr>
<td>19:45-22:00 h</td>
<td>Reception and Conference Dinner (Buffet)</td>
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<tr>
<td>22:00 h</td>
<td>Return by Bus to Hotel</td>
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**Wednesday 24th**

<table>
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<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>until 10:00 h</td>
<td><strong>departure from hotel</strong></td>
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<tr>
<td></td>
<td>unless reservation for an extension has been made</td>
</tr>
<tr>
<td>9:30-13:00</td>
<td>possibility to visit the <a href="#">Max Born Institute</a></td>
</tr>
<tr>
<td></td>
<td>please register for this visit as early as possible at the conference office</td>
</tr>
</tbody>
</table>
The James Franck Lecture
Coherent Control: From concept to reality

Shapiro\textsuperscript{1}, Moshe

\textit{Chemical Physics Department, Weizmann Institute of Science}
\textit{76100 Rehovot, Israel}

The concept of "coherent control" and its theoretical and experimental evolution will be reviewed, with special emphasis on symmetry breaking, chiral purification, and molecular BEC formation via adiabatic passage photo-association.

\textsuperscript{1} Moshe Shapiro is Jacques Mimran Professor of Chemical Physics at the Weizmann Institute of Science, Rehovot, Israel, and Canada Research Professor, Dept. of Chemistry and Physics at the University of British Columbia. He received his BSc, MSc, and PhD from the Hebrew University of Jerusalem. He pioneered the field of quantum control with groundbreaking theoretical investigations.
Abstracts of invited talks
Shaped nozzles in supersonic beams

Even, Uzi

School of Chemistry, Tel Aviv University, Israel
Bivalent metal clusters revisited

Cheshnovsky, Ori

*School of Chemistry, Tel Aviv University, Israel*

We present PES studies on Zn\(_n\)- in the size range of \(n=4-117\). We show that zinc clusters exhibit a distinct transition in their electronic structure characteristics as a function of their size. At small sizes up to \(n=18\) the clusters follow the Bloch-Wilson picture with a gradual band gap decrease. At higher sizes as the valence electrons delocalize, which leads to an almost perfect free electron density of states. This is demonstrated by discussing the spectra in the light of standard free electron models and by the comparison to the results on sodium clusters. The general aspects of Metal to Isulator Transitions in clusters will be discussed in view of the Zn results.

The second half of the talk will present new results on thermalization dynamics in mercury clusters. We show that when the possibility of electron-electron scattering is blocked, thermalization of electrons is substantially slower than in other metal clusters.
Real-time Experiments of Doped Helium Nanodroplets: Coherence and Relaxation

Stienkemeier, Frank\textsuperscript{(1,2)}; Claas, Patrick\textsuperscript{(2)}; Droppelmann, Georg\textsuperscript{(2)}; Schulz, Claus-Peter\textsuperscript{(3)}

\textsuperscript{(1)}Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, D-79104 Freiburg, Germany
\textsuperscript{(2)}Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld, Germany
\textsuperscript{(3)}Max-Born-Institut, Max-Born-Str. 2a, D-12489 Berlin, Germany
email: frank.stienkemeier@physik.uni-freiburg.de

Real-time dynamics in superfluid helium nanodroplets is studied by means of femtosecond pump-probe techniques. In particular, a beam of helium droplets is doped with alkali atoms. The formation of alkali-helium exciplexes upon electronic excitation of the alkalis is followed in real time. Formation times are determined, especially comparing superfluid $^4$He and normalfluid $^3$He droplets [1]. Furthermore, we observe quantum interference structures both in the ionization rates of desorbed single atoms as well as exciplex molecules. Analysis of the interference oscillations reveals a detailed view of the level structure of the molecules, providing a novel approach to characterize vibrational structures and dynamics of transient species. Moreover, in this way even the time evolution of energies can be studied.

Fig.1: Quantum interferences of Rb atoms as well as Rb$^+$He exciplex molecules. Rb atoms were attached to helium nanodroplets, electronic excited ($5p \leftarrow 5s$) by a femtosecond laser and detected mass selectively. The insets show the resolution of the optical frequency and the structure of the amplitude modulation.

From Large Molecules to Small Systems

Christen, Wolfgang

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The intact transfer of solids into the gas phase is an important, necessary process in science, technology, and industry. This task is especially challenging for nonvolatile, thermally unstable, large molecules. Experimental methods explored so far include electrospray ionization (ESI [1]), laser desorption, or matrix-assisted laser desorption and ionization (MALDI [2]). Another possibility is the expansion of supercritical solutions into a molecular beam. In the latter approach the idea is to dissolve the solid substance at high pressure, exploiting the supercritical fluid’s solvent power, and precipitate it by expansion into vacuum. The use of supercritical fluids as solvents offers various advantages: Due to the high compressibility of the solvent, the density and hence the solvent power of a supercritical fluid can be adjusted between gas- and liquid-like extremes with only moderate changes in pressure. Second, solvents such as supercritical carbon dioxide are compatible with hydrocarbon-free ultrahigh vacuum conditions. And finally, supersonic beam expansions are especially attractive because they allow the generation of internally cold and electrically neutral molecules, a feature not readily available otherwise. Here we present recent results extending our previous work on the supersonic expansion and vacuum deposition of solid caffeine [3] to naphthalene, vitamin K₃, L-phenylalanine-tetbutylester, and C₆₀.

The second part of the talk introduces a new initiative for the efficient, fast, and free exchange of scientific information: The new Journal of Small Systems (http://jsmallsystems.org) presents a new concept in communicating quality scientific results in an open-access environment. It is intended to combine the best of the two most prominent models of publishing scientific results: peer-reviewed conventional journals with no open access, and open-access Web archives with no quality control, and add additional services by using the full potential of the Internet.

Multifragmentation in cluster-surface collisions

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The multifragmentation dynamics of a large molecule/cluster impacting a solid surface is of both fundamental and practical importance. Disintegration or shattering of an object (either macroscopic or microscopic) is an elementary process which may reveal universal patterns. This collisional event (for tightly bound species) is expected to play a central role in a variety of applied processes involving ion-surface impact such as deposition and growth of ultra-thin layers using energetic cluster ion beams, nano-processing of surfaces using large ionic projectiles, various surface induced analytical mass spectrometry methods, etc. Recently, due to the increased importance of C\textsubscript{60} projectiles in both static and dynamic SIMS (secondary ion mass spectrometry) measurements there is a specific interest in the surface induced multifragmentation of fullerenes over a broad range of impact energies. In this work we are using fullerene collisions to address the issue of a disintegration event which is completed away from the surface (Post-collision) as compared with a disintegration event which is completed while the collider is still in close contact with the surface (During-collision). We have carried out detailed measurements of kinetic energy and angle distributions of C\textsubscript{n}\textsuperscript{-} (n=2-12) fragment anions resulting from the impact induced disintegration of C\textsubscript{60}\textsuperscript{-} projectiles at a gold surface for different incidence configurations and impact energies (80-900 eV). The experimental results obtained provide evidence for both Post-collision and During-collision type multifragmentation processes.
Clusters on Solid Surface

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The fundamental properties of metal clusters are modified in touch with a solid surface because of the interaction between the clusters and the solid surface. In this regard, we investigated, by use of STM, the geometric and electronic structures of size-selected platinum clusters on a silicon (111)7x7 surface at a single cluster level. In practice, size-selected platinum cluster cations (the sizes up to 40) were deposited on the silicon surface at a temperature of 300 K and a pressure of 10-8 Pa, and then were measured by STM. The clusters were found to be held firmly on the surface without suffering any aggregation and dissociation.

STM images of platinum clusters show that they have single-layered two dimensional structures in contrast to three dimensional structures of platinum clusters in the gas phase; the average diameter remains to be about 1 nm up to the cluster size of 20 and then increases gradually with the size. It follows that the average interatomic distance in a cluster which is the largest at the smallest size decreases with the size until the size of 20 and levels off above it as the size increases. The finding of the size-independent cluster diameter in the size range smaller than 20 is explained by a picture that there are reactive surface sites with a diameter of 1 nm, which can accommodate less than 20 platinum atoms.

On the other hand, the tunneling spectrum of a single platinum cluster exhibits several peaks originating from the d-electrons of the constituent platinum atoms and an energy gap. The energy gap changes from cluster to cluster even at the same size; the data scattering seems to be more prominent in the size range below 20 in accordance with the presence of the reactive surface sites as described above. In average, the energy gap tends to decrease with the size, as expected from the decease of the average interatomic distance with the size. The local density of states for the platinum cluster was also derived from the tunneling spectrum as a function of the distance from the center of the cluster. It was found that the electronic wavefunctions of the platinum are confined inside it.

Key words:
Spatially-resolved tunneling spectrum
Size-selected platinum cluster
Si(111)-7x7 surface
Electronic structure
Geometric structure
STM
Impact-heated cluster technique provides a controlled and systematic tool to explore the properties of matter under extreme conditions. Considerable attention has been given to the heating of a molecular cluster by the impact at a hard surface. Here we report on another aspect, the high matter density of the cluster that can be achieved during the compression at the wall. Of course, this pressure rise is transitory as the hot and dense cluster rapidly shatters. On the other hand, while the extreme conditions reached by the collision do not last long, they do last long enough for reactions to take place.

During the impact a high material density is achieved. The computational and theoretical characterization of this ultrahigh compression is our objective.

The ultra fast changes and spatial inhomogeneity in the cluster during impact create a difficulty in defining average values (such as density, pressure and volume) in the non-equilibrium unbound system. We face this difficulty by applying constraints on the cluster and employing an analogous to the virial theorem. By constrained molecular dynamics simulations we define instantaneous pressure. We show that for rare gas clusters the pressure can reach the teraPascal range and that it scales with the initial kinetic energy and with the mass of the particles in the cluster.
Electron Impact Ionization of Atomic Clusters in Ultraintense Laser Fields

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We report on computer simulations of inner ionization of Xe\(_n\) clusters (n = 55 – 2171) in ultraintense Gaussian laser fields (peak intensity I = 10\(^{15}\) – 10\(^{20}\) Wcm\(^{-2}\), pulse width \(\tau\) = 25-100 fs, frequency 0.35 fs\(^{-1}\)). The cluster inner ionization process is induced by the barrier suppression ionization (BSI) mechanism and by electron impact ionization (EII), which occurs sequentially with the BSI. We address electron impact ionization of clusters, which pertains to inelastic reactive processes of the high-energy (100 eV – 1 keV per electron) nanoplasma. We utilized experimental data for the energy dependence of the electron impact ionization cross sections of Xe\(^{j+}\) (j = 1 – 10) ions, which were fit by an empirical three-parameter Lotz-type equation, to explore EII in clusters by molecular dynamics simulations. Information was obtained on the yields and time-resolved dynamics of the EII levels (i.e., number \(n_{imp}\) of electrons per cluster atom) in the Xe\(_n\) clusters and their dependence on the laser intensity and cluster size. The relative long-time (t = 90 fs at \(\tau\) = 25 fs) yields for EII, \(n_{imp}/n_{ii}\) (where \(n_{ii}\) is the total inner ionization yield), increase with decreasing the laser intensity and with increasing the cluster size. In the intensity range I = 10\(^{15}\) – 10\(^{16}\) Wcm\(^{-2}\), \(n_{imp}/n_{ii}\) = 0.21 for n = 2171 and \(n_{imp}/n_{ii}\) = 0.09 – 0.14 for n = 459, while for I = 10\(^{18}\) – 10\(^{20}\) Wcm\(^{-2}\), \(n_{imp}/n_{ii}\) = 0.01 – 0.05. The difference \(\Delta n_{imp}\) between the EII yield at long time and at the termination of the laser pulse reflects an ionization dynamics by the nanoplasma when the laser pulse is switched off. For Xe\(_{2171}\) in the lower intensity domain, \(\Delta n_{imp}\) = 0.9 at I = 10\(^{15}\) Wcm\(^{-2}\) and \(\Delta n_{imp}\) = 0.4 at 10\(^{16}\) Wcm\(^{-2}\), reflecting on EII by the persistent nanoplasma under “laser free” conditions, while in the higher intensity domain of I = 10\(^{17}\) – 10\(^{18}\) Wcm\(^{-2}\), \(\Delta n_{imp}\) is negligibly small due to the depletion of the transient nanoplasma. The marked increase of the EII yields with increasing \(\tau\) opens avenues for the control of extreme multielectron ionization.
Probing Molecular Dynamics: Learning in the Loop

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The advent of shaped femtosecond pulses, which are optimized in feedback-loops by means of genetic algorithms, allows to address specific photo-induced dynamical pathways. Examples for these are the generation of selective high harmonics in gases, the formation of plasma filaments, photo-isomerisations or even photo-reactions. In other words: The shape of the pulse decides if a molecular bond is formed, or if it is broken. We have demonstrated the feasibility of this approach in photo-ionization, -dissociation, and -association experiments of alkali dimer and trimer systems. The obtained pulse shapes reveal interesting details on the chosen dynamical pathway. Various optimization and pulse cleaning schemes will be presented, and the resulting optimum pulse shapes will be discussed and compared with the results from theory. In those experiments, the reactive pathway always led across an electronically excited intermediate target. Future experiments will also concentrate on the possibility of control Schemes in the electronic ground state using charge reversal spectroscopy schemes.
Theoretical exploration of ultrafast processes in clusters and their complexes

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We present a theoretical approach for the exploration and control of ultrafast processes in complex systems based on a combination of the adiabatic and nonadiabatic ab initio MD "on the fly" with the Wigner distribution approach. This allowed us to accurately simulate fs-spectra in atomic clusters involving both ground as well as excited electronic states, to get insight into the underlying dynamical processes and to develop a new strategy for the optimal control in complex systems [1].

The simulation of ultrafast dynamics will be illustrated on the following examples: i) NeNePo signals and time resolved photoelectron spectra for noble metal clusters and their reactions involving ground state dynamics and ii) pump-probe signals for cluster complexes involving excited electronic states and nonradiative relaxation processes. The analysis of dynamics and comparison with experiments allowed to identify different processes.

For the optimal control of ultrafast processes by tailored light fields, two aspects will be addressed: i) Can underlying processes be revealed from the shapes of optimized pulses and ii) are complex systems controllable by introducing new control strategies? The control of isomerization and fragmentation processes in clusters, biomolecules and their complexes will be presented.

Two-dimensional electronic spectroscopy of molecular complexes

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In general, time-resolved optical spectroscopy is used for monitoring transient changes in quantum-mechanical populations. Yet the fundamental cause of such evolution, namely the couplings that lead to transitions between levels, is usually inferred only indirectly. This deficiency is overcome in the novel technique of multidimensional spectroscopy of electronic transitions [1,2]. Here electronic couplings can be measured directly, for example in natural photosynthetic pigment-protein complexes [3,4]. Thus the energy transport pathways can be made visible, giving insight into the driving force of biological light harvesting. The excitation energy does not simply cascade stepwise down the energy ladder; rather the detailed spatial properties of delocalized excited-state wavefunctions are relevant. This spectroscopic methodology opens the door for similar investigations of electronic coupling and energy transport in any photoactive assembly, macromolecule or other nanoscale system.

In addition, a very different new spectroscopic scheme for ultrafast spectroscopy is proposed and analyzed which delivers direct and simultaneous nanometer spatial and femtosecond temporal resolution [5]. It could thus yield information similar to multidimensional spectroscopy, but with a direct spatiotemporal probing scheme. This is achieved in a combination of femtosecond polarization laser pulse shaping and nano-optics [6], allowing to control the spatial and temporal evolution of optical near-fields. The near-field is tailored with a learning algorithm such that pump and probe excitations occur not just at different times but also at different positions. The two excitations can be restricted spatially to far below the diffraction limit and are separable on a nanometer length scale. Experimental realization of this technique will thus enable the direct spatial probing of nanoscale energy transfer or charge transfer processes.

Ultrafast Charge Transfer in Solution and Zeolites

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Recent developments in ultrafast technology allow the generation and routine use of sub-20 fs pulses tunable throughout the visible and near infrared. This allows the investigation of ultrafast chemical processes with unprecedented temporal resolution. Most important, the wide tunability of the light sources and their full synchronization make it possible to choose the excitation and detection wavelengths according to the spectral features of the investigated system. With this capability on hand, a large range of new problems can be tackled.

In triphenylmethane lactones we observe charge separation in as little as 50 fs. This means that the electron transfer occurs faster than the time scale of the inertial solvation dynamics [1]. The polarity of the solvent can be used to moderate the speed of the electron transfer and cause an additional ring opening in the lactone part of the molecules. In crystal violet lactone a charge transfer state $^1\text{CT}_{A\alpha}$ localized on the 6-DMAPd subunit is initially excited. The polar solvent shell starts to rearrange and this in turn lowers the energy position of the highly polar $^1\text{CT}_{B}$ state until a second electron transfer becomes possible [2].

Chemical reactions in a restricted geometry can be investigated when the molecules are incorporated in the nanoporous voids of zeolites. The in situ incorporation of 2-(2′-hydroxyphenyl)benzothiazole (HBT) inside the supercages of nanosized FAU and MFI zeolites is possible by the use of HBT as a cotemplate in the precursor colloidal solution [3]. The sub-100 nm size of the resulting crystals renders an optically clear suspension that can be investigated both with steady state and time resolved spectroscopic methods [4]. Contrary to HBT in cyclohexane solution, the molecule can be initially in its keto state. The UV excitation leads to a backconversion to the enol state, that is energetically favored. The HBT photoconversion takes place via an ultrafast deprotonation within 1.5 ps as detected by femtosecond transient absorption spectroscopy [5].

Multi-frequency EPR spectroscopy*

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Multi-frequency time-resolved EPR (TREPR) spectroscopy is very powerful in studying photoinduced processes. In this lecture, experiments in this line will be discussed. In the photosynthetic models, in which the donor and acceptor moieties are linked together by hydrogen bonds, we have determined the nature of the radical pair states by combining X-band (9 GHz) and W-band (94 GHz) TREPR spectroscopy. In addition, the donor-acceptor electronic coupling via the hydrogen-bonded network was found to be similar to that via covalent linkage. In different model system, we were able to follow the multi-step electron transfer (ET) by employing Q-band (35 GHz) experiments. ET was found to proceed simultaneously through two channels, namely, originated from the singlet and triplet states of the electron donor.

In a related study, the interactions between photoexcited triplets and free radicals in covalently linked and free diffusion complexes were investigated. In these studies, a new electron spin polarization (ESP) mechanism, generated in linked fullerene-TEMPO complexes was determined. The ESP was explained in terms of selective transitions between composite trip-doublet and trip-quartet states and spin-conserving decay to the ground state. As to the free diffusion systems, the magnitude of the ESP was measured at X- and S-band (4 GHz) TREPR. As predicted by theory, we have demonstrated that the ESP magnitude is inversely proportional to the Zeeman magnetic field.

* This study is based on three Ph.D. theses: 1. A. Blank (HUJ, Levanon); 2. E. Stavitski (HUJ, Levanon) and 3. U. Heinen (University of Freiburg, Kothe). This work was supported by the Israel Ministry of Science, the US-Israel BSF, the Israel Science Foundation, and the DFG (Möbius). The Farkas Research Center is supported by the Bundesministerium für die Forschung und Technologie and the Minerva Gesellschaft für Forschung GmbH, FRG.
Correlated Dynamics in Confined Suspensions

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We investigate theoretically and experimentally the hydrodynamically correlated lateral motion of particles in a suspension confined between two surfaces. The correlations are long-range, decaying as $1/r^2$ with the inter-particle distance $r$. The transverse correlation is negative, i.e., particles exert "anti-drag" on one another as they move perpendicular to their connecting line. Despite the long range of the correlations the concentration of the suspension has an effect only at short inter-particle distances for which the static pair-correlation function is nonuniform. These findings differ qualitatively from the known behavior of unconfined suspensions.
Interaction of metal, semiconducting and functionalized tips with semiconductor nanocrystals; physical mechanisms and basis for imaging below the diffraction limit.

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We investigate the modification of photoluminescence (PL) from single dipolar emitters in proximity of metal and semiconducting Atomic Force Microscope (AFM) tips. The presence of the tip alters the radiative decay rate of an emitter via interference and opens efficient non radiative decay channels via energy transfer to the tip material. These effects cause quenching, and in some cases enhancement of the emitter's PL intensity, as a function of its distance from the interacting tip. We directly measure the PL intensity of Single semi-conductor Quantum Dots (QDs) as a function of the tip distance, and compare our results to predictions made by a fully classical theoretical model describing an oscillating dipole interacting with a planar mirror.

We take advantage of this highly distance dependent effect to realize a contrast mechanism for high resolution optical imaging. Semiconductor nanocrystals are used to functionalize an atomic force microscope (AFM) tip. QDs are chemically bound to the surface of an AFM tip by three coating methods, utilizing organo-silane linker molecules. The resulting tips remain sharp, retaining the benefits of AFM imaging, while possessing photophysical properties of the attached nanocrystals. Emitting probes with various emission colors can be prepared and easily tailored for specific applications. These functionalized probes are especially attractive for imaging schemes based on FRET. When used as acceptors, the probes were used to quench the emission of donor nanocrystals thus recording images with a lateral optical resolution of 20-30nm. The nature of the FRET interaction serves to confine the active photonic volume to the tip apex, thus enhancing potential imaging resolution with such probes.
Metallic nano-clusters growth and film patterning via weakly bound buffer layer

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Growth of metallic nano-clusters and control over their size are critically important for catalysis. Development of film patterning at the nanometer scale has significant impact on future lithography. In this work we present a novel approach to grow metallic nano-clusters and control their size using a weakly bound buffer layer as an intermediate substance to control the clusters size at the range 1-15 nm. Using optical probes, the size selected diffusion of gold nano-clusters on metallic and oxygen modified surfaces has been studied. Information on clusters mobility is critical for understanding and control over thermal stability of clusters toward the development of sintering resistant catalysts.

The same technique was further developed at thicker film thickness to pattern the layer at the sub-micron to nanometer scale employing a single laser pulse. This technique is discussed as a potential alternative for photo-lithography.
Interfaces with and within magnetic clusters and nanoparticles

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At sizes of the order of nanometers, small particles intrinsically possess a large fraction (20-100%) at interfaces, either within the nanoparticles (core shell structures) or at the interface to their surrounding. As a consequence, the properties of such particles are strongly influenced if not dominated by the interfacial interactions. This proves to be particularly true in the case of magnetic properties of transition metal clusters and nanoparticles. Their study using polarized synchrotron radiation will be introduced and examples ranging from the single atom up to the 10 nm scale will demonstrate the importance of understanding and controlling the interface properties.
Quantum control spectroscopy of biomolecules

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The combination of traditional spectroscopic methods, like transient absorption or Raman scattering with coherent control provides a novel type of difference spectroscopy. Instead of preparing small chemical or structural changes to the molecular system under study, e.g. by adding additional side groups, replacing the chromophore or changing the solvent, we make small changes to the excitation of the system by modifying the laser pulse using shaped femtosecond laser pulses and applying coherent control techniques.

The approach of difference spectroscopy is demonstrated by our studies on the energy flow in carotenoids embedded in light harvesting complexes or surrounded by solvent molecules [1]. So far, the ultrafast energy flow in carotenoids [2] has mostly been studied with linear spectroscopy, where a visible pump pulse excites the S0-S2 transition and a probe pulse records the time resolved absorption and/or fluorescence of the deactivation process. Inspired by the Tannor-Rice scheme of coherent control [3], we now use an additional 'depletion' pulse to manipulate the excited state population [4]. The depletion pulse can be tuned in delay and wavelength to the Franck-Condon window of a specific absorption/emission band, thus intercepting the natural photoreaction. The correlation of the changes that are induced on the different signals helps for their attribution within a rate-equation model. In the next step, we excited S2 in LH2 with shaped VIS pulses and optimized the excitation shape for maximum ratio of internal conversion compared to excitation energy transfer [5]. From the characteristic modulation of the optimal multipulse excitation one can extract a frequency shown in the figure that can be identified with the mode that promotes S2 – S1 internal conversion [1].

The extension of the spectroscopic techniques to non-linear methods gives additional insight into the structure and dynamics of the molecular system and allows to study the fundamental control mechanism more systematically. In order to measure the important vibrational modes in carotenoids we again combined coherent anti-Stokes Raman spectroscopy (CARS) and coherent control techniques allowing us to detect low-frequency vibrational modes of carotenoids [6] which are relevant for internal relaxation and to selectively excite different vibrational ground state modes [7]. This again underlines the power of coherent control techniques for spectroscopy.

6. B. von Vacano, W. Wohlleben, and M. Motzkus, J. of Raman Spectrosc., (accepted for publication)
Excited state dynamics of microsolvated DNA bases and base pairs

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The photochemical stability of DNA bases may be enhanced by ultrafast excited state relaxation, which efficiently quenches reactive electronically excited states. We characterized internal conversion pathways and dynamics in DNA base pairs, the corresponding water clusters and model compounds by femtosecond time-resolved electron and mass spectroscopy. Several relaxation pathways were observed and involve excited states of \( \pi-\pi^* \), \( n-\pi^* \), \( \pi-\sigma^* \) and excimer character. The propensity of different relaxation channels was sensitive to both, the composition and the structure of the cluster.

The results of our gas phase experiments provided a direct test of theoretical predictions and thus lead to a detailed understanding of photochemical reaction mechanisms. The investigation of microsolvated clusters thus carries promise to bridge the gap between the detailed understanding of processes in the gas phase and complex observations made in the condensed phase.

References


Proteins have a well defined three dimensional structure which is essential for their function. An important secondary structure element is the $\beta$-sheet. We investigate isolated peptides and peptide clusters with $\beta$-sheet binding motifs in molecular beam experiments. The chosen combined IR and UV methods are mass-, isomer-, and state-selective yielding an IR spectrum for each individual isomer. Due to our development of a new narrow band-width and high power IR laser we are able to obtain spectra in the complete region from 1000 – 4000 cm$^{-1}$. By investigating isolated clusters we would like to answer the questions (a) what are the driving forces of peptides to form either inter- or intramolecular hydrogen-bonds, (b) how strong are the individual hydrogen bonds which form stable $\beta$-sheet structures and (c) what are the best templates to inhibit pathogenic $\beta$-sheet structures. Our group has started with the investigations of smaller $\beta$-sheet models containing clusters of protected amino acids (phe, trp, tyr). We now present results both on the larger isolated tri- and tetrapeptides and extended $\beta$-sheet models formed by the clusters of the tripeptides. These are the largest aggregates investigated up to now with the chosen highly selective methods.
Ultrafast Solvation of Methyl-Quinolone Probes Local IR Spectrum

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When zwitterionic N-methyl-6-quinolone is excited with femtosecond laser pulses, its dipole moment is suddenly decreased. A polar surrounding responds with oscillatory motion leading to a new solvation equilibrium. The process is not only launched but also reported by the dye molecule, as shift of the fluorescence band which can be directly monitored. The relaxation is reproduced quantitatively by the continuum theory of dipolar solvation, and in this way the connection to IR spectroscopy is made.

For example we measure the C-O stretching vibration of methanol at 1030 cm$^{-1}$, or the O...O stretching vibration of H-bonded water around 170 cm$^{-1}$, as frequency modulation of the time‐resolved Stokes shift. Applications to DNA are discussed.
Recent development in atomchips

Ron Folman

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The field of matter wave optics has been progressing rapidly in recent years. The tools named Ion Chip and Atom Chip, have contributed much to this advance. Specifically, in the past year numerous coherent phenomena have been observed on these chips.

In this presentation we will describe these tools, advantages and drawbacks. In particular, we will focus on the interaction between the nearby surface and the atoms, and how the new fabrication facility in Ben-Gurion University (www.bgu.ac.il/nanofabrication) together with the Atom Chip Laboratory (www.bgu.ac.il/atomchip) intend to address some of the problems and further develop the capability of present day chips.
On the Conversion of Ultracold Fermionic Atoms to Bosonic Molecules via Feshbach Resonances

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Recently much progress has been made in the achievement of increasingly degenerate regimes of trapped atomic Fermi gases. In such ultracold gases magnetically tuned scattering resonances, known as Feshbach resonances, allow to control and vary the interaction strength between atoms over a very broad range. We will describe recent experiments[1,2] in which a gas of ultracold fermionic atoms having two spin components was transformed into molecules employing a Feshbach resonance. Through such experiments molecular condensates have been produced, and moreover such systems offer to unique possibility of experimentally studying the crossover from a Bose-Einstein condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) super fluid which has for decades attracted considerable attention in manybody theory.

We shall theoretically analyze the dynamics of an adiabatic sweep through a Feshbach resonance focusing on the experimental efficiency observed in the conversion of ultracold Fermi gases of 40K and 6Li atoms into diatomic Bose gases. More specifically we shall resolve [3], through symmetry considerations, the mystery of 0.5 efficiency limit in the production of bosonic molecules observed in some of the Feshbach sweep experiments. We will also illustrate how for adiabatic Feshbach sweeps that convert degenerate fermionic atoms to diatomic molecules, the Landau-Zener behavior for a single pair of particles is dramatically changed due to many-body effects [4]. The fraction of unconverted atoms is shown to be a power-law in the sweep rate, rather than exponentially small as predicted by an essentially single-particle, linear Landau-Zener model.

Poster Contributions
Aggregation and solvation: Proton transfer and solvent dynamics probed by IR and THz spectroscopy

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The accessory chlorophyll and not P700 is the primary electron donor in photosystem I

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The energy transfer and charge separation kinetics in several core photosystem I particles of *Chlamydomonas reinhardtii* with point mutations around the $P_A$ and $P_B$ reaction center chlorophylls (Chls) have been studied using ultrafast transient absorption in the femtosecond to nanosecond time range in order to characterize the influence on the early electron transfer processes. The adequate description of the transient absorption kinetics requires three different radical pairs in the time range up to $\approx 100$ ps. Also a charge recombination process from the first radical pair back to the excited state is present in all the mutants, as already shown previously for the wild type $^1, ^2$

In all mutants the primary charge separation occurs with the same effective rate constant within the error limits as in the wild type ($\approx 350$ ns$^{-1}$), which implies an intrinsic rate constant of charge separation of $<1$ps$^{-1}$. The rate constant of the secondary electron transfer process is slowed down by a factor of approx. 2 in the mutant B-H656C which lacks the ligand to the central metal of Chl $P_B$. For the mutant A-T739V, which breaks the hydrogen bond to the keto carbonyl of Chl $P_A$, only a slight slowing down of the secondary electron transfer is observed. Finally for mutant A-W679A, which has the Trp near the $P_A$ Chl replaced, either no pronounced effect or, at best, a slight increase on the secondary electron transfer rate constants is observed. Our data strongly suggest that the Chls of the $P_A$ and $P_B$ pair, constituting what is traditionally called the "primary electron donor P700", are not oxidized in the first electron transfer process, but rather only in the secondary electron transfer step. We thus propose a new electron transfer mechanism for photosystem I where the accessory Chl(s) function as the primary electron donor(s) and the $A_0$ Chl is the primary electron acceptor(s). This new mechanism also resolves in a straightforward manner the difficulty with the previous mechanism, where an electron would have to overcome a distance of approx. 14 Å in less than one ps in a single step. If interpreted within a scheme of single-sided electron transfer our data suggest that the B-branch is the preferentially active branch. It is interesting to note that the new mechanism proposed is in fact analogous to the electron transfer mechanism in photosystem II, where also the accessory Chl plays the role of the primary electron donor, rather than the “special Chl pair” P680 $^3$.


Theoretical Approach to Ultrafast Femtosecond Non-Resonant Multiphoton Transitions and Applications to CpMn(CO)$_3$

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Fragmentation and control in $C_{60}$ - a model case for large finite systems in (moderately) strong laser fields

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