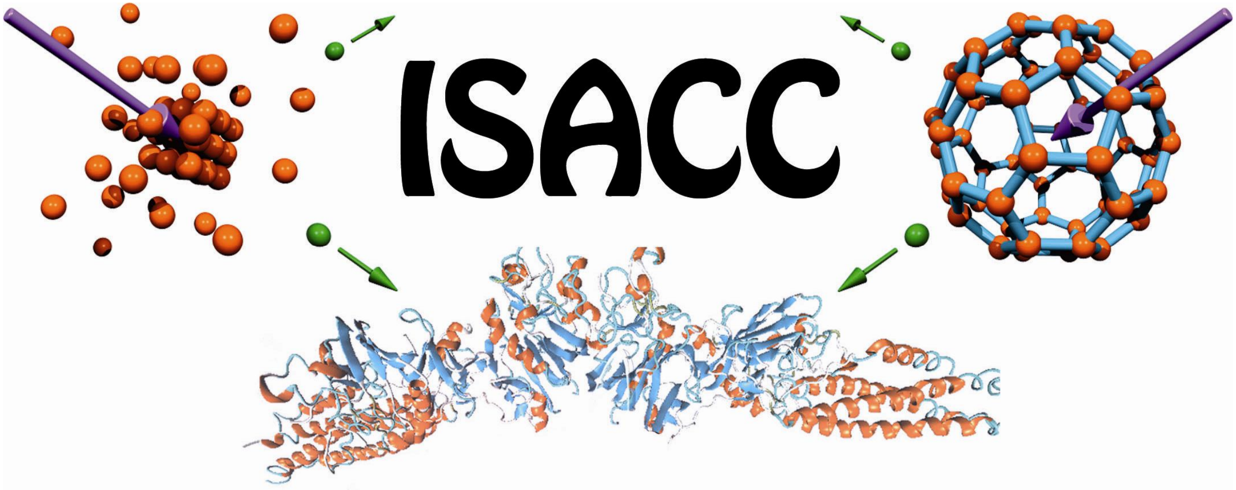
FHI der MPG HZB Helmholtz Zentrum Berlin FIAS Frankfurt Institute for Advanced Studies

# The Fifth International Symposium "Atomic Cluster Collisions"

## *ISACC 2011*

Berlin, Germany
July 20 - 25, 2011



St. Michaels Heim, Berlin

**co-sponsored by**
**Deutsche Forschungsgemeinschaft DFG**
**& King Saud University, Riyadh, Saudi Arabia**

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# Preface

The Fifth International Symposium “Atomic Cluster Collisions" (ISACC 2011) will take place in July 21-25, 2011 in Berlin, Germany. The venue of the meeting will be the St.-Michaels-Heim a lovely place located within a garden area of Berlin-Grunewald. The ISACC 2011 is organized by the Fritz-Haber-Institute of the Max-Planck Society along with the King Saud University, Rhiyadh and by the Frankfurt Institute for Advanced Studies (FIAS), Frankfurt am Main, Germany.

ISACC started as the international symposium on atomic cluster collisions in St. Petersburg, Russia in 2003. The second ISACC was held at the GSI, Darmstadt, Germany in 2007. Both first and second symposia were satellites of the International Conferences on Photonic Electronic and Atomic Collisions (ICPEAC). The third ISACC has returned to St. Petersburg, Russia in 2008. The last ISACC took place in Ann Arbor, again as a satellite meeting of the ICPEAC. Initially the symposium was mainly focused on dynamics of atomic clusters, especially in atomic cluster collisions, but since then its scope has been widened significantly to include dynamics of nanosystems, biomolecules, and macromolecules with the emphasis on the similarity of numerous essential clustering phenomena arising in different branches of physics, chemistry, and biology. After the four ISACC meetings it has become clear that there is a need for an interdisciplinary conference covering a broad range of topics related to the Dynamics of Systems on a Nanoscale. Therefore in 2010 it was decided to expand upon this series of meetings with a new conference organized under the new title "Dynamics of Systems on the Nanoscale", the DySoN Conference, since this title better reflects the interdisciplinary character of the earlier ISACC meetings embracing all the topics of interest under a common theme. The first DySoN Conference took place in Rome, Italy in 2010.

The fifth ISACC symposium will be again a satellite of the ICPEAC. The ISACC 2011 will promote, as all former ones, the growth and exchange of scientific information on the structure, properties and dynamics of complex nuclear, atomic, molecular, cluster, nanoscopic and biological systems studied primarily by means of photonic, electronic and heavy particle collisions. In the symposium, particular attention will be devoted to new developments such as the employment of Free Electron Lasers FEL’s for the study of dynamical, in particular time dependent phenomena, many-body effects taking place in clusters, nanostructures, molecular and biological systems, which include problems of fusion and fission, fragmentation, collective electron excitations, phase transitions, radiation damage and many more. Nonlinear phenomena in the photoionization of clusters are explored by the new excitation possibilities in the VUV and soft X-ray regime for the first time. Both experimental and theoretical aspects of cluster physics uniquely placed between nuclear physics on the one hand and atomic, molecular, and solid state physics on the other will be subjects of this symposium.

## *Sponsors*

The symposium will be held under the auspices of the following sponsors:

- Helmholtz-Zentrum-Berlin für Materialien und Energie
- Frankfurt Institute for Advanced Studies, Frankfurt
- Fritz-Haber-Institute of the Max-Planck-Gesellschaft, Berlin
- Technische Universität Berlin
- Freie Universität Berlin
- Humboldt Universität Berlin

## *Important Dates*

| | |
|---|---|
| Distribution of the first announcement | February 15, 2011 |
| Distribution of the second announcement | May 1, 2011 |
| Deadline for abstracts | June 1, 2011 |
| Deadline for early-bird registration | May 15, 2011 |

## *Scientific Program*

The scientific program for this symposium will consist of sessions, which will include invited lectures, review talks and progress reports. A number of contributed papers will be chosen as special reports by the International Advisory Committee of the ISACC 2011. Other contributed papers will be presented in a poster session. Suggestions about possible candidates for invited speakers should be sent to one of the Co-Chairmen of the ISACC 2011.

## *Topics*

- Structure and dynamics of atomic clusters and nanoparticles
- Electron & photon cluster collisions
- Ion-cluster collisions
- Cluster structure and dynamics on a surface
- Formation, transformation and fragmentation dynamics of clusters and biomolecules
- Clustering in systems of various degrees of complexity
- Structure and dynamics of clusters and biomolecules
- Collision processes with clusters and biomolecules
- Clusters and biomolecules in external fields: electric, magnetic, laser etc
- Cluster and biomolecular research at FEL

## *Symposium venue*

The venue of the meeting will be the St Michaels Heim at Bismarckallee 23, 14193 Berlin. The detail information on how to reach the ISACC 2011 venue can be found on the symposium webpages.

## *Symposium language*

The language of the symposium is English.

## *Social Program*

| **Event** | **Date/Time** |
|---|---|
| Symposium reception | Wednesday, July 20, 2011<br>18:00 - 22:00 |
| Symposium Banquet in the Citadel Spandau | Saturday, July 23, 2011<br>19:00 - 22:30 |
| Symposium tour through the famous castles of Potsdam with a barbecue in the evening at a lake nearby | Sunday, July 24, 2011<br>10:00 - 21:00 |

A guided tour program for participants and accompanying persons can be arranged upon request.

## *Symposium program*

*Wednesday, 20 July 2011*

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|---|---|
| $16^{00} – 22^{00}$ | **Participants registration and Symposium reception (18-22h)** |

*Thursday, 21 July 2011*

| | |
|---|---|
| $9^{15} – 9^{30}$ | **ISACC 2011 Opening**<br>**Uwe Becker, Andrey V. Solov'yov** |
| $9^{30} – 11^{00}$ | **Morning session I: Structure and dynamics of atomic clusters and nanoparticles**<br>**Chair: Andrey V. Solov'yov**<br>**Shiv N Khanna**, Virginia Commonwealth University, Richmond, USA<br>*Atomic, Electronic & Magnetic Structure of free, supported & oxidized* $Pd_n$ *cluster*<br>**Julius Jellinek**, Argonne National Laboratory, Illinois, USA<br>*Density functional theory studies of pure and mixed Pt/Mo*<br>**Atsushi Nakajima**, Keio University, Yokohama, Japan<br>*Phase transition of self-assembled monolayers studied by soft-landing experiments & by two-photon photoemission spectroscopy* |
| $11^{00} – 11^{30}$ | **Coffee break** |
| $11^{30} – 13^{00}$ | **Morning session II: Structure and dynamics of atomic clusters and nanoparticle**<br>**Chair: Julius Jellinek**<br>**Philippe Dugourd,** CNRS and University Lyon 1, France<br>*Combining ion chemistry & photo-excitation in an ion trap: spectroscopy of organo-Ag cluster*<br>**Eric Suraud,** Université Paul Sabatier, Toulouse, France<br>*Dynamics of clusters & molecules in extreme light*<br>**Riccardo Ferrando,** Dipartimento di Fisica Università di Genova, Italy<br>*Structure and thermal stability of AgCu nanoparticles* |
| $13^{00} – 14^{30}$ | **Lunch** |
| $14^{30} – 16^{00}$ | **Afternoon Session I: Electron & photon cluster collisions**<br>**Chair: Uwe Becker**<br>**Andrey Korol,** Frankfurt Institute for Advanced Studies, Germany<br>*Auger processes in endohedral fullerenes*<br>**Steven Manson,** Atlanta University, USA<br>*Ionization of atoms confined in fullerenes by photons and charged-particle impact*<br>**Alfred Müller**, Giessen University, Germany<br>*Single-photon interactions of endohedral fullerenes* |
| $16^{00} – 16^{30}$ | **Coffee break** |
| $16^{30} – 18^{00}$ | **Afternoon Session II: Electron & photon cluster collisions**<br>**Chair: Matthias Neeb**<br>**Paul-Gerhard Reinhard**, University of Erlangen, Germany<br>*Laser excitation of clusters - observables from electron emission*<br>**Lorenz Cederbaum**, Heidelberg University, Germany<br>*Intermolecular Coulombic decay in clusters*<br>**Andre Fielicke** Fritz-Haberer Institut, Berlin, Germany<br>*Shedding IR light on gas phase metal clusters: insights into structures and reactions* |

*Friday, 22 July 2011*

| | |
|---|---|
| $9^{30} – 11^{00}$ | **Morning session I: Clustering in systems of various degrees of complexity**<br>**Chair: Ludger Wöste**<br>**Catherine Brechignac**, CNRS, Paris, France<br>*Corrosion at the nanoscale: the case of silver*<br>**Walter Greiner**, Frankfurt Institute for Advanced Studies, Germany<br>*Clusters of matter, antimatter and strange matter*<br>**Torsten Siebert,** Freie Universität Berlin, Germany<br>*Ultrafast Supercontinuum Spectroscopy: for a closer look at spin and charge in cluster-based chemical reactions* |
| $11^{00} – 11^{30}$ | **Coffee break** |
| $11^{30} – 13^{00}$ | **Morning session II: Ion-cluster collisions**<br>**Chair: Alfred Müller**<br>**Bernd A. Huber**, CIMAP-CEA, Caen, France<br>*PAH molecules and clusters interacting with ions*<br>**Sanja Korica,** Institute of Nuclear Sciences 'Vinca', Belgrade, Serbia<br>*Plasmon excitations in fullerenes*<br>**Lokesh Tribedi,** Tata Institute of Fundamental Research, Mumbai, India<br>*Ionization of fullerenes and RNA base molecules by fast ions: collective response* |
| $13^{00} –13^{15}$ | **Conference photo** |
| $13^{15} – 14^{30}$ | **Lunch** |
| $14^{30} – 16^{30}$ | **Afternoon session I: Cluster structure and dynamics on a surface**<br>**Chair: Catherine Brechignac**<br>**Maria J. Lopez,** University of Valladolid, Spain<br>*Palladium clusters supported on graphene: structure and hydrogen adsorption*<br>**Amedeo Palma,** Instituto per lo Studio dei Materiali Nanostrutturati, CNR – ISMN, Monterotondo, Italy<br>*Self-assembling and chirality transfer in D-alaninol on the Cu(100) surface.*<br>**Gregor Kowarik,** Institute of Applied Physics, Wien, Austria<br>*Electron emission from solids due to cluster impact*<br>**Ramli Ismail,** University of Birmingham, United Kingdom<br>*Theoretical study of the structures of AuPd nanoparticles on MgO (100)* |
| $16^{30} – 18^{00}$ | **Poster session & Coffee** |

*Saturday, 23 July 2011*

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|---|---|
| $9^{30}$ – $11^{00}$ | **Morning session I: Clusters and biomolecules in external fields: electric, magnetic, laser, etc.**<br>**Chair: Thomas Schlathölter**<br>**Eugene Surdutovich,** Oakland University, USA<br>*Multiscale approach to ion-beam radiotherapy: towards understanding the cluster damage in DNA molecules*<br>**Alexander Yakubovich** , Frankfurt Institute for Advanced Studies, Germany<br>*Biomolecules under nanoscale thermomechanical stress*<br>**Florent Calvo**, Universite de Lyon 1, France<br>*Vibrational transparency of water clusters under collisions: experiment & molecular simulation* |
| $11^{00}$ –$11^{30}$ | **Coffee break** |
| $11^{30}$ –$13^{00}$ | **Morning session II: Electron & photon cluster collisions**<br>**Chair: Joachim Ullrich**<br>**Michel Broyer,** Universite de Lyon 1 and CNRS, France<br>*Linear optical spectroscopy & Pump-Probe studies of small metallic and bimetallic clusters*<br>**Vadim Ivanov,** Saint Petersburg State Polytechnical University, Russia<br>*Photoionization processes with negative ions of atomic clusters*<br>**Arion Tiberiu,** Max-Planck-Institut für Plasmaphysik, Garching, Germany<br>*Complexity in atoms & molecules investigated by electron-electron coincidence methods* |
| $13^{00}$ –$14^{30}$ | **Lunch** |
| $14^{30}$ –$16^{00}$ | **Afternoon session I: Cluster and biomolecular research at FEL**<br>**Chair: Kiyoshi Ueda**<br>**Joachim Ullrich**, Max-Planck-Institut für Kernphysik, Heidelberg, Germany<br>*FELs: Imaging Clusters, Aerosols, Viruses & Nanocrystals*<br>**Karl-Heinz Meiwes-Broer,** University Rostock, Germany<br>*Tailoring photoemission in strong-field laser cluster ionization*<br>**Andriy Kostyuk**, Frankfurt Institute for Advanced Studies, Germany<br>*Crystalline undulator & crystalline undulator based GAMMA laser: current status & perspectives* |
| $16^{00}$ –$16^{30}$ | **Coffee break** |
| $16^{30}$ –$18^{00}$ | **Afternoon session II: Formation, transformation and fragmentation dynamics of clusters and biomolecules**<br>**Chair: Michael Broyer**<br>**Harald Schoebel,** Universität Innsbruck, Austria<br>*Formation of ionic complexes in doped helium droplets*<br>**Frank Filsinger**, Fritz-Haber Institut, Berlin, Germany<br>*Embedding biomolecular ions in liquid helium nanodroplets*<br>**Wolfgang E. Ernst**, Graz University of Technology, Austria<br>*Alkali atoms & molecules on cold helium clusters: spin relaxation due to collisional interactions* |
| $19^{00}$ - $22^{30}$ | **Conference banquet at Citadel Spandau** |

*Sunday, 24 July 2011*

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|---|---|
| $10^{00}$ – $21^{00}$ | **Conference tour through the famous castles of Potsdam with a barbecue in the evening at a lake nearby** |

*Monday, 25 July 2011*

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| $9^{30}$ – $11^{00}$ | **Morning session I: Structure and dynamics of clusters and biomolecules**<br>**Chair: Lorenz Cederbaum**<br>**Henrik Cederquist**, Stockholm University, Sweden<br>*Fragmentation and protection of biomolecules - the effects of attaching a few water molecules*<br>**Chris Calvert,** Queen's University of Belfast, United Kingdom<br>*Intense femtosecond laser studies of biomolecules*<br>**Yang Wang**, Departamento de Quimica C-13, Universidad Autónoma de Madrid, Spain<br>*Shell effects on helium-*$C_{60}^{+}$ *complexes in helium droplets* |
| $11^{00}$ –$11^{30}$ | **Coffee break** |
| $11^{30}$ –$13^{00}$ | **Morning session II: Collision processes with clusters and biomolecules**<br>**Chair: Steven Manson**<br>**Thomas Schlathölter,** University of Groningen, The Netherlands<br>*Dissociation of free peptides and oligonucleotides by energetic photons and keV ions*<br>**Ilia Fabrikant**, University of Nebraska-Lincoln, USA<br>*Resonances and threshold effects in dissociative electron attachment to biological molecules.*<br>**Lorenzo Avaldi**, CNR-Istituto di Metodologie Inorganiche e dei Plasmi (IMIP), Monterotondo Scalo, Italy<br>*(e,2e) experiments on C60 in gas Phase* |
| $13^{00}$ –$14^{30}$ | **Lunch** |
| $14^{30}$ –$16^{30}$ | **Afternoon session I: Clusters and biomolecules in external fields: electric, magnetic, laser, etc.**<br>**Chair: Karl-Heinz Meiwes-Broer**<br>**Kiyoshi Ueda,** Tohoku University, Sendai, Japan<br>*Experiments at Spring-8 FEL: From EUV to X rays*<br>**Thomas Fennel**, University Rostock, Germany<br>*Ionization heating in rare-gas clusters under intense XUV laser pulses*<br>**Knut Asmis**, Fritz-Haber Institut, Berlin, Germany<br>*Microhydration of conjugate base anions probed by gas phase vibrational spectroscopy*<br>**Eckhard Rühl,** Free University Berlin, Germany<br>*Ultra short pulse excitation of free nanoparticles* |
| $16^{30}$ –$16^{45}$ | **ISACC 2011 Closing** |

***Registration fees***

| Level of Participation | Symposium Fee | |
|---|---|---|
| | **before May 15, 2011** | **after May 15, 2011** |
| Regular Participant | 280 Euro | 330 Euro |
| Student Participant | 160 Euro | 210 Euro |
| Accompanying Person | 60 Euro | 110 Euro |
| Banquet Ticket | 50 Euro | 50 Euro |
| Banquet Ticket (ages 4 to 12) | 30 Euro | 30 Euro |
| Symposium Tour to Potsdam and barbeque | 60 Euro | 60 Euro |

The fee includes the book of abstracts, coffee breaks and the symposium reception. The fees can be paid by credit card, bank transfer of by cash at the registration desk. Please note that if you decide to pay by cash at the registration desk we cannot offer you the reduced early-bird registration option.

## *Meals*

Meals (lunches and dinners) will be served at the symposium venue. At the registration the ISACC 2011 participants are inquired about their choices and preferences for the meals during the symposium days. The ISACC 2011 Local Organizing Committee recommends the participants to take the organized catering service because there are no restaurants in the nearest vicinity of the symposium venue.

## *Accommodation*

We ask all participants of the symposium to make their own reservation directly with the hotel of their choice. **Please book the hotels ONLY VIA E-MAIL with the code word "ISACC 2011" in the subject.** The conventional booking of the hotels via thier webpages does not provide the discount and can be declined in case of a special agreemnet with a hotel to pre-reserve the rooms for the conference participants. Additionally the „Studentshostel“ at Hubertusallee is reserved to students and postgraduates only. The number of rooms is fixed (13) and this reservation is organized and paid by the local organizing team (please use the Reservation E-mail only). These rooms will be **offered for free** for students who qualify as students, including doctoral students. These participants should fill out the **registration form** as soon as possible. The suggested hotels are located rather within vicinity of the symposium venue.

## *Official invitation and visa*

Symposium participants are advised for checking passport and visa requirements for travel to the Germany well in advance before departure. More information regarding the visa formalities will be provided with the second announcement and can also be found on the ISACC 2011 web pages. An official letter of invitation to attend the ISACC 2011 can be sent to any participant upon request. This invitation implies no obligation, financial or otherwise, by the symposium Organizing Committee.

## *Support*

A selected number of participants, mainly young scientists from less favorite regions, will be sponsored by the organizing committee. The number of grants is limited. Grants will cover partially the registration fee and/or accommodation in a student's residence. The support will be limited to participants who submit a contribution and accompany it with the request for support and CV. Applications for (partial) support should be made by **June 1, 2011.**

## *Conference Chair*

**Prof. Dr. Uwe Becker**
Chairman of the Local Organizing Committee, ISACC 2011
Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft
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## *Local Organizing Committee*

- B. Langer (Freie Universität Berlin, Germany)
- T. Lischke (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin)
- A. Meißner (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin)
- Th. Möller (Technische Universität Berlin, Germany)
- M. Neeb (Helmholtz-Zentrum Berlin, Germany)
- E. Prohn (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, *Conference Office*)
- K. Rademann (Humboldt Universität Berlin, Germany)
- D. Radulescu (Institute for Theoretical Physics, Goethe University, Frankfurt am Main)
- L. Wöste (Freie Universität Berlin, Germany)
- A.V. Yakubovich (Frankfurt Institute for Advanced Studies, Germany)

## *International Advisory Committee*

- U. Becker (Fritz-Haber-Institute of the Max-Planck-Gesellschaft & College of Science, King Saud University)
- C. Brechignac (Laboratoire Aime Cotton, Orsay, France)
- M. Broyer (University of Lyon, France)
- A.W. Castleman (Penn State University, USA)
- J.-P. Connerade (Imperial College London, London, UK)
- F. Gianturco (University of Rome "La Sapienza", Rome, Italy)
- W. Greiner (Johann Wolfgang Goethe University, Frankfurt am Main, Germany)
- H. Haberland (University of Freiburg, Freiburg, Germany)
- B. Huber (Centre Interdisciplinaire de Recherche Ions Lasers, CIRIL - GANIL, Caen, France)
- J. Jellinek (Argonne National Laboratory, Argonne, Illinois, USA)
- S. Khanna (Virginia Commonwealth University, Virginia, USA)
- A.V. Solov'yov (Frankfurt Institute for Advanced Studies, Germany, Chair)

### *Registration and general inquiries*

Registration is opened now. The registration form can filled in and submitted on the symposium website. Please follow the following link to access the registration form:
http://fias.uni-frankfurt.de/isacc2011/index.php/participants/add
General inquiries related to the symposium can be addressed to the **Co-Chairmen** of the ISACC 2011:

### *Symposium's web page*

Updated information on the symposium is available at the following Internet address:
http://fias.uni-frankfurt.de/isacc2011

### *Symposium's e-mail*

isacc2011@fias.uni-frankfurt.de

### *Location of Conference office at St. Michaels Heim*

„Bismarck Zimmer“

### *Location of oral sessions*

„Kinosaal”

### *Poster area and Reception:*

„Großer Saal“

***Location: “Kinosaal”***

# Thursday, 21 July 2011

## 9:15-9:30h: ISACC 2011 Opening

## Morning Session I: 9:30-11:00h

Structure and dynamics of atomic clusters and nanoparticles............ 14

*Coffee break 11:00-11:30h*

## Morning Session II: 11:30-13:00h

Structure and dynamics of atomic clusters and nanoparticles............ 17

*Lunch 13:00-14:30h*

## Afternoon Session I: 14:30-16:00h

Electron and photon cluster collisions................................................ 20

*Coffee break 16:00-16:30h*

## Afternoon Session II: 16:30-18:00h

Electron and photon cluster collisions................................................ 24

# Atomic, Electronic, and Magnetic Structure of free, supported and oxidized $Pd_n$ Clusters

S. N. Khanna
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Palladium clusters present unique electronic, magnetic, and chemical behaviors. While bulk Pd is paramagnetic, small $Pd_n$ clusters display magnetic order. $Pd_n$ clusters are also important catalysts. For example, small clusters of palladium supported on oxide supports constitute an important class of heterogeneous catalysts employed in a variety of industrially relevant processes including methane combustion and elimination of pollutants like CO. Consequently, identifying atomic, electronic, and magnetic character of clusters is an important undertaking.

I will first present our results of the first principles density functional studies on free $Pd_n$ clusters and in particular $Pd_{13}$. I will show that a bi-layer ground state structure that can be regarded as a relaxed bulk fragment is most compatible with the experimental results from Stern Gerlach measurements. An icosahedral structure, considered to be the ground state in numerous previous studies, is shown to be around 0.14 eV above the ground state. A detailed analysis of the molecular orbitals reveals the near degeneracy of the bi-layer or icosahedral structures is rooted in the stabilization by p- or d- like cluster orbitals. The importance of low-lying spin states in controlling the electronic and magnetic properties of the cluster will be highlighted.

I will then talk about our work on $Pd_n$ clusters supported on various supports and in particular on $TiO_2$. Since the $Pd_n$ clusters are important oxidation catalysts, I will present our work on the effect of oxygen absorption on the atomic and electronic structure. In particular, I will show how the absorption of oxygen can lead to structural rearrangements in cluster and strong relaxations of the support. The talk will highlight the microscopic origin of the strong metal-support interaction and the existence of “spill over” O states.

# DENSITY FUNCTIONAL THEORY STUDIES OF PURE AND MIXED Pt/Mo NANOCATALYSTS

Julius Jellinek[1,2], Aslihan Sumer[1]

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Results of an extensive density functional theory study on structural, electronic, and chemical reactivity properties of pure Pt and Mo, and mixed Pt/Mo catalytic clusters will be presented and discussed. The discussion will include analyses of isomeric forms, bonding energetics, and electronic features of the pure clusters as a function of their size, and how these are affected by admixing Mo to Pt clusters and vice versa. The issue of the energetically preferred homotopic conformations (particular placement of different types of atoms among the cites of a given isomeric form) and the role of the stoichiometric composition will be addressed as well. The chemical reactivity of the nanocatalysts will be analyzed for the case of CO adsorption. The energetic and electronic aspects of this reaction will be characterized as a function of cluster size, structure, and composition. The issues of site and coverage dependence will also be addressed. The implications of our findings for the well-known problem of CO-poisoning of Pt catalysts will be pointed out. Finally, we will remark on the role of the synthesis pathway in defining the structural and, consequently, chemical reactivity characteristics of mixed Pt/Mo nanocatalysts.

## Acknowledgments

This material is based upon work supported as part of the Institute for Atom-efficient Chemical Transformations (IACT), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, and by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, U.S. Department of Energy under Contract No. DE-AC-02-06CH11357.

# PHASE TRANSITION OF SELF-ASSEMBLED MONOLAYERS STUDIED BY SOFT-LANDING EXPERIMENTS AND BY TWO-PHOTON PHOTOEMISSION SPECTROSCOPY

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Self-assembled monolayer (SAM) has been recently attracted much attention from the viewpoints of molecular electronics and designing surface functionalities. In order to characterize the fundamental properties of SAMs, the geometric and electronic structures should be clarified in details. The former has been studied widely with microscopic and spectroscopic methods, while the latter has been scarcely exemplified. Especially, the information on the unoccupied states of SAMs has been hardly obtained so far, although the unoccupied states play an important role in dominating an energy barrier to inject electrons from the substrate to SAMs. Here, we present the specroscopic resluts on the electronic structures of alkanethiol SAMs on Au(111) surface; dodecanethiol (C12)-, octadecanethiol (C18)-, and docosanethiol (C22)-SAMs, where they form “standing-up” phase unchoring sulfur atom on Au atom. We employed two-photon photoemission (2PPE) spectroscopy that is a versatile tool to probe the electronic states below and above Fermi level (EF). In 2PPE, the first photon excites an electron from an occupied state to an unoccupied state, and the excited electron is photoemitted by the second photon. For the C18-SAM, adsorption-induced electronic states at EF+3.68, +1.23, and -2.83 eV were observed at 80 K. With incleasing sample temperature up to 330 K, the unoccupied state of EF+3.68 eV which is presumably formed at the Au-S interface was shifted toward EF. In the temperature range of 80-330 K, it is known that the tilt angle of alkyl chain of SAMs relative to surface normal becomes small with the temperature. By comparing chain length dependence of the energy shift against the temperature, we conclude the origin of the energy shift is attributed to the change in chemical condition of anchoring atoms depending on tilt angle of SAMs.

Furthermore, gas-phase synthesized organomatallic sandwich clusters of M(benzene)$_2$ (M = Ti, V, and Cr) are soft-landed onto a self-assembled monolayer of *n*-octadecanethiol (C18-SAM) and that of fluorinated alkanethiol (C10F-SAM) at a collision energy of 10–20 eV. The resulting adsorption states and thermal desorption kinetics of the soft-landed complexes are studied with infrared reflection absorption spectroscopy and temperature-programmed desorption. The complexes keep their native sandwich structure intact on the SAM substrate even after the “hyperthermal” deposition event. The soft-landed clusters are oriented with their molecular axes largely tilted off the surface normal of the SAM substrate, and exhibit unusually large desorption activation energies ($E_d$ = ~130 kJ/mol). For comparison, thermal deposition (~25 meV) of Cr(benzene)$_2$ vapor onto the C18-SAM, carried out using a physical vapor deposition technique, showed that the complexes are weakly physisorbed ($E_d$ = ~70 kJ/mol) on the SAM with a random orientation. Only a hyperthermal collision event allows the incident clusters to penetrate into the SAM matrix. The desorption of the embedded clusters in the SAM is then suppressed to around room temperature, and may be associated with the crystal-rotator phase transitions of the SAM matrix.

# COMBINING ION CHEMISTRY AND PHOTO-EXCITATION IN AN ION TRAP: SPECTROSCOPY OF ORGANO-SILVER CLUSTER COMPLEXES AND OF RADICAL PROTEINS.

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During this presentation, we will show how the combination of ion chemistry and laser spectroscopy in an ion trap can be used to produce, isolate and characterize reactive intermediates, which chemistry and reactivity are otherwise purely understood. In the first part, we will describe the formation of small organic-silver cluster complexes that are used to mimic C-C bond formation on silver surfaces. The comparison between the experiment and theoretical data allowed us to identify the most stable structures of these molecules and to identify the central role of the silver part on the optical absorption of these species [1]. In the second part, we will focus on the formation, structural characterization and photofragmentation of peptide and protein radical ions [2]. In particular, we will show how photoexcitation can be used to monitor the position of the radical on a peptide or protein sequence, and to get a better understanding of fragmentation methods that are based on radical reactivity.

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# Clusters and molecules in extreme light

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The progress in laser technology over the last decades has opened up new avenues for the exploration of properties of clusters and molecules. A laser pulse is characterized by its frequency but also by the laser intensity as well as the laser time profile. While for years the variations of these parameters were heavily constrained by technology, the last two decades and even more so the last years have seen tremendous increases in the range of attainable parameters. This is true for intensity, which since the 1990's can reach huge values which can lead to very large energy deposits and possibly violent disintegration of the irradiated species. But this is also true for the tunnig of the time profile which can now be tailored up to time scales of the order of magnitude of electronic motion and even below. This allows the follow up of the detail of electronic dynamics at its own "natural" time. The latest breaktroughs were attained in terms of laser frequency with the ongoing possibility of reaching very large frequencies up the X domain. This opens up new possibilities of imaging which are progressively being explored.

We shall discuss these various directions of investigation, taking examples in cluster and molecular physics. We shall especially discuss the case of high intensity and short time pulses for which a sizable amount of results have already been attained. We shall also briefly discuss the case of very short times (attoseconds) and very large frequencies (several hundreds of eV) which are becoming more and more studied.

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# Structure and thermal stability of AgCu nanoparticles

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A class of nanoclusters possessing the highest degree of chiral symmetry, the chiral icosahedral symmetry, is found by a combination of global optimization searches and first-principle calculations. These nanoclusters are core-shell nanoalloys with a Cu core and a chiral Ag shell of monatomic thickness. The chiral shell is obtained by a transformation of an anti-Mackay icosahedral shell by a concerted rotation of triangular atomic islands which breaks all mirror symmetries. This transformation becomes energetically favorable as the cluster size increases. Other chiral nanoalloys, belonging to a different structural family of C5 group symmetry, are found in the size range between 100 and 200 atoms. The driving forces favouring the chiral structures are rationalized by simple arguments, that apply to a variety of systems besides AgCu (for example, AgNi, AgCo, AuNi). The thermal stability of the chiral AgCu icosahedra is checked by molecular dynamics simulations. It is shown that these structures melt in the same temperature range as the pure Ag clusters of comparable size. Finally, the structures of Ag-rich AgCu clusters are determined, showing that Cu forms off-center cores.

# AUGER PROCESS IN ENDOHEDRAL ATOMS: THE ROLE OF NON-CENTRAL POSITION OF THE ATOM

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We demonstrate that the rate of atomic non-radiative decay in an endohedral system A@$C_N$ strongly depends on the location of the atom inside the fullerene cage. In particular, the width of the Auger decay can be varied by orders of magnitudes by increasing the atomic displacement *a* from the cage center [1]. As *a* increases the most pronounced enhancement of the width occurs for the transitions whose energy lies in the vicinity of the fullerene surface plasmon of high multipolarity.

To analyze the influence of the fullerene electron shell on the atomic decay we consider two physical mechanisms.The first one accounts for the change in the electric field at the atom due to the dynamic polarization of the shell by the Coulomb field of the transferring atomic electron [2]. Within the second mechanism the energy, released in the atomic transition, is transferred via the Coulomb interaction to the fullerene electron which becomes ionized. In [3] this mechanism was called interatomic Coulombic decay, thus pointing out its close relationship with the interatomic decay process in various molecular clusters.

It is demonstrated that in many cases the additional channels can dominate over the direct Auger decay resulting in pronounced broadening of the atomic emission lines. The case study, carried out for $Sc^{2+}$@$C_{80}^{6-}$, shows that narrow autoionizing resonances in an isolated $Sc^{2+}$ within the range $\omega = 30\ldots45$ eV are dramatically broadened if the ion is located strongly off-the-center.

Using the developed model we carry out quantitative analysis of the photoionization spectrum for the endohedral complex $Sc_3N$@$C_{80}$ and demonstrate that the additional channels are partly responsible for the strong modification of the photoionization spectrum profile detected experimentally [4].

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# Ionization of Atoms Confined in Fullerenes by Photons and Charged-Particle Impact

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The properties of an atom confined inside a fullerene cage such as $C_{60}$, both static and dynamic, are altered owing to the interaction of the confining structure with the enclosed atom. Using a variety of theoretical models, calculations have been performed that illustrate a variety of phenomena in ionization of these endohedrally-confined atoms owing to the interaction of the central atom with the confining cage. Among the theoretical predictions are confinement resonances [1], oscillations in the cross section owing to interferences between electrons ejected directly and those scattered off the confining walls. The existence of confinement resonances has recently been confirmed experimentally in the Xe@$C_{60}$ system [2]. The details of these confinement resonances depend upon the specific subshell, the specific atom, and the specific confining potential in the ionization process. They also depend upon the confined atom being at (or, at least near) the center of the confining cage [3,4]. These confinement resonances are generally found at low photoelectron energy, but owing to interchannel coupling (configuration interaction in the continuum) it is predicted that such resonances can be found at very high photoelectron energy [5]. And, it is not just the cross sections that will be affected, but the angular distribution and photoelectron spin polarization as well. Furthermore, it is predicted that ionization of endohedral atoms by charged particle impact will also exhibit confinement resonances [6].

In addition, various new phenomena have been theoretically predicted arising from the interaction of the electrons of the entrapped atom with the valence electrons of the fullerene shell itself. Among these are the huge transfer of oscillator strength from the surface plasmon to the trapped atom [7], and the hybridization of atomic levels with the levels of the valence electrons of the confining shell leading to dramatic changes in the cross sections of both the atom [8] and the shell [9]. These effects require experimental scrutiny, which has not yet been forthcoming.

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# SINGLE-PHOTON INTERACTIONS OF ENDOHEDRAL FULLERENES

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Gas-phase experiments have been carried out to study single and multiple photoionization of endohedral $Ce@C_{82}^{+}$ fullerene ions with and without fragmentation of the fullerene cage. Effects of 4d photoexcitation of the encapsulated cerium on net single and double ionization of the $Ce@C_{82}^{+}$ parent ion could be isolated [1]. These measurements were extended to reaction channels of the type

$$h\nu + Ce@C_{82}^{+} \rightarrow Ce@C_{82-2n}^{(m+1)+} + m\,e^{-} + n\,C_2 \quad m=1,2,3\,;\quad n=1,2,\ldots 9\,.$$

A single photon with energy 125 eV can cause substantial destruction of the fullerene cage, e.g. with n=9 $C_2$ units and m=2 electrons ejected. When the photon is absorbed by the encapsulated cerium the cross section for such an event is almost 8 times larger than that observed with absorption of the photon by the cage itself.

Small quantities of $Xe@C_{60}$ could be synthesized by bombarding thin layers of $C_{60}$ with accelerated $Xe^{+}$ ions. Measured cross sections for the photon-induced production of $Xe@C_{58}^{3+}$ from parent $Xe@C_{60}^{+}$ ions provide first experimental evidence for the presence of confinement resonances [2].

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# LASER EXCITATION OF CLUSTERS: OBSERVABLES FROM ELECTRON EMISSION

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We study the dynamics of clusters following a short and intense laser pulse. A variety of different cluster configurations is considered, e.g., free metal clusters, fullerenes, or metal clusters in contact with inert substrate. The early phase (several 10 fs) of a laser induced reaction concerns predominantly electron dynamics. A first scan of the dynamics is performed in terms of optical response sorting out resonant regions and regions of inert response. More details are worked out analyzing the process with observables of electron emission: net ionization, photo-electron spectra (PES), and photo-electron angular distributions (PAD). We will briefly explain the computation of PES and PAD, also addressing the strategy for the necessary orientation averaging in case of free clusters. We will present results for optical response, PES and PAD from a variety of cluster systems.

# Intermolecular Coulombic decay and ultrafast energy transfer

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How does a microscopic system like an atom or a small molecule get rid of the excess electronic energy it has acquired, for instance, by absorbing a photon? If this microscopic system is isolated, the issue is much investigated and the answer to this question is more or less well known. But what happens if our system has neighbors as is usually the case in nature or in the laboratory? In a human society, if our stress is large, we would like to pass it over to our neighbors. Indeed, this is in brief what happens also to the sufficiently excited microscopic system. A new mechanism of energy transfer has been theoretically predicted and verified in several exciting experiments. This mechanism seems to prevail "everywhere" from the extreme quantum system of the He dimer to water and even to quantum dots. The transfer is ultrafast and typically dominates other relaxation pathways.

# Shedding IR light on gas phase metal clusters: insights into structures and reactions

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Clusters are frequently used as model systems for low coordinated sites of extended surfaces and their study can provide valuable insights into the mechanisms of heterogeneous catalytic reactions. In many cases, however, there is still a lack of information on their structures and the relationship between structure and chemical behavior. Vibrational spectroscopy of gas-phase clusters can provide insights into the clusters' structure and the chemistry of adsorbed species.[1]

In the last years we have intensively utilized mass-selective vibrational spectroscopy of neutral and charged cluster complexes by multiple photon excitation down to the far-infrared (<100 $cm^{-1}$). This technique requires an intense and widely tunable IR light source, in our experiments the Free Electron Laser for Infrared eXperiments (FELIX), which generates IR light between 40 and 3500 $cm^{-1}$ and is therefore well suited to induce, e.g., photodissociation by excitation of ligand related vibrations as well as of internal cluster modes.

Far-IR multiple photon dissociation (MPD) spectroscopy on weakly bound complexes between metal clusters and rare gas atoms can provide the unique vibrational fingerprints of the metal clusters. The comparison with IR spectra calculated using density functional theory allows determination of the clusters' structures and provides insights into the growth mechanism. The capabilities of structure determination via far-IR MPD spectroscopy are demonstrated for neutral gold [2] and cationic rhodium [3] clusters. Finally, recent results on the investigation of neutral and cationic magnesium oxide clusters will be presented. Their structures are assigned by comparing with DFT calculations using global optimization techniques. While bulk MgO is a prototype of a simple cubic solid, many small MgO clusters show rather different structural motifs.[4]

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***Location: "Kinosaal"***

# Friday, 22 July 2011

## Morning Session I: 9:30-11:00h

*Coffee break 11:00-11:30h*

## Morning Session II: 11:30-13:00h

***Conference photo*** *13:00-13:15h*
*Lunch 13:15-14:30h*

## Afternoon Session I: 14:30-16:30h

## Afternoon Session II: 16:30-18:00h

# CORROSION AT THE NANOSCALE: THE CASE OF SILVER

Catherine Brechignac

CNRS, Paris, France

# CLUSTERS OF MATTER, ANTIMATTER AND STRANGE MATTER

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The extension of the periodic system into various new areas is investigated. Experiments for the synthesis of superheavy elements and the predictions of magic numbers are reviewed. Further on, investigations on hypernuclei and the possible production of antimatterclusters in heavy-ion collisions are reported. Various versions of the meson field theory serve as effective field theories at the basis of modern nuclear structure and suggest structure in the vacuum which might be important for the production of hyper- and antimatter.

# ULTRAFAST SUPERCONTINUUM SPECTROSCOPY
# for a closer look at spin and charge in cluster-based chemical reactions

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Fundamental for gaining insight to the complex interplay of electronic and geometric degrees of freedom that determine the mechanism underlying chemical reactions is the capability to spectroscopically address the time scales as well as resonance conditions involved. In order to approach this circumstance, a filament-based light source offering a coherent bandwidth of up to 300 THz over the visible to near infrared range and sub 5 fs temporal resolution has been developed [1]. The supercontinuum generation is combined with the control of the spectral phase over the full white-light envelope via chirped mirrors and a liquid crystal modulator for precise pulse compression and the transcription of parametric phase functions in the frequency synthesis of a desired pulse form. This configuration is developed for exploring the influence of varying spin and charge states on the course of a bimolecular reaction mediated in the electronic environment of a metal cluster. Specifically, the application to the spectroscopy of the $[Au_2O_2CH_4]^{-/0/+}$ cluster complex in achieving a photo-induced partial oxidation of methane is discussed. Sequential ultrafast photo-electron detachment, electronic excitation and photo-ionization within the manifold of electronic potentials available to the negative neutral and positive charge states of a reaction complex are presented as a spectroscopic strategy for systematically varying electronic configurations on the time-scale of chemical reactivity.

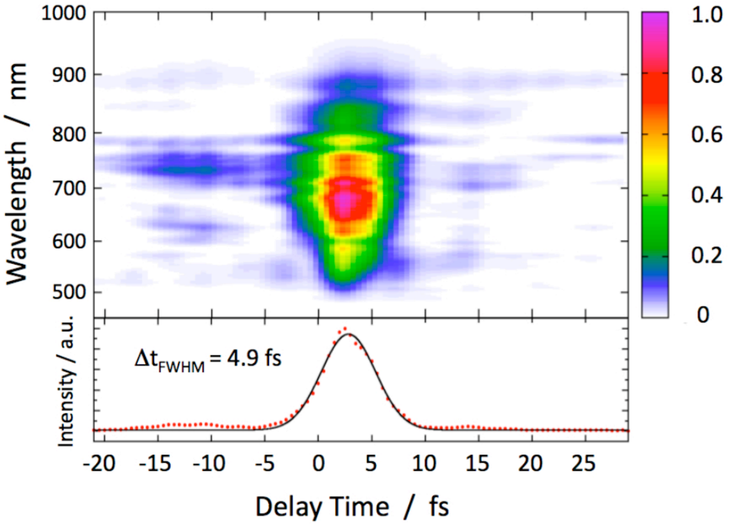

Figure 1: Frequency resolved optical gating via transient phase gratings for the characterization of a supercontinuum laser pulse

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# PAH MOLECULES AND CLUSTERS INTERACTING WITH IONS

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Polycyclic Aromatic Hydrocarbons (PAHs) are widespread atmospheric pollutants produced by e.g. fuel burning, and are therefore of major concern in environmental and health sciences. PAHs are also omnipresent in the interstellar medium as manifested by strong contributions to the infrared (IR) spectrum of many interstellar sources [1]. The electronic properties and structures of PAHs have thus been studied in great detail for a number of years, in particular concerning their interaction with photons and electrons. In the present work, we will discuss the interaction of PAH molecules and PAH clusters with low energy ions.

In the experiment, ions in low and high charge states ($He^+$ and $Xe^{20+}$) are produced in an ECR ion source. They collide with a PAH target, either in form of isolated molecules which are evaporated from a heated powder, or in form of clusters which are produced in a cluster aggregation source. Positively charged reaction products are analyzed with the aid of time-of-flight mass spectrometry.

We will discuss the importance of different decay channels as H-loss, loss of $C_2H_x$ molecules and the production of charged $C_xH_y$ fragments (see fig.1). The experimental findings for different targets (monomers and clusters) and different projectile charge states are explained by taking into account i) calculated ionization potentials which increase only slowly with the charge state and which increase the importance of multi capture processes, ii) the high charge mobility within a charged cluster, iii) the energy transfer during the electron capture collision and iv) fragment heating due to Coulomb explosion.

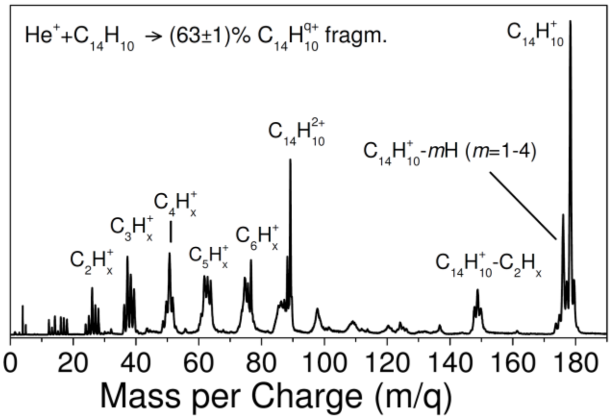

**Figure 1:** Positively charged ions produced in collisions of $He^+$ projectiles with the PAH molecule anthracene [2].

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# PLASMON EXCITATIONS IN FULLERENES

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Since the discovery of the C60 molecule in 1985 many studies have been performed to investigate its fundamental properties. These properties are mainly driven by its unique molecular structure like its spherical shell. One of the important characteristics of this molecule is the collective response of its valence electron cloud to electromagnetic radiation. This collective behavior gives rise to the occurrence of the giant dipole resonance a surface plasmon in the absorption spectrum centered around 20 eV, which has been analyzed theoretically by various authors. In addition, our photoionization cross-section measurements reveal a resonance near 40 eV, a volume plasmon analogous to observations made for C60 ions. Time-dependent density functional calculations confirm the collective nature of this feature as corresponding plasmon excitation. A third excitation of this kind is predicted but not experimentally confirmed. Concerning photoelectron emission, plasmonic excitations are characterized by a particular intensity behavior near threshold. They follow the threshold behavior law predicted for the first time by Thomas Derrah[1]. Our measurements of the C60 plasmon excitations above the C1s ionization threshold confirm this law very well and are in unexpectedly good agreement with the corresponding behavior of K-shell satellite excitations in atoms such as neon.

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# Ionization of fullerenes and RNA base molecule Uracil: collective response

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Mechanism of electron emission in collisions with clusters including fullerene or large biomolecules are governed by more complicated processes than that in ion-atom collisions. Besides fundamental interest in the study of ion-molecule collision aspects, investigations of biologically relevant molecules have recently found application for modeling the radiation damage process in hadron therapy. Generally GeV energy protons and C-ions are used in hadron therapy. The Bragg peak for energy loss in such cases happens to be in the MeV (or lower) energy region. The basic collision processes and its microscopic details in this energy range are therefore of immense important to help modeling of hadron-therapy [1-4]. The charged particle radiation can cause single and double strand breaking in DNA/RNA which in turn causes mutation. Uracil is one of the four nucleo-bases found in RNA.

Fullerenes are known to exhibit *giant dipole plasmon resonance* (GDPR) (Ref. several works by Solovyev et al and Connerade et al.) and has been observed in photo-ionization through the detection of photo-ions. The effect of Plasmon resonance on single and double ionization under heavy ion impact has been reported by our group [1-6] by using recoil-ion mass spectroscopy. The plasmon excitation de-excite through emission of electrons of particular energy, which is characteristic of the plasmon frequency. This presents a unique possibility of observing the GDPR peak in the low energy electron spectrum of $C_{60}$. Such a Plasmon electron peak has been now observed at different emission angles, for the first time [7]. Very recently we have extended these studies to the RNA base molecules, such as, Uracil ($C_4H_4N_2O_2$). We have used ion beams of $C^{4+}$ on awide energy range (90 keV-60 MeV) by using a newly built ECR-based ion-accelerator as well as 14 MV Pelletronaccelerator at TIFR, Mumbai. The recoil-ion TOF spectrum clearly indicates the single ionization and fragmentation peaks. No double ionization was observed, as against that for $C_{60}$ breakup spectrum. The total single-ionization and fragmentation (e.g. at mass 69 and 42) cross sections were obtained which were put on an absolute scale by choosing a suitable normalization procedure which allowed us to provide a stringent test to the theoretical models developed recently, for the first time [8]. This will find applications in case of modeling the hadron therapy (for cancer treatment) in the Bragg-peak region. Interestingly a connection can be made between the results obtained for many body systems like fullerene and uracil using electron emission spectroscopy.

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# PALLADIUM CLUSTERS SUPPORTED ON GRAPHENE: STRUCTURE AND HYDROGEN ADSORPTION

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Doping carbon porous materials with palladium might enhance their hydrogen storage capacity by surface reactions [1], especially by hydrogen spillover which consists in the dissociation-storage-recombination of hydrogen in the material.

To gain some insight on the possible structures formed by palladium on nanoporous carbons and on the role played by palladium in the storage of hydrogen, we have performed density functional calculations (DFT) on the adsorption of palladium on a graphene surface and the adsorption/dissociation of molecular hydrogen on those clusters. Our calculations show that [2], even at the earlier stages of Pd deposition on the graphene surface, the Pd atoms have a strong tendency to form clusters. Three--dimensional clusters are more stable than planar clusters and the transition from planar to three--dimensional Pd clusters adsorbed on graphene occurs very early as a function of cluster size, at $Pd_4$. This tendency is a consequence of the strong Pd-Pd interaction. We have also investigated the adsorption-and/or-dissociation of molecular hydrogen on the deposited Pd clusters as a function of cluster size. The mechanism for the activation of the hydrogen molecule and its possible subsequent dissociation is discussed. We also discuss the implications for the hydrogen storage capacity of Pd-doped nanoporous carbon materials.

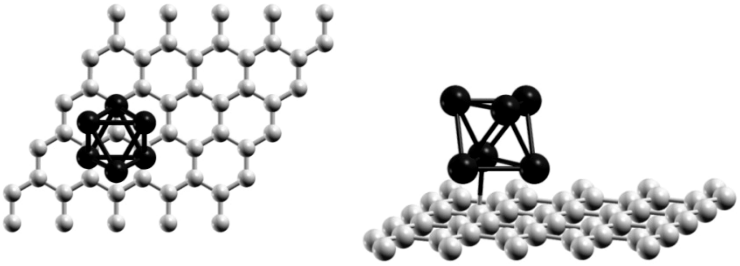

Figure 1: Octahedral structure of the $Pd_6$ cluster supported on a graphene surface.

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# SELF-ASSEMBLING AND CHIRALITY TRANSFER IN D-ALANINOL ON THE CU(100) SURFACE.

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Control of chirality transfer from a single molecule to surface superstructures is still a challenging problem for tailoring the properties of 2D nanostructure.
In this contribution we present a coupling of scanning tunneling microscopy and low energy electron diffraction measurements with an original theoretical approach, which combines essential dynamics and DFT calculations, to investigate self assembled chiral structures formed when alaninol adsorbs on Cu(100) surface at differnt coverages. Our results suggest that the distinctive orientation of the self-assembled monolayer originates from a balance of cooperating forces which start acting only when alaninol tetramers pack together to form small clusters.

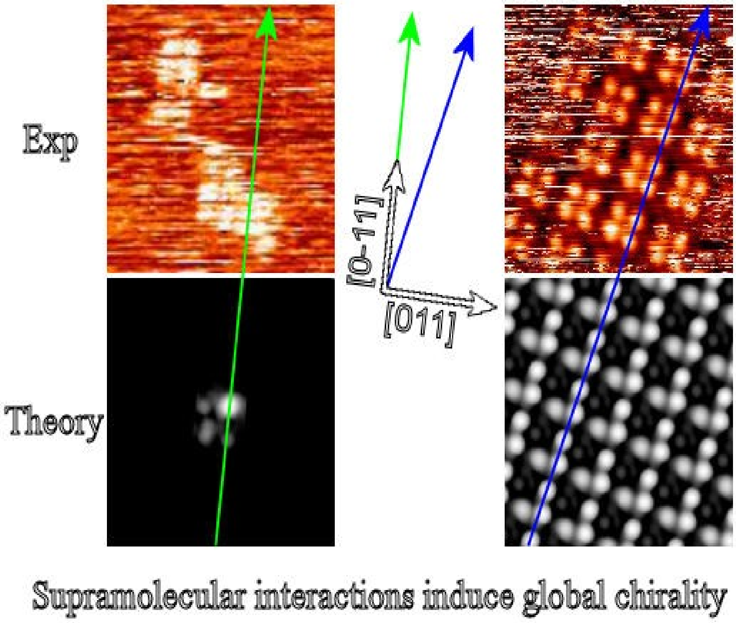

Figure 1: D-Alaninol molecules on the Cu(100) surface. Experimental and theoretical STM images.

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# ELECTRON EMISSION FROM SOLIDS DUE TO CLUSTER IMPACT

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Electron emission from surfaces caused by ion bombardment has been intensively studied in the last decades (see e.g. [1]) but still there remain some open questions concerning the fundamental processes. Especially the occurrence of electron emission below certain threshold impact velocities is still drawing attention (see e.g. [2] and references therein).

We measured electron emission statistics from metal (Au) and insulating surfaces (LiF) under the bombardment with singly charged copper clusters $Cu_n^+$ ($n \approx 2-10000$) in the kinetic energy regime between 1.5 keV and 4 keV provided by the magnetron sputter cluster source available in the ARIBE facility at Ganil, located in Caen [3]. The projectile velocities reach values well below the classical threshold for kinetic electron emission.

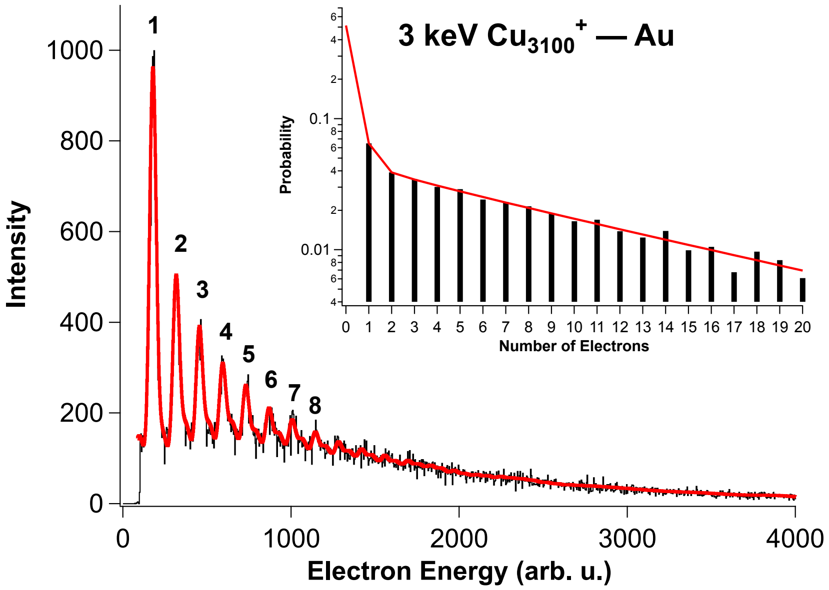

Figure 1: Example Electron Emission statistics as measured from a Au target under bombardment with $Cu_{3100}^+$ clusters. The raw data are fitted by a law from the literature [4]. The extracted number statistics can be described with a combination of a Poisson and a Polya probability function, as illustrated in the insert. This eventually yields the mean number of emitted electrons per impact event.

We used an existing setup for the electron number statistics measurements described elsewhere [5]. The emitted electrons are collected from the sample by an electric field and afterwards accelerated to 30 keV. These electrons hit a surface barrier detector, which gives a signal proportional to the deposited energy, thus the number of electrons detected within the integration time. The acquired

spectrum, as illustrated in figure 1, shows a peak structure corresponding to the number of emitted electrons and can be fitted with a well known function [4].
We are presenting systematic experimental data on the electron emission statistics from Au and LiF surfaces under cluster bombardment in the mentioned energy and mass regime.

Financial support by the European Project ITS LEIF (RII3026015) is gratefully acknowledged.

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# THEORETICAL STUDY OF THE STRUCTURES OF PD-AU NANOPARTICLES ON A MGO (100)

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Pd-Au nanoparticles are particularly interesting from the view point of their catalytic properties [1], for example for selective hydrogenation and alcohol oxidation. The electronic structures of Pd-Au clusters are quite distinct from Pd or Au, due to their differing atomic electron configurations and electronegativities [2]. A variety of structures (fcc truncated octahedra, icosahedra and decahedra) appear to have very similar energies, so that transitions between different states are possible [3]. To be relevant to catalysis, one should study these particles supported on the types of supports (e.g. metal oxides) used in real catalytic systems. For this reason, the interaction of bimetallic clusters with magnesium oxide (MgO) supports has been attracting the attention of many researchers. In this work, structures and chemical ordering (atomic segregation) of Pd-Au clusters supported on MgO(100) for sizes of 30 atoms (composition 8-22, 15-15, 22-8) and 40 atoms (composition 10-30, 20-20, 30-10) have been studied with combined empirical potential and Density Functional Theory (DFT) calculations using the Quantum Espresso plane wave DFT code. For comparison, free Pd-Au particles of the same size and composition also been calculated. In addition, calculations on 38-atom nanoalloy clusters have been carried out as an extension to our existing data base of Pd-Au nanoalloys. Analysis of the results show that the energy differences between structures are very close and resulting in structural crossover. Interactions with MgO substrate were predicted to enhance the structural transformations of Pd-Au nanoparticles and are corroborated by experimental findings in which several structural motifs were found to co-exist.

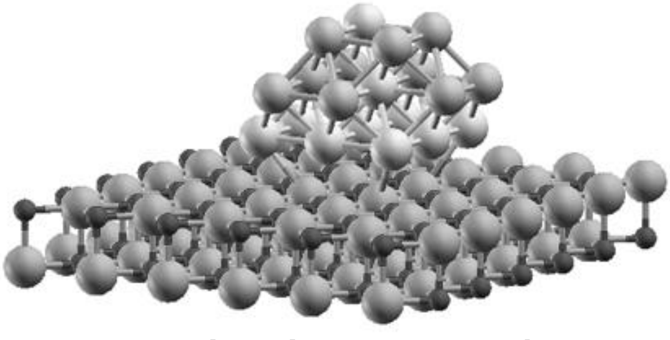

Figure 1: Pd-Au clusters on MgO substract

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***Location: “Kinosaal”***

# Saturday, 23 July 2011

## Morning Session I: 9:30-11:00h
Clusters and biomolecules in external fields ...................................... 40

*Coffee break 11:00-11:30h*

## Morning Session II: 11:30-13:00h
Electron and photon cluster collisions................................................ 43

*Lunch 13:00-14:30h*

## Afternoon Session I: 14:30-16:00h
Cluster and biomolecular research at FEL ......................................... 46

*Coffee break 16:00-16:30h*

## Afternoon Session II: 16:30-18:00h
Formation, transformation and fragmentation dynamics
of clusters and biomolecules ............................................................. 49

*19:00-22:30h*
***Conference banquet*** *at Citadel Spandau*

# ASSESMENT OF CLUSTER DAMAGE OF DNA IRRADIATED WITH IONS

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We present the analysis of complex damage of DNA irradiated by ions. The assessment of complex damage is important because cells in which it occurs are less likely to survive because the DNA repair mechanisms may not be sufficiently effective. This assessment is made in the framework of the multiscale approach to ion-beam cancer therapy. The multiscale approach to the radiation damage induced by irradiation with ions is aimed to the phenomenon-based quantitative understanding of the scenario from incidence of an energetic ion on tissue to the cell death [1]. This approach joins together many spatial, temporal, and energetic scales involved in this scenario. The success of this approach will provide the phenomenon-based foundation for ion-beam cancer therapy, radiation protection in space, and other applications of ion beams. Main issues addressed by the multiscale approach are ion stopping in the medium [2], production and transport of secondaries produced as a result of ionization and excitation of the medium [2,3], interaction of secondaries with biological molecules, most important with DNA [1], the analysis of induced damage, and evaluation of probabilities of subsequent cell survival or death. Evidently, this approach is interdisciplinary, since it is based on physics, chemistry, and biology. Moreover, it spans over several areas within each of these disciplines.

In Ref. [4], the radial dose distribution has been addressed. Traditionally, the radial dose is related to the radial distribution of damage. However, this does not include the complexity of damage, considered within the multiscale approach in Ref. [5]. It is still not clear how to relate the dose with complexity of damage. Our present work is a step in this direction. We consider several possible approaches to the calculation of complex damage and calculate radial distributions of clustered damage around the ion's track. We calculate the radial dose distribution, compare it to the simulations and derive the distribution of complexity from it. As expected, the radial distribution of complex damage is different from that of the dose. The comparison with experiments may solve the question of what is more lethal for the cell, damage complexity or absorbed energy. We suggest a way to calculate the probability of cell death based on complexity of damage.

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# THERMO-MECHANICAL DAMAGE OF BIOMOLECULES BY HEAVY IONS

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The structural nano-scale transformations in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state and vice versa (also known as (un)folding process) occur in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes, etc. [1].

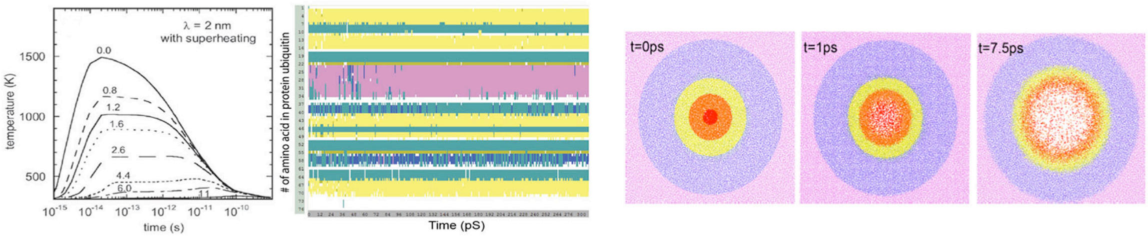

Figure 1. Left: Energy deposition in eV/atom on the molecular subsystem versus time assuming a superheating scenario. The calculations have been performed for C ions at 0.5 MeV/u with an electronic energy loss of 0.91 keV/nm [2]. Center: The dependence of the secondary structure of protein ubiquitin on time obtained using molecular dynamics simulations. The protein is exposed to the heat spike produced by the propagation of an energetic particle. Prominent disturbance of the secondary structure is observed during first 100 ps after the propagation of a particle [3]. Right: The snapshots of molecular dynamics simulation of the heat spike. Only oxygen atoms of water molecules are shown. Three images correspond to 0, 1 and 7.5 ps after ion's passage, respectively. By violet, yellow, orange and red colors are shown water molecules initially located 10nm, 5nm, 3nm and 1nm away from the ion's track, respectively. From the left figure it is seen the formation of a strongly vacuated cylinder with radius of ~ 3-5*nm* at 7*:*5*ps* after ion's passage.

We focus on the transformations in biomolecules caused by the near passage of energetic particles – carbon ions. In particular we consider the possibility of the creation of the shock waves in the vicinity of the ion tracks. We demonstrate that at the initial stages after ion's passage the shock wave is so strong that it can contribute to the DNA and protein damage due to large pressure gradients developed at the distances of a few nanometers from the ionic tracks. This novel mechanism of damage of biomolecules provides an important contribution to the cumulative biodamage caused by low-energy secondary electrons, holes and free radicals.

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# MOLECULAR MODELING OF COLLISION- AND LASER-INDUCED CLUSTER FRAGMENTATION

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Dissociation experiments remain a powerful method to determine physical and chemical properties of atomic and molecular clusters. Those properties are not always accessible by static (quantum chemical) calculations, and dynamical processes might sometimes be important. In this work, we report on the use of explicit molecular dynamics simulations, coupled with statistical analyses, to assist the interpretation of two classes of dissociation experiments. In the first example, water molecules collide on protonated water clusters and sticking and fragmentation cross sections are measured at low and high collision energies, respectively. Classical and quantum (path integral) trajectories are performed, providing a great deal of details in the energy redistribution process, the roles of impact parameter and vibrational delocalization. Our second example deals with laser-induced fragmentation, as exploited in vibrational predissociation (argon tagging) and infrared multiphoton experiments. A completely classical modeling of the laser field for a chemically realistic alkali halide cluster was undertaken to calculate action (dissociation) spectra that can be compared with linear absorption spectra. For the first time, the results allow differences in the line widths and broadenings to be fully quantified.

# Linear optical spectroscopy and pump-probe studies of small metallic and bi-metallic clusters

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Metallic and bimetallic clusters are produced in a laser vaporization source. They are selected in size and co-deposited with a transparent matrix ($SiO_2$ or $Al_2O_3$). Their optical properties may be measured as a function of size and composition for various systems: pure silver, gold and platinum clusters and bimetallic clusters such as AgAu, AgPt, AgNi, CuNi, AgCo. The cluster size range varies from 1.2 nm to 4 nm in diameters (70 to about 1500 atoms)

Firstly the optical absorption spectra of pure and bimetallic clusters are measured for cluster sizes ranging from 1 nm to 4 nm. These results are compared to the cluster structure deduced from electron microscopy (TEM) and Low Energy Ion Scattering (LEIS). For AuAg the optical spectra are in agreement with an alloy structure, while for AgNi, AuNi and AgCo they are in agreement with a segregated one. For AgPt clusters the optical properties are not in agreement with a core shell structure predicted at OK, but they are in better agreement with the alloy core/pure Ag shell obtained at 305 K by F. Calvo[1] using exchange Monte Carlo simulations.

These bimetallic clusters as well as pure clusters may also be studied by femtosecond pump-probe spectroscopy. This allows us to measure the electron-lattice energy exchange time $\tau_{ephonon}$ [2] and the acoustic response of these clusters [3]. For pure Ag and Au clusters $\tau_{e\text{-}phonon}$ decreases with the size in the scalable size regime, but increases below 2 nm due a change of paradigm associated to quantum confinement. For $Au_xAg_{1-x}$ alloy clusters having the same size, we have shown that the electron-lattice energy exchange time $\tau_{e\text{-}phonon}$ varies linearly with x between the values for pure Au and Ag clusters. This is not the case for core-shell structures.

Finally acoustic response of metallic clusters is also measured and may be interpreted from a macroscopic approach based on the continuous elastic model even for very small clusters (70 atoms) For bimetallic clusters the acoustic properties depend also of the structure (alloy versus core-shell).

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# PHOTOIONIZATION PROCESSES WITH NEGATIVE IONS OF ATOMIC CLUSTERS

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This report presents the results of calculations of photoprocesses in metal cluster negative ions and $C_{60}^-$ obtained by the Frankfurt Institute of Advanced Studies and St. Petersburg Polytechnic University theoretical groups [1]. We apply the consistent many-body theory to calculate the partial and total photodetachment cross sections, and the photoelectron angular distributions. The main attention is paid to the investigation of the role of many-electron interactions in these processes. The many-electron correlations are taken into account within the Random Phase Approximation with Exchange, which is based on the Hartree-Fock approximation for the delocalized electrons and the Jellium Model for the ionic core.

Our calculations demonstrate the dominant role of the many-body effects in the formation of cross sections and angular distributions of photoelectrons emitted from sodium clusters and are in a good agreement with existing experimental data [2]. The concrete comparison of the theory and experiment has been performed for the photodetachment from $Na_7^-$, $Na_{19}^-$, $Na_{39}^-$, $Na_{57}^-$ anions possessing only the closed shells of delocalized electrons. As an example, Fig. 1 shows the good agreement of the calculated angular asymmetry parameter with experimental data [2]. Note that this result has been achieved only with accounting for the dynamical correlation effects [1].

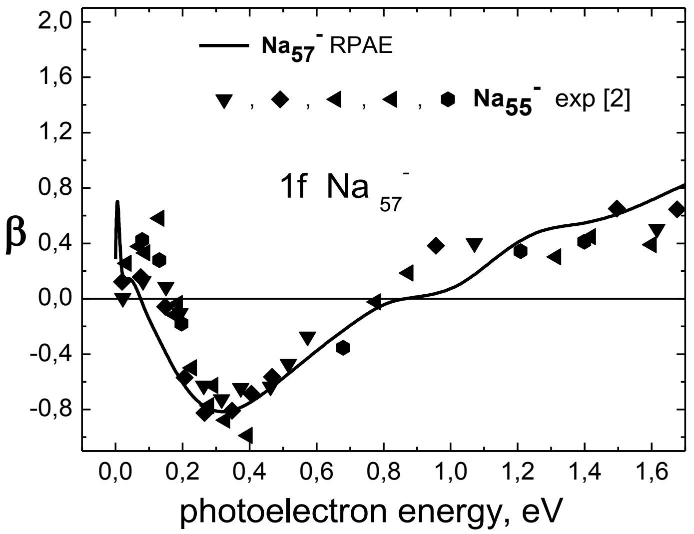

Figure 1: The angular asymmetry parameter of photodetachment from 4f electron shell in $Na_{57}^-$. Experimental data are from [2].

The similar approach has been used for the calculation of the photodetachment cross section and photoelectron distribution for the $C_{60}^-$ anion. The results will be presented at the conference.

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# COMPLEXITY IN ATOMS AND MOLECULES INVESTIGATED BY ELECTRON, ELECTRON COINCIDENCE METHODS

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In the past one and a half decades, non-local autoionization processes have attracted a growing interest, by the prediction of two new such phenomena in 1997 [1] and 2001 [2]. Ever since, a great deal of effort has been invested in proving their occurrence and in understanding their implications, as these decay mechanisms, now known as Interatomic Coulombic Decay (ICD) and Electron Transfer Mediated Decay (ETMD) were predicted to be universally occurring.

Although ICD has been experimentally demonstrated some time ago [3], only recently was it possible to record electrons emerging from the non-local autoionization of water clusters [4]. This has been achieved by using an electron-electron coincidence technique, in which, from a process leading to the ejection of two electrons, both are collected and guided towards the detector.

Further on, experiments on mixed Ne-Kr clusters have shown that ICD is the only open decay channel after Ne 2s ionization. Our systematic study as a function of the initial mixture composition shows that on increasing the Kr percentage, the ICD feature shifts towards higher kinetic energies, but not on increasing the cluster size at the same mixing ratio. This was interpreted by the change in the polarizability of the clusters as the cluster size increases due to Kr enrichment, thus leading to a lowering of the initial and the final states, with the latter being lowered more than the former. Furthermore, Kr enrichment yields a shoulder on the high kinetic energy side of the ICD peak, indicating the involvement of surface Kr atoms in the decay process in Kr-poor clusters, whereas in big mixed cluster both surface and bulk components seem to play an important role.

In recent experiments we have shown the existence of the so called Electron Transfer Mediated Decay (ETMD) process [5] (see also [6]). This decay starts with an inner-valence shell ionization, where the hole is filled by an electron from a valence shell of a adjacent atom, with the subsequent ejection of a third electron from the same (ETMD (II)) or different atom (ETMD(III)).

Our newest experimental work has focused on autoionization processes occurring in ArXe heterogeneous clusters. Systematic investigations on aggregates with a Xe percentage of 1-5 % in the original mixture indicate an ICD-ETMD competition, consistent with recent theoretical results predicting both paths as viable decay channels [7], depending on the size of the cluster.

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# FREE ELECTRON LASERS: DYNAMICS AND SRUCTURE TOWARDS FEMTOSECOND TIME AND NANOMETER SPATIAL RESOLUTION

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***F***ree ***E***lectron ***L***asers (FEL) are innovative, accelerator-driven light sources that now have been demonstrated to deliver, for the first time, intense coherent light in a wavelength regime from tens of nanometers down to even one Ångström. Pulse intensities surpass those of 4th generation synchrotrons by a factor of one billion and the light flashes, with a duration of less than ten femtoseconds (1 fs = $10^{-15}$ s), are more than thousand times shorter than achievable up to now. Thus, FELs penetrate a *terra incognita* in light-matter interaction opening a new chapter in science throughout all disciplines, in physics, material science, chemistry or biology.

The talk will highlight the working principles of FELs and the performance of the first machines operational worldwide, the FLASH in Hamburg, the SCSS in Japan and the LCLS in Stanford. Exploiting the capabilities of a new instrument, the ***C***FEL-***A***SG ***M***ulti ***P***urpose (CAMP) end-station [1] that allows the simultaneous momentum resolved detection of electrons, ions, scattered as well as of fluorescence photons, pioneering results of in atomic, molecular and cluster physics have been achieved pointing to the rich future potential. Can we record “the molecular movie”, i.e., follow in time the motion of atoms and the rearrangement of electrons, e.g., at transition states during chemical reactions, for light-harvesting molecules and will it be possible to realize the vision determining the structure of single biomolecules – proteins, viruses – or nanoparticles in gas or liquid phases without the need of crystallization?

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# Tailoring photoemission in strong-field laser cluster ionization

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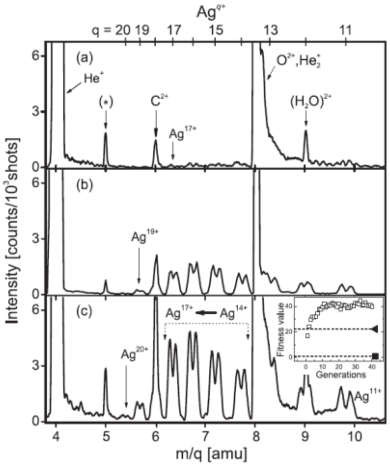
Atomic clusters in intense laser fields are a nice playground to study the non-linear coupling of electromagnetic radiation into matter [1]. Experiments on cluster beams (see e.g. [1-4]) as well as corresponding theoretical work [1,4,5] have shown that excitation with optically delayed dual pulses provides a powerful way to control the coupling of the radiation to these finite systems. Both the yields of highly charged atomic ions as well as the kinetic energy of emitted electrons [6] are strongly enhanced for a particular optimal delay and laser polarization [7]. Non-stationary plasma effects lead to pronounced dynamics in the optical response, which itself depends on the cluster size. In general, it has become clear that by shaping the exciting field photoemission can be tailored within a wide range.

In this contribution we will first present results of laser intensity resolved measurements which show that high charged (up to q=24 in the case of $Xe_N$) atomic ions can be generated at an unexpectedly low threshold intensity of $10^{14}$ W/cm$^2$. Good agreement between these observations and a molecular dynamics analysis allows us to identify the mechanisms responsible for the highly charged ion production and the surprising intensity threshold behavior of the ionization process [4].



In a second approach we study the influence of shaping the intense laser pulses in amplitude and phase. The figure shows how – just by pulse shaping – the charge state distributions Ag$^{q+}$ from the Coulomb explosion of silver clusters embedded in Helium droplets can be modified [8]:
top: unshaped 50 fs pulse,
middle: 500 fs linearly downchirped pulses,
bottom: laser pulses fully optimized in amplitude and phase within a control experiment based on iterative feedback with genetic algorithm. By this the yield of highly charged ions significantly increases.

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# CRYSTALLINE UNDULATOR AND CRYSTALLINE UNDULATOR BASED GAMMA LASER: CURRENT STATUS AND PERSPECTIVES

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Recent advances in the theory of novel sources of hard electromagnetic radiation: Crystalline Undulator (CU) and Crystalline Undulator based Laser (CUL) will be presented. The operating principle of CU is based on the channelling phenomenon. Channelling takes place if a particle enter a crystal at a small angle to major crystallographic planes or axes. The particle becomes confined by the planar or axial potential and moves preferably along the plane or axis following its shape.

If the planes or axes are periodically bent, the channelling particles move along nearly sinusoidal trajectories. Similarly to what happens in ordinary undulator, relativistic charged particles radiate electromagnetic waves in the forward direction. The advantage of the crystalline undulator is an extremely strong electromagnetic field inside the crystal which can steer the particles much more effectively than the most advanced superconductive magnets. This allows one to make the period of CU two or even three orders of magnitude smaller then that of the conventional undulator. As a result the frequency of the radiation can reach the hard x-ray and gamma-ray range.

The radiation becomes much more powerful and coherent if the density of the particles that enter the undulator is modulated along the beam direction with the period equal to the wavelength of the produced radiation. In this case the electromagnetic waves emitted by different particles have nearly the same phase and therefore the intensity of the radiation becomes proportional to the particle density squared in contrast to the linear proportionality in the case of unmodulated beam.

The beam can be modulated in ordinary (magnetic) undulator tuned to the wavelength of auxiliary light which is integer multiple of the wavelength of the crystalline undulator radiation (here called 'main radiation'). The auxiliary wavelength should be in the optical or soft X ray range which is attainable in the present state-of-the-art magnetic undulators and free electron lasers.

Due to the interaction with the auxiliary wave and the field of the magnetic undulator, the beam will be spatially modulated with the period equal to the wavelength of the auxiliary radiation. But the Fourier decomposition of the density profile will contain also higher harmonics with shorter wavelength including the wavelength of the main radiation. The necessary harmonic can be substantially amplified if the initial particle beam has a layered energy profile.

In the recent patent application we have described CUL: a device in which the crystalline undulator is placed near the exit from the magnetic undulator. This tandem of magnetic and crystalline undulators allows the intensive generation of coherent radiation in hard X-ray or gamma ray range.

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# FORMATION OF IONIC COMPLEXES IN DOPED HELIUM DROPLETS

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Superfluid helium nano-droplets (HND) are an excellent medium to investigate atomic and molecular complexes at ultracold temperatures. Due to the unique properties of the droplets it is possible to synthesize and study novel complexes [1]. In addition, helium droplets provide a perfect environment in which metastable excited He atoms (He*) are easily formed and Penning ionization processes can be investigated.

In the present work we report on the discovery of a novel ionization mechanism of ions embedded in helium nano-droplets. An electronically excited He atom (He*) collides with a singly-charged cation preformed inside the HND and transfers its internal energy which result in the formation of a doubly-charged cation. This mechanism can be attributed to a Penning-like process of the following form:

$$He^* + X^+ \rightarrow He + X^{2+} + e^-$$

This reaction was discovered during our investigations of methyl iodide embedded in helium nano-droplets and the formation of doubly-charged iodine was observed [2].

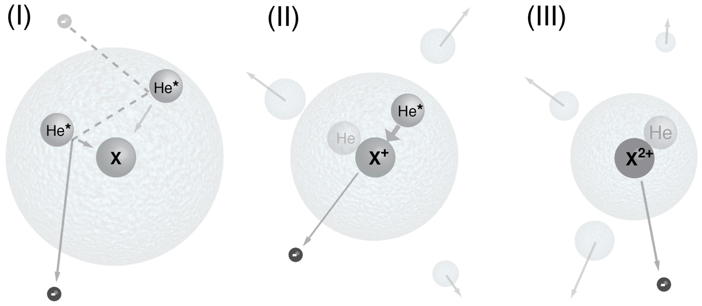

Figure 1: Scheme of a sequential Penning ionization process. An initial electron with sufficient high energy forms two or more metastable excited helium atoms (I). In a multiple step process the He* atoms can transfer successive their internal energy to the dopant and can cause among others the formation of doubly charged species (II+III) [2].

*Acknowledgement:* This work was supported by the *Fonds zur Förderung der wissenschaflichen Forschung* FWF, Wien (P 19073) and the University of Innsbruck via the *Doktoratsstipendium aus der Nachwuchsförderung der Universität Innsbruck*. AM gratefully acknowledges a FWF Erwin-Schrödinger-abroad fellowship (J 2973-N20). As holder of a Canada Research Chair in Physical Chemistry, DKB also thanks the support of the Canada Research Chair Program.

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# EMBEDDING BIOMOLECULAR IONS IN LIQUID HELIUM NANODROPLETS

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Superfluid helium droplets provide an isothermal ultracold environment for embedded molecules and are ideal matrices for optical spectroscopy [1]. Recently, we set up a new experiment to dope He droplets with biomolecular ions [2]. In this approach, biomolecules are brought into the gas phase via electrospray ionization (ESI) and are then selected according to their mass-to-charge ratio using a quadrupole mass spectrometer. The mass-to-charge selected ions are stored in a linear ion trap, from which they are picked up by a pulsed beam of helium droplets. While in the initial experiments very large He droplets (composed of $10^{10}$-$10^{12}$ atoms) were observed [2], a new He droplet source enables us now to embed amino acids, peptides, and even small proteins in droplets consisting of $10^4$ to $10^6$ He atoms, depending on the dopant molecules and the source conditions. We will discuss how the size of the doped droplets can be directly measured by accelerating the doped droplets in an electric field. Furthermore, we will present our progress towards IR spectroscopy of the embedded molecules aiming on detailed structural information on these cold species.

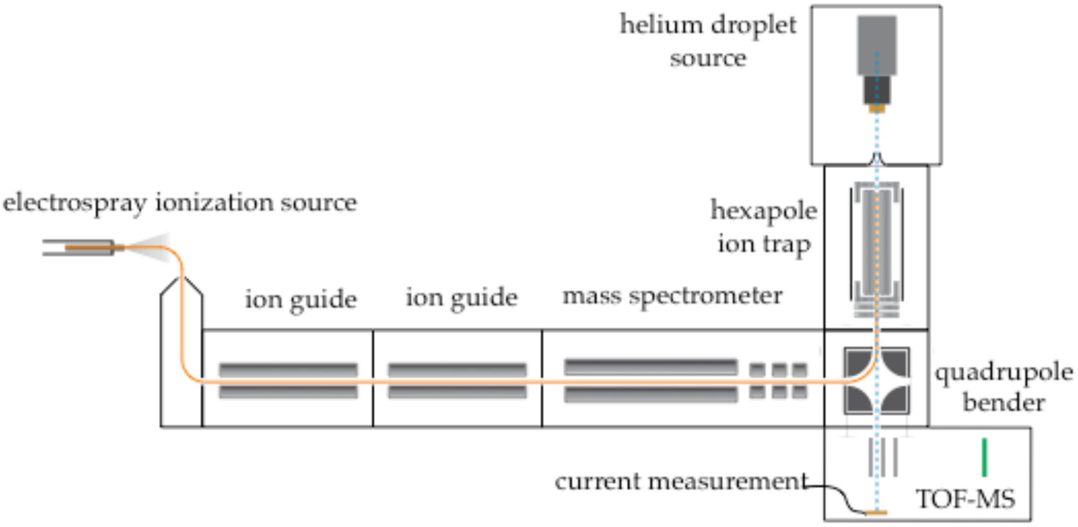

Figure 1: Schematic overview of the experimental setup. Ions are brought into the gas phase via electrospray ionization and are stored in a linear ion trap, from which they are picked up by a pulsed beam of He droplets.

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# Alkali Atoms and Molecules on Cold Helium Clusters: Spin Relaxation due to Collisional Interactions

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Alkali atoms deposited on large helium clusters stay at the cluster surface and form molecules in cold collisions. Through evaporation of helium atoms, the internal temperature is automatically maintained at 0.4 K, the equilibrium temperature of the cluster. Laser spectroscopy of the created molecules has been accompanied by our own quantum chemical calculations that allow state assignments for alkali dimers and trimers in various spin states [1]. By measuring the circular dichroism in the presence of a magnetic field, the populations of Zeeman sublevels in alkali atoms, dimers, and trimers on helium clusters were probed. No dichroism was observed for the atomic alkali sample (K, Rb, Cs) on helium droplets, indicating that the sublevels have not thermalized [2]. The Zeeman sublevels of dimer and trimer molecules, however, turn out to be populated according to a temperature of 0.4 K, implicitly allowing the first determination of the droplet's surface temperature [3]. In an optically detected electron spin resonance experiment [4], long electron spin life times were confirmed for the atomic species. This result seems to be of similar origin as the observation of slow spin relaxation in cold collisions between metal atoms and helium [5] and fast relaxation in molecule-helium collisions [6].

High resolution ESR spectroscopy of K and Rb on the helium cluster surface shows the influence of the helium cluster size on the electron spin density at the alkali nucleus [6]. The corresponding change of the Fermi contact interaction can be modeled in a similar way as a collision induced hyperfine shift.

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# **Sunday, 24 July 2011:** 10:00-21:00h

Conference tour through the famous castles of Potsdam with a barbecue in the evening at a lake nearby

***Location: “Kinosaal”***

# Monday, 25 July 2011

## Morning Session I: 9:30-11:00h

*Coffee break 11:00-11:30h*

## Morning Session II: 11:30-13:00h

*Lunch 13:00-14:30h*

## Afternoon Session I: 14:30-16:30h

## 16:30-16:45: ISACC 2011 Closing

# FRAGMENTATION AND PROTECTION OF BIOMOLECULES – THE EFFECTS OF ATTACHING A FEW WATER MOLECULES

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We have studied fragmentation of water embedded adenosine 5'-monophosphate (AMP) anions after collisions with neutral sodium atoms [1]. At a collision energy of 50 keV, loss of water molecules from the collisionally excited cluster ions is the dominant process while fragmentation of the AMP itself is almost completely prohibited if the number of attached water molecules is larger than thirteen [2]. However, regardless of the initial number of water molecules attached to the ion, capture of an electron, i.e. formation of a dianion, always leads to loss of a single hydrogen atom accompanied by evaporation of water molecules [3]. This damaging effect becomes more important as the size of the water cluster increases, which is just the opposite behaviour of that observed for collision induced dissociation (CID) without electron transfer. For both cases, the loss of water molecules within the experimental time frame (of the order of 10 μs) is qualitatively well described by means of a common model of an evaporative ensemble. Comparisons with this model indicate characteristically different distributions of internal energy for CID and electron capture induced dissociation [1]. A slightly different approach to this problem has also been taken in which we ascribe each final cluster size (number of kept water molecules) to a small, unique, interval of internal energy in the mother cluster. This approach yields semi-empirical internal energy distributions for the two processes – CID and electron capture induced dissociation – which exhibit the same main features as those assumed for the model [4].

Interestingly, similar ideas may be used to qualitatively explain high probabilities for long series of evaporations of single intact molecules from singly charged, loosely bound, clusters of polycyclic aromatic hydrocarbon (PAH) molecules [5-6].

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# INTENSE FEMTOSECOND LASER STUDIES OF BIOMOLECULES

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Intense femtosecond (fs) laser pulses provide unique tools for influencing and observing molecular dynamics on ultrashort timescales [1]. Whilst such pulses have been applied for time-resolved studies in the most fundamental molecules (e.g. see [2] and references therein), there is increasing interest in using this technology for studying bond fragmentation in molecules of biological importance. For example, there is significant promise in sequencing of peptides [3] and of selective bond cleavage in prototypal amino acids [4].

At the meeting, I will report on recent experimental studies of fs laser interactions with molecules of biological interest, namely small peptides and DNA bases. In a novel experimental approach, we utilise Laser Induced Acoustic Desorption [5] to produce a gas phase target of neutral molecules, which are subsequently exposed to an fs laser pulse. Ionisation and fragmentation products are extracted electrostatically and mass analysed in either a time-of-flight device or a linear electrostatic ion trap, with the latter providing high resolution mass spectra [6]. These formative studies have been carried out using pulses of 100 fs duration, and provide insight into how these small biomolecules behave in an intense laser field. This provides a valuable platform for future studies where ultrashort pulses (<10fs) promise to enable observation and control of biomolecular fragmentation on sub-vibrational timescales.

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# SHELL EFFECTS ON HELIUM-$C_{60}^+$ COMPLEXES IN HELIUM DROPLETS

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Novel molecular complexes may be grown within ultracold helium droplets. Recent experiments have found the formation of helium-fullerene complexes embedded in helium droplets. The mass spectra interestingly show “magic” numbers of the particles of the monocation series fullerene–$He_n$, corresponding to abrupt drops in the cluster abundance.

Stimulated by these fascinating experimental results, we have performed quantum chemistry computations and molecular dynamics (MD) simulations on these $C_{60}$-$He_n^+$ ($n$=1–66) systems. By the assessment based on the CCSD(T)/CBS results for He-benzene systems, the best density functional has been determined and applied from more than 200 functionals. Then the potential energy surface (PES) is explored for the $C_{60}$-$He^+$ system, by using 676 3D-sampling grid points. It is found that hexagonal faces of $C_{60}$ are global minima of the PES with binding energy (BE) of ~10 meV, while pentagonal faces correspond to local minima (BE=~9 meV). In order to investigate the multiple-helium and fullerene clusters $C_{60}$-$He_n^+$, MD simulations are performed utilizing the fitted $C_{60}$-$He_n^+$ force field and He-He force field. In this talk, I will present these simulation results and explain the origin of the shell effects observed in experiments.

# DISSOCIATION OF FREE PEPTIDES AND OLIGONUCLEOTIDES BY ENERGETIC PHOTONS AND KEV IONS

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The response of isolated biomolecules upon VUV and soft X-ray photoabsorption and energetic ion impact is of great interest in the context of astrobiology and radiobiology. Key questions concern e.g. ion chemistry in the interstellar medium, the possibility of transport of intact gas phase biomolecules from space to earth and the molecular mechanisms underlying biological radiation damage. We have developed a novel apparatus in which a home built electrospray ionization (ESI) source is combined with a radiofrequency (RF) ion trap and a time of flight mass spectrometer. First experimental campaigns focused on the investigation of dissociation dynamics in various protonated peptides *in vacuo*. For photoionization studies, the system was interfaced with the U125/NIM VUV beamline at the BESSY II facility (Berlin) and with the I411 MAXII soft X-ray beamline at MAX-lab (Lund). Complementary experiments on keV ion induced peptide fragmentation where performed in-house, using a 14 GHz electron cyclotron resonance ion source.

VUV photodissociation of protonated leucine enkephalin was found to predominantly induce the loss of aromatic side-chains and related fragments [1]. These channels are very likely due to fast bond-scission following e.g. population of a dissociative state *before* internal energy is equilibrated over the peptide and statistical fragmentation can set in. A systematic investigation of this process as a function of peptide size revealed a quenching of these fast channels in larger peptides. Furthermore, soft X-ray induced N 1s ionization localized on the leucine enkephalin backbone was found to trigger fast scissions in the adjacent side chain. No such site selectivity could be observed in the core ionization induced fragmentation of oligonucleotides.

Ion induced dissociation of various protonated peptides at keV energies was found to induce similar fragmentation patterns dominated by side-chain related fragments [2,3]. This finding implies that here the initial process is single (or multiple) electron capture of peptide valence electrons in glancing collisions – a process similar to VUV photoionization. For head-on collisions, much higher excitation energies are expected, leading to complete disintegration of the peptide.

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# RESONANCES AND THRESHOLD EFFECTS IN DISSOCIATIVE ELECTRON ATTACHMENT TO BIOLOGICAL MOLECULES

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Recent progress in studies of dissociative electron attachment (DEA) processes was stimulated by the development of new experimental techniques involving electron beams with high energy resolution. This allowed detailed investigation of threshold phenomena in low-energy dissociative attachment to diatomic and polyatomic molecules: vibrational Feshbach resonances (VFRs) and threshold cusps.[1] A VFR occurs when the electron is captured by the long-range field of the molecule with the simultaneous excitation of molecular vibrations. Further investigations showed that VFRs and threshold cusps are very general phenomena, also observed in DEA to biological molecules in the gas phase. Particular outstanding examples are sharp peaks in DEA cross sections for uracil[2,3] and thymine[4].

Recent calculations[5,6] based on the resonance R-matrix theory[7] showed that VFRs and threshold cusps in these systems can be described by a model incorporating a very short-lived $\sigma^*$(O-H) resonance leading to the loss of a hydrogen atom from the carboxyl group to form the dehydrogenetated anion $(M\text{-}H)^-$. *Ab initio* calculations were performed for formic acid and uracil. More recent calculations for alanine, β-alanine, and α-, β- and γ-aminobutanoic acids are based on a model with R-matrix parameters for the formic acid, which is modified then to take into account the actual values of dipole moments and polarizabilities of these molecules. The isotope effect is investigated too, and results confirm experimental findings for deuterated uracil and thymine.

For practical applications to radiation damage it is important to know how DEA processes are modified in condensed-matter environments. It is known that the long-range effects are significantly suppressed in this case. On the other hand, polarization of the environment by the negative ion and the lower density of electron states in the medium lead to the DEA enhancement observed for several molecules in the past. Therefore investigation of competition between these several effects is important. A particular interesting example is a suppression of the VFR effect in DEA to the $CH_3I$ molecule observed experimentally[8]. Recent calculations[9] confirm that the cross section for DEA to the $CH_3I$ molecule physisorbed on a surface of the Kr film is reduced by an order of magnitude as compared to the gas phase DEA cross section.

This work was performed in collaboration with G. A. Gallup, V. Vizcaino, and S. Denifl, and was supported by the US National Science Foundation and a Marie Curie International Incoming Fellowship (IIF) FP7-PEOPLE-2009-IIF – 252714.

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# (e,2e) EXPERIMENTS ON $C_{60}$ IN GAS PHASE

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The ionization of $C_{60}$ in gas phase has been studied by (e,2e) experiments at about 1000 eV in asymmetric kinematics and 0.6 a.u. momentum transfer. The binding energy spectrum has been compared with previous gas phase[2] as well as solid state [2] photoemission data and theoretical calculations [3]. The measured coincidence angular distributions corresponding to the ionization of the HOMO and HOMO-1 states have been compared with calculations that account for the ionic symmetry and electronic structure of $C_{60}$ [4].

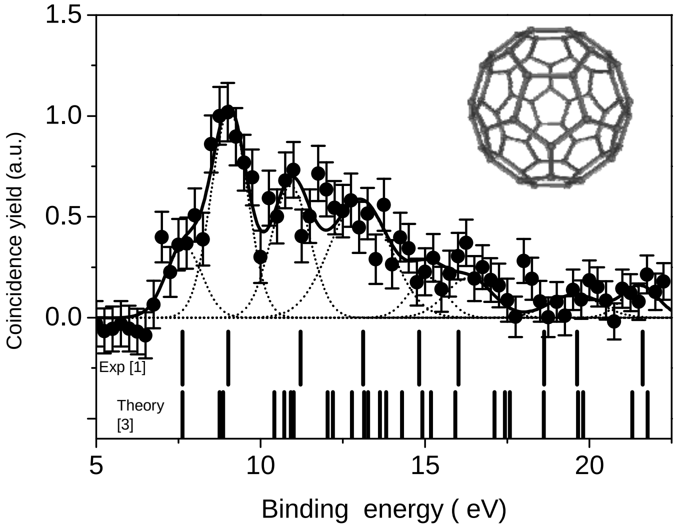

Figure 1: Binding energy spectrum of $C_{60}$ measured at $E_a$=1000 eV, $E_b$=20 eV, $\theta_a$=4° and $\theta_b$=80°. The bars below the spectrum are the positions of the electronic bands measured in [1] and calculated in [3]. The *a,b* labels represent the scattered and ejected electrons respectively.

The (e,2e) measurements well reproduce the electronic structure which was established by previous calculations and measurements, both in the gas and condensed phases thus confirming the weak interaction of $C_{60}$ molecules in the solid. The differences observed in the comparison between calculations and experiment in the case of the angular distributions hint to the role of the screening and its consequences for the interactions between the continuum state electrons.

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# MULTIPLE EXCITATION, ELECTRONIC DECAY, AND CHARGE TRANSFER IN RARE-GAS CLUSTERS IRRADIATED BY EUVFEL PULSES

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Following FLASH operation in Germany [1], SPring-8 Compact SASE Source (SCSS) test accelerator in Japan [2] started user operation in 2008. This test facility provides EUVFEL pulses in the photon energy range between 20 and 24 eV. Most of the atoms can be photoionized at huge cross sections in this energy range. As a result, if atomic clusters are irradiated by the tightly focused EUVFEL beam, sequential multi-photon ionization and excitation take place. We have been studying these multiphoton multiple excitation and subsequent decay in rare gas clusters [3-10].

In brief, we have carried out 3D ion momentum spectroscopy and 2D electron spectroscopy and confirmed the following scenario. Up to a certain charge state of the cluster, single photon ionization takes place sequentially. With the increase in the charge states of the parent cluster, however, the single photon ionization (outer ionization) becomes energetically forbidden due to Coulomb blockade. Even after that, photo-excitation (inner ionization) proceeds. These multiply excited states (nano-plasma) decay electronically emitting low energy electrons. The created charges are distributed in the cluster in such a way that the total energy is minimized before Coulomb explosion takes place. We will report the results of measurements that prove this scenario.

The planned experiments at SACLA, the XFEL in Japan, will also be described.

The author is grateful to all the collaborators listed above and authors for Refs. [3-10]. The work is supported in part by X-ray Free Electron Laser Utilization Research Project of MEXT.

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# MICROHYDRATION OF CONJUGATE BASE ANIONS PROBED BY GAS PHASE VIBRATIONAL SPECTROSCOPY

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Conjugate base anions are ubiquitous species in aqueous phase chemistry. However, how these anions are hydrated at the molecular level is far from completely understood. A molecular-level understanding of ion hydration is also important in understanding the surface speciation and reactivity of aerosols, which play a key role in atmospheric and oceanic chemical cycles. We use infrared multiple photon dissociation spectroscopy over the spectral range of 550-4000 cm$^{-1}$ as a structural probe of size-selected clusters in which the polyatomic anions $HCO_3^-$, $NO_3^-$, $HSO_4^-$, $SO_4^{2-}$, $H_2PO_4^-$ and $(CH_2)_n(COO^-)_2$ are hydrated by a known number of water molecules.[1-3] The experiments follow how the hydrogen-bonded solvent network around these anions evolves, one water molecule at a time. Structural assignments are made by comparing the experimental infrared spectra to those obtained from electronic structure calculations. Our results show how changes in anion structure, symmetry, charge state and acidity have a profound effect on the structure of the solvent network and, vica versa, how hydration can markedly affect the structure of the anion core in a microhydrated cluster.

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# CLUSTERS IN INTENSE XUV PULSES: IONIZATION HEATING AND TIME-RESOLVED IMAGING OF CLUSTER POTENTIALS

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A key issue for many applications of short wavelength FEL light is how the nature and dynamics of intense laser-matter interactions develop as function of wavelength. Promising prototypes for exploratory studies on finite targets are atomic clusters, as great experience in their experimental and theoretical investigation is available [1].

In this contribution we discuss the dynamics of small $Ar_N$ in intense XUV laser fields, where experiments have shown strong evidence for the presence of a multistep ionization process and the disappearance of collisional plasma heating [2]. To study the microscopic laser-cluster dynamics we use Monte-Carlo- and molecular dynamics simulations [3]. It turns out that the cluster excitation mechanisms in intense XUV and soft x-ray pulses strongly differ from the response behavior in the well-studied near-infrared and VUV wavelength regimes. Whereas the heating of delocalized electrons in the nanoplasma is the dominant energy capture mechanism in optical and VUV fields, energy absorption due to the excitation of localized electrons, i.e. by the inner ionization processes itself, becomes increasingly importantat high photon energy. An implication of this ionization heating mechanism is the possibility to produce nanoplasmas with well controlled density and temperature [3,4]. Further, the formation of a nanoplasma is substantially delayed due to direct photoemission in early stages. The resulting signatures in electron spectra due to the multistep ionization process and subsequent thermal electron evaporation from the nanoplasma are analyzed via molecular dynamics simulations, cf. Fig. 1.

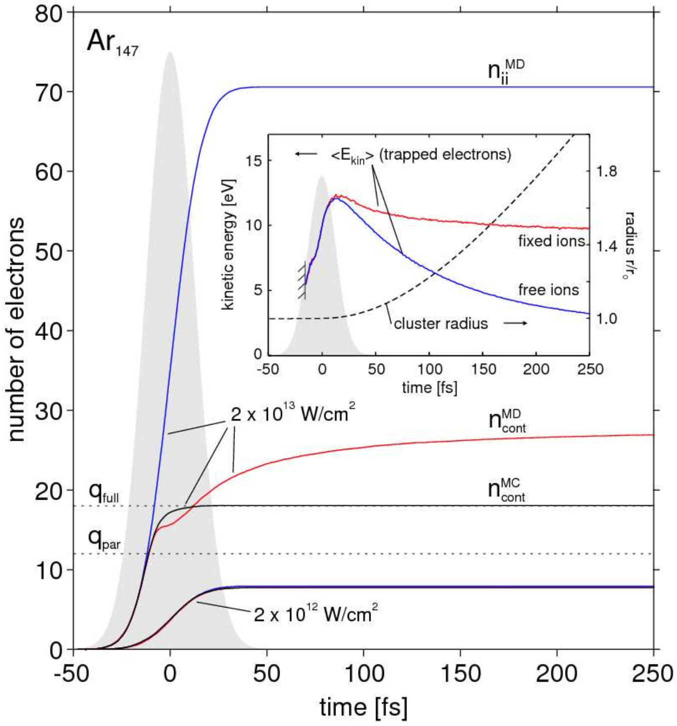

Figure 1: Calculated ionization dynamics of $Ar_{147}$ for excitation with 30 fs laser pulses at 32 nm (intensities as indicated). Evolutions of total inner ionization $n_{ii}$ and the number of continuum electrons $n_{cont}$ are given for MD and MC simulations. The inset depicts the evolution of the mean kinetic energy of trapped electrons for free vs. fixed ions dynamics.

We further propose a non-optical scheme to directly measure the cluster ionization and explosion dynamics together with the evolution of the nanoplasma by tracing the cluster space-charge potential in a two color pump-probe experiment. Numerical results on this time-resolved potential streaking will be discussed and it will be shown that our approach offers a promising new route to access ultrafast ionization dynamics in finite samples [5]. The direct access to the cluster space-charge potential is of high relevance for assisting x-ray single shot diffraction measurements because of the possibility to extract so far inaccessible properties of the nanoplasma.

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# ULTRA SHORT PULSE EXCITATION OF FREE NANOPARTICLES

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Nanoscopic systems prepared from nanoparticles as unique building blocks have the advantage that their properties depend critically on the single nanoscopic units and their assembly on substrates. Single nanoparticles show often size and composition dependent optical, electronic, structural, and dynamical properties. This includes quantum size effects, which are efficiently modified by the internal structure of the nanoparticles and their surroundings

Recent progress in chemical syntheses of structured nanoparticles as well as properties of single nanoparticles is presented. Single, free nanoparticles without any contact to other particles or substrates are either prepared in traps or focused nanoparticle beams. These approaches allow us to study the intrinsic size- and composition dependent properties of isolated nanoscopic matter and their photon-induced dynamics. Results from a variety of different experimental approaches making use of synchrotron radiation and ultra-short laser pulses are presented. These provide specific information on the electronic structure, plasmonic excitations, the location of the emitted electrons from nanoparticles, the dynamics of electron emission and cation formation, as well as the dynamics of collective electronic excitations in the femtosecond time domain.

*Location: “Großer Saal”*

# Poster session & coffee

# SURFACE IMPACT COLLISIONS OF ENDOHEDRALLY COMPLEXED FULLERENES

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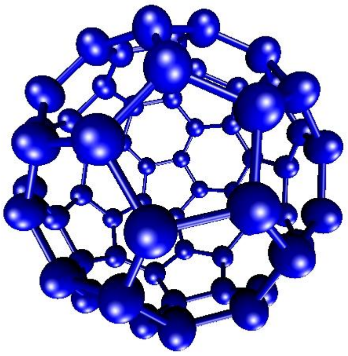
Classical molecular simulations of collisions between graphene barriers and the endohedral compound Xe@$C_{60}$ were performed. A Tersoff potential modeled the interactions between the carbon atoms while the endoatom-carbon interactions were obtained from a Lennard-Jones potential.

Sixteen different targets were explored, varying in number of layers (1 - 4) and number of Carbon atoms per layer (276, 496, 780, 1128). The peripheral atoms on the top, bottom, and sides, of each barrier were secured. The projectile, Xe@$C_{60}$, was given various initial velocities and launched 76 times for given velocity for a given barrier. The spectrum of initial velocities for the 1-layer (2-layer, 3-layer, 4-layer) thick barrier was .06-.14 (.06-.21, .06-.24, .06-.28) Å/fs, with increments of .005 Å/s. Overall, 520 batches of 76 simulations per batch were performed. During each batch, the initial displacement of the barrier was randomized within its smallest non-symmetrical region. The initial orientation of the fullerene projectile was systematically rotated by small increments, spanning its smallest non-symmetrical region.

Using results from previous investigations, a testing system was implemented to determine the qualitative effect of the collisions. This was done in order to determine the minimum size of the wall and number of layers needed to run accurate future simulations.



$C_{60}$ Fullerene

# STABILITY OF MULTIPLY CHARGED RARE GAS CLUSTERS

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A multiply charged cluster with charge $Z$ is stable if the cluster size $N$ is larger than the appearance size $N_c(z)$. Echt et al. [1] estimated the appearance sizes for different multiply charged van der Waals clusters using the liquid drop model. Their calculation reproduced the appearance sizes for many multiply charged clusters measured in experiments. However, a recent experiment [2] has shown that the observed appearance sizes for doubly and triply charged neon clusters are much smaller than those expected by the model. There has been an attempt to shed light on this problem. Nakamura [3] has calculated the appearance size accounting for the geometrical shell effects. The discrepancy between the theory and experiment has been improved. Still the model cannot explain sufficiently well the discrepancy for the case of Ne clusters. Furthermore Calvo [4] has recently introduced the effects of nuclear motion in the liquid drop model. However, the discrepancy between the model and the experiment has not yet been drastically improved.

In this work we suggest a different approach. In the calculations performed so far, the excess charge is supposed to be distributed uniformly within the cluster volume. Instead, here we assume the uniform charge distribution over the cluster surface. Such distribution could be justified by the repulsion and the migration of the excessive positively charged sites in the system. As shown in Table below, the appearance sizes calculated within this model are much lower than those reported in the previous works. The present model gives the appearance sizes for doubly and triply charged neon clusters that are quite close to the earlier reported experimental values.

Additionally we will analyse the fragmentation of multiply charged rare gas clusters using the molecular dynamics approach.

This work has been financially supported by bilateral scientist exchange program between Germany and Japan by DAAD and JSPS.

Table: Theoretical and experimental values for appearance sizes $n_c(z)$ of multiply charged clusters with charge $Z$. Values in parentheses are the results of calculation accounting for the geometrical shell effects

| Rg | $Z$ | Experiment[1,2] | Echt[1] | Nakamura[3] | Present model |
|---|---|---|---|---|---|
| Ne | 2 | 287 | 868 | 635(657) | 257(257) |
|  | 3 | 656 | 2950 | 2209 | 660(667) |
| Ar | 2 | 91 | 122 | 92(97) | 61(61) |
|  | 3 | 226 | 333 | 251(255) | 134(135) |
| Xe | 2 | 46 | 51 | 40(36) | 26(30) |
|  | 3 | 107 | 114 | 87(83) | 50(53) |

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# SILVER INTERACTION IN THE PRION OCTAREPEAT DOMAIN

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PRION, proteinaceous infectious particle, is an infectious agent composed of protein in a misfolded form. This new structure, which is influenced by metal binding, becomes pathological and is involved in many diseases such as Creutzfeldt-Jakob.

The prion protein is known to binds metal in its N-terminal octarepeat domain [1]. This domain is composed of tandem repeats of the sequence PHGGGWGQ. Recent work [2] showed that each HGGGW (Histidine, Glycine and Tryptophan) segment may accommodate on metal ion. We aim at investigating the coordination of silver in this amino acid sequence and his influence on the peptide conformation.

Using a mass spectrometer coupled with OPO lasers in the UV and IR regions, we measured the optical and vibrational spectra of the $[HGGGW+Ag]^+$ complex and of several other sequences. Optical properties, binding site and peptide confirmation will be discussed. We will also report ion mobility spectroscopy and theoretical results.

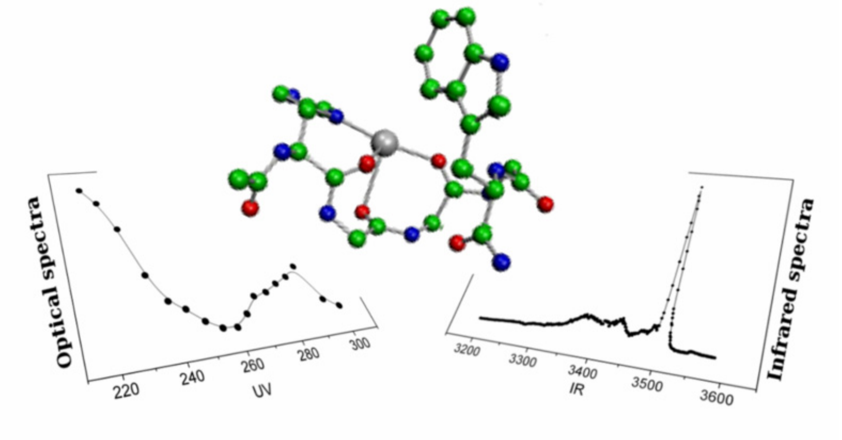

Figure 1: Using mass spectrometer coupled with OPO lasers, we measured optical and vibrational spectra of Ag-PRION complex.

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# STRONG COUPLING REGIME IN METALLIC CLUSTERS IN MICRORESONATORS

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We investigate theoretically the photoabsorbtion of the metallic cluster embedded into a single mode quantum microcavity. We show that when the energy of the giant plasmon resonance lies close to the energy of the cavity mode, the strong coupling between plasmons and cavity photons can occur, which is characterized by mode anticrossing and emergence of the doublet structure in ptotoabsorbtion crossection. The characteristic values of the Rabi splitting are expected to be several orders of magnitude larger than those observed in other 0D objects, e.g. single quantum dot- cavity systems.

The photoabsorption of the metallic cluster without a cavity has been calculated taking into account the dynamical polarization effects by using random phase approximation with exchange (RPAE). It's well known that in that case the theory predicts appearance of the giant plasmon resonance in the photoabsorption spectrum (see inset in figure 1) [1]. The ground and excited electronic states of clusters are obtained within the Jellium model using Hartree-Fock approximation for wave functions and one-electron energies calculations.

We develop a new theoretical model based on Feynman diagram technique aimed at finding out a diagram representation of the dipole photoabsorption amplitude which includes processes of direct photoabsorption, influence of the dynamical polarizability within the RPAE and gives rise the plasmon excitation with multiple re-emissions and re-absorptions of the cavity photons. Note, that to find a solution of the corresponding non-linear equation for amplitude is equivalent to detection of conditions of the strong coupling between transitions in cluster and cavity photon. As a result it describes the formation of the hybrid plasmon- photon excitations in cluster – cavity system [2].

We consider a $Na_8$ cluster embedded in a photonic cavity. Figure 1 shows spectrum of the absorption of the cavity cluster system when the energy of giant plasmon resonance is tuned in resonance with the photonic mode energy $\omega_0$. Rabi splitting $\Omega_R$ decreases at the photon lifetime being decreased and finally disappears at $\gamma \approx 8$ meV. Figure 2 shows dependence of real parts of the eigen frequencies on the cavity energy $\omega_0$ for different linewidths of the cavity (in meV). The Rabi splitting varies from ≈0 meV ($\gamma \approx 8$ meV) to 17 meV (for $\gamma = 0.1$ meV). The inset illustrates dependence of the splitting on $\gamma$.

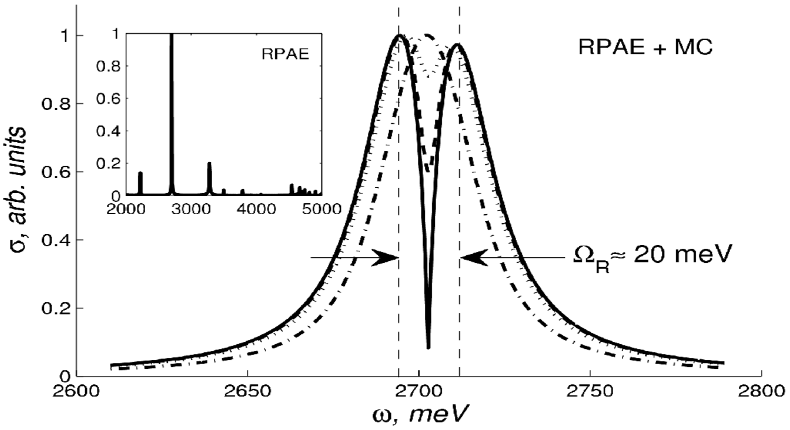

Figure 1: Photoabsorption cross sections of Na$_8$ cluster cased in microresonator for different lifetimes γ of cavity photons (in meV): 0.1 – solid, 2.0 – dashed, 4.0 – dotted and 8.0 – dash-dotted. Inset shows the photoabsorption spectrum of Na$_8$ without of cavity.

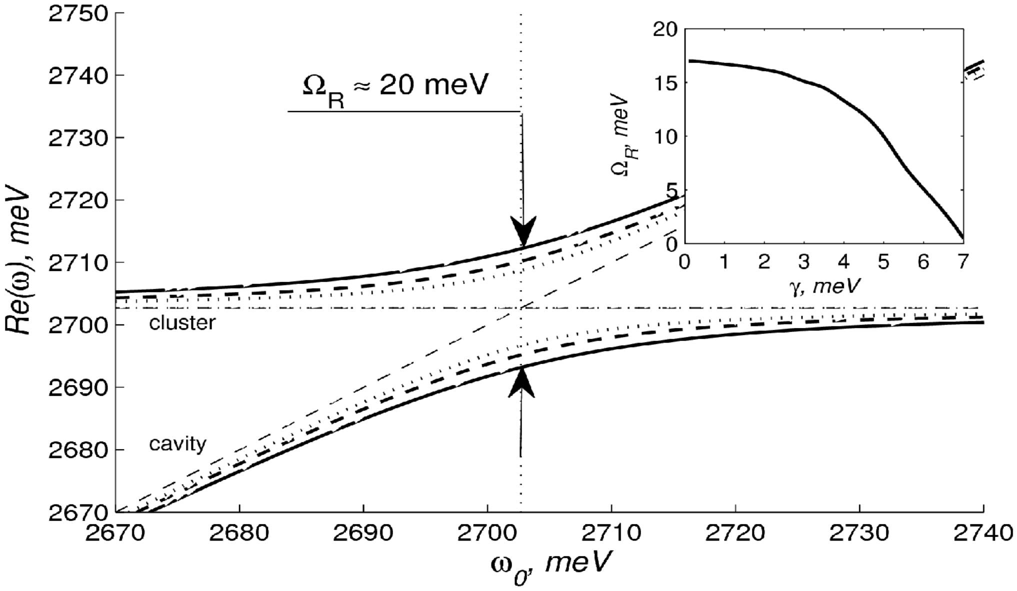

Figure2: Eigen frequency real part dependence on the microcavity mode wavelength for different lifetimes of the photons (in meV): 0.1 – solid, 2.0 – dashed, 4.0 – dotted. Illustration of the crossover from strong- to weak-coupling regime.

In conclusion, we have shown that in the region of the giant plasmon resonance the regime of strong coupling between plasmon and cavity photon can be achieved, which manifests itself by formation of the Rabi doublet and mode anticrossing.

The authors thank V.K.Ivanov for useful discussions. The work was supported by Rannis "Center of Excellence in Polaritonics" and FP7 IRSES project "POLAPHEN". R.G.P. thanks the University of Iceland for hospitality.

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# DISCOVERING STABLE STRUCTURES OF ATOMIC AND MOLECULAR CLUSTERS

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Structural optimization is a major issue in the study of atomic and molecular clusters. Global optimization algorithms have been applied either to map in detail the energy landscape of a cluster system modeled with analytical potentials or to explore promising regions of the configuration space that can be subsequently studied with ab initio or DFT methods. Over the last twenty years, many optimization procedures have been proposed to deal with such challenging problem (see, e.g., Refs.[1-4]). We have developed completely unbiased evolutionary algorithms (EAs) for the global geometry optimization of atomic and molecular clusters (see, e.g., Refs. [5, 6] and references therein). Specifically, we have applied our EAs to discover with success the global minimum of several cluster systems: argon (up to $Ar_{78}$) [7], Morse (up to 80 atoms) [5], binary Lennard-Jones (up to 55 atoms) [8, 9], water (up to 20 molecules) [6] and benzene (up to 30 molecules) [6]. In the case of binary Lennard-Jones clusters [8], the EA was even able to update the global minimum for $n$=38 and size ratio 1.05 that it is reported in the Cambridge Cluster Database [10].

In this communication, we present the main features of our EAs and compare the results of their application to Morse clusters with those obtained with other methods, *e.g.*, the big-bang algorithm, which has also been studied in our group [11]. We will also discuss new results on mixed rare-gas, $Ar_nC_6H_{12}$ [12] and benzene-cation clusters [6].

Acknowledgments: This work was supported by Fundação para a Ciência e Tecnologia (FCT), Portugal, under grant PTDC/QUI/69422/2006, which is financed by Programa Operacional Factores de Competitividade (COMPETE) of QREN and FEDER programs.

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# SUPERIMPOSING ALGORITHM FOR THE IDENTIFICATION OF CHIRAL STRUCTURES (SAICS): APPLICATION TO CLUSTERS

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We report a ready-to-use computational program [1] that extends the scope of a recently proposed superimposing method [2] to include the enantiomer assignment. This is relevant for many chemical applications, because this computational tool is able to qualify a particular difference (i.e., chirality) between two structures, which is sometimes nontrivial to assign. The method uses a probability driven approach, which involves the application of the Hungarian algorithm [3,4] to several randomly generated orientations of one of the comparing structures, followed by reorientation to tune for the best superposition. Basically, the identification of enantiomers is achieved by applying such scheme, a second time, to the mirror-image of one of the comparing structures. As a test of the algorithm for discovering chiral molecules, we have applied the SAICS program to the enantiomer structures of bromochlorofluoromethane, 2,3-dibromobutane, 2-cloro-3-bromo-butane, hexahelicene and [6.6]chiralane. In addition, we have used SAICS to identify enantiomers of water and benzene clusters that arise from global geometry optimization. The results show that the algorithm is robust and effective for the comparison of chemical structures and in discovering pairs of enantiomers resulting, *e.g.*, from geometry optimization. The SAICS program is freely available from the web-site at the University of Coimbra: http://apps.uc.pt/mypage/faculty/qtmarque/en/software/.

Acknowledgments: This work was supported by Fundação para a Ciência e Tecnologia (FCT), Portugal, under grant PTDC/QUI/69422/2006, which is financed by Programa Operacional Factores de Competitividade (COMPETE) of QREN and FEDER programs.

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# CONFINEMENT RESONANCES IN PHOTOIONIZATION OF Xe@$C_{60}$ AND $Xe^+$@$C_{60}$

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Recently the photoionization of Xe@$C_{60}$ [1] and $Xe^+$ [2] have been measured in the energy region of the Xe 4d giant resonance. The experiment [1] confirmed the predicted significant distortion of the giant resonance by the $C_{60}$ shell. Here the photoionization of both the Xe and $Xe^+$ confined inside $C_{60}$ have been investigated using our recently developed $C_{60}$ model potential [3] and the random phase approximation with exchange (RPAE) method for the former and the open-shell RPAE method for the latter. The calculation included all the intershell couplings among the transitions 4d-εf, 5s-εp, 5p-εs and 5p-εd. The results demonstrate significantly stronger correlated confinement resonances in the photoionization of Xe@$C_{60}$ (see Fig. 1) and $Xe^+$@$C_{60}$.

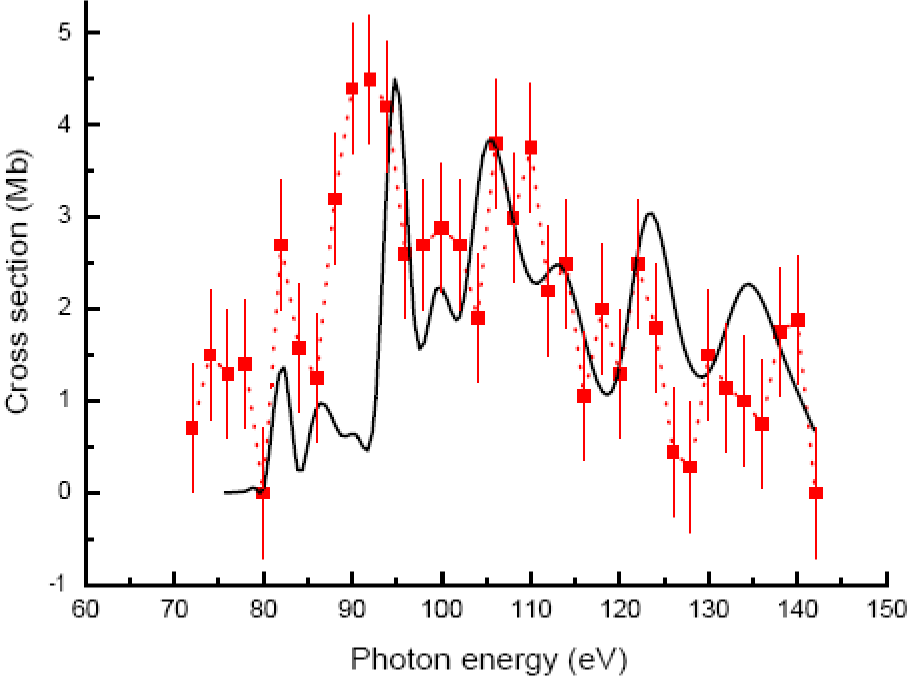

**Figure 1**: Photoionization cross sections for Xe@$C_{60}$. Solid curve represents our results normalized to the experimental data, solid squares with error bars [1]

Also, our results yield better agreement with the measurement for Xe@$C_{60}$[1] and for Xe [2] and demonstrate strong intershell coupling between the 4d-εf and 5s-εp transitions.

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# VALENCE TRANSFORMATIONS OF METAL IONS IN OXIDE CRYSTALS INDUCED BY CHANGES IN AMBIENT PARTIAL OXYGEN PRESSURE

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Oxide crystals are commonly used as hosts for different metal ions, for example as laser gain materials, or light absorbers. At elevated temperatures, the crystal may loose lattice oxygen when exposed to an ambient reducing atmosphere, thus creating oxide vacancies, and possibly free electrons and holes, overall maintaining an average electro-neutrality. Oxygen diffusion in oxide crystals is of interest in relation to color centers related to oxygen vacancies, as well as an agent for valence transformation of embedded metal ions (dopants).

Three types of oxygen vacancies were considered, depending on the ionization state: a neutral vacancy, and a singly or a doubly ionized one. The vacancy interaction with the metal ions always involves a donation of a single electron. A donating neutral vacancy attaches to the metal ion, creating an immobile vacancy/metal-ion complex. In the case of a singly or a doubly ionized vacancy, the electron capture by the metal ion involves interaction with the free electron-hole system. The charged vacancy remains mobile, yet with an ambipolar diffusivity dictated by the spatial electroneutrality.

Oxidation and reduction processes of the metal ions are induced by changes in the ambient partial oxygen pressure. The vacancy diffusion induced by pressure variation, hence changes in the metal ionic state, exhibit quite a complex behavior. Under some conditions, the vacancy diffusion may be described by a constant diffusivity, and is symmetric with respect to oxidation and reduction. However, under a wide range of conditions, the vacancy diffusivity is strongly concentration dependent, and the ionic state changes are highly asymmetric with respect to oxidation and reduction. For example, for a neutral vacancy, a very narrow reaction front might establish during reduction. The different metal ion populations (reduced vs. non-reduced) then exhibit a very steep change. In the inverse process (namely oxidation), on the other hand, changes in the different metal ion population are quite smooth. Differences between dynamic oxidation and reduction characteristics occur in special cases of ionized vacancies as well. An interesting example is a case where a very large ambipolar diffusivity develops in a near surface region during reduction. A virtually constant metal-ion concentration results, establishing in fact a "quenched" reaction region. However, the said region front progresses into the crystal with a characteristic diffusivity that is orders of magnitude smaller than the ambipolar diffusivity.

Such features allow for experimental assessment of different process parameters by measuring the metal ion concentrations during oxidation and reduction. This further allows the process analysis in terms of a reaction rate and a reaction zone [1– 3].

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# SELF-CONSISTENT DESCRIPTION OF ENDOHEDRAL FULLERENES' ELECTRONIC STRUCTURE WITHIN THE HARTREE-FOCK AND THE LOCAL DENSITY APPROXIMATIONS

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The results of many-body theory calculations of electronic structure and photoionization cross section of noble gas endohedral fullerene Ar@$C_{60}$ are presented. The total electronic system of the endohedral compound consists of all the electrons of the encapsulated atom and 240 valence electrons of $C_{60}$ which are distributed with the ratio of 3:1 over the $\sigma$ (none-node) and $\pi$ (one-node) orbitals correspondingly. The fullerene ionic core is described by a uniform distribution of positive charge (Z=240) over a spherical layer of finite thickness [1]. All the electrons are treated within the Hartree-Fock and the local density approximation with the field of the ionic core and the point nuclear charge of the embedded atom placed at the center of the system.

The electrons of the encaged atom and the delocalized electrons of $C_{60}$ are treated simultaneously within the unified electronic configuration which allows one to implement the Pauli exclusion principle.

Accounting for the non-local exchange interaction within the Hartree-Fock approximation leads to the significant hybridization of the 3p shell (solid black line in Fig. 1a) and the modification of the 4d shell (solid black line in Fig. 1b) of the compound. The local exchange interaction within the local density approximation doesn't reveal any significant hybridization of the shells (grey solid lines in Fig. 1) that corresponds to the LDA results reported earlier in [2].

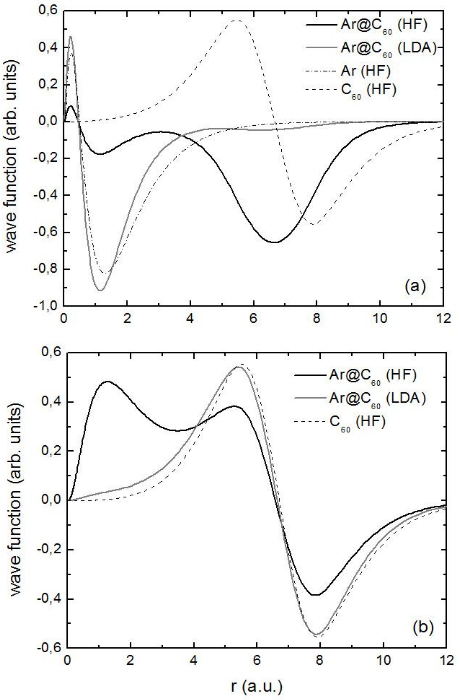

Figure 1. Top: Wave function of the *3p* shell in isolated Ar (dash-dotted), pristine $C_{60}$ (dashed) and in Ar@$C_{60}$ calculated within HF (solid black) and LDA (solid grey). Bottom: Wave function of the *4d* shell in pristine $C_{60}$ and Ar@$C_{60}$.

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# Alignment-Resolved (e,2e) Study of Deuterium Molecules

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The dependence of electron-molecule ionization cross sections on molecular alignment and orientation has been the subject of recent interest [1-3]. It provides very strict tests of our understanding of electron impact ionization of molecules. Here we present alignment-resolved experimental results for the electron-impact-induced dissociative ionization of deuterium molecules, significantly extending our earlier results for the $H_2$ molecule [4]. The measurements were performed using time-coincidence techniques enabling, for each individual ionization event, the momenta of fragment electrons and ions to be determined. The study was performed at an electron collision-energy of 176eV and scattered- and ejected-electrons of 100eV and 40eV energies respectively were measured in toroidal-sector electrostatic energy analyzers. $D^+$ ions of energies up to 12eV were collected over $4\pi$ steradians using a pulsed extraction field and their momenta determined using position- and time-sensitive detectors. By analyzing ion momenta, the orientation of the molecular axis, prior to collision, was inferred. Furthermore, by measuring the energies of electrons and ions comprising each dissociative ionization event, partial cross sections for transitions to specific dissociative states of $D_2^+$ could be resolved.

Here we present relative triple differential cross sections for transitions from the $1s\sigma_g$ ground state of the deuterium molecule to the dissociative excited-states $2p\sigma_u$ and $2s\sigma_g/2p\pi_u$ of $D_2^+$ as a function of both molecular alignment and the momentum transferred from the projectile electron to the deuterium molecule. The results show rate of dissociative ionization to be strongly dependent on *both* the symmetry of the excited state *and* on the direction of molecular alignment. For the kinematic range spanned by our measurement, the magnitude of the triple differential cross section for dissociative ionization is shown to depend strongly on the magnitude of momentum transfer, while the relative rates for dissociative ionization for different alignment directions depends weakly on this quantity.

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# DFT STUDY OF FORMING CF3CF2 FROM CF2 AND CF3 COADSORBED ON CU(111) SURFACE

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Total energy calculations based on density functional theory in connection with ultrasoft pseudopotential, generalized gradient spin-polarized approximation, and the partial structural constraint path minimization method have been used to investigate the energetically possible reaction pathways to form $CF_3CF_{2(ads)}$ from $CF_{2(ads)}$ and $CF_{3(ads)}$ coadsorbed on the Cu(111) surface. The calculated results suggest that the bridge site of $CF_{3(ads)}$ will firstly diffuse into the top site and then continue moving toward energetically favorable bridge site of $CF_{2(ads)}$ to form $CF_3CF_{2(ads)}$ through insertion process on the Cu(111) surface. In addition, the energy barrier for the formation of $CF_3CF_{2(ads)}$ is higher than $CF_2=CF_2$ coupling reaction on the Cu(111) surface. It is in reasonable agreement with the temperature programmed reaction/desorption (TPR/D) experimental observation. Furthermore, the calculated partial density of states of $CF_{2(ads)}$, $CF_{3(ads)}$ and Cu atoms on the Cu(111) surface clearly illustrate how electronic factors govern the energy barriers along the reaction pathway. Finally, simulated infrared spectrum of $CF_{2(ads)}$, $CF_{3(ads)}$, and $CF_3CF_{2(ads)}$ adsorbed on the Cu(111) surface are in good agreement with the experimental reflection-adsorption infrared spectroscopy.

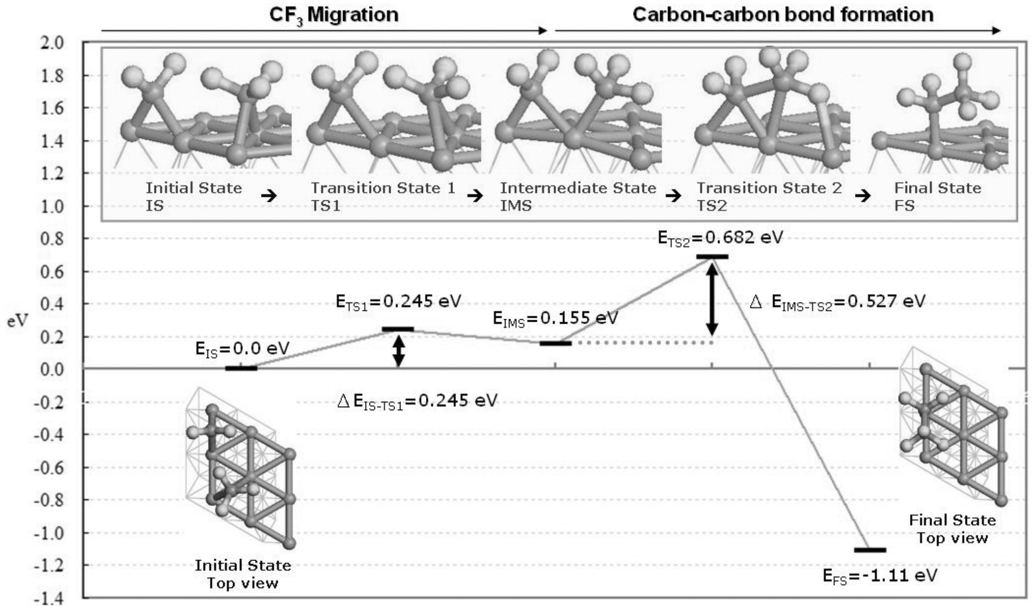

Figure 1: Energy profile and structural patterns from initial state to final state in optimized mechanism..

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# ELECTRICAL CHARGE DEPENDENCE OF GOLD NANOPARTICLE ABSORPTION AND PHOTOLUMINESCENCE

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The aim of our research is to create an electro-optical switchable device that exploits the charge state dependent optical properties of nanoparticles. Hereto we intend to incorporate size selected nanoparticles in a capacitor-like configuration allowing controlled charging of the nanoparticles and measuring their absorption or photoluminescence.

Monolayer-protected immobilized gold nanoparticles (MPN) are both relatively stable and conductive, and easy to design. When dissolved in an electrolyte solution, the metal-like core of the MPN can be electrically charged by coming into contact with an electrode/electrolyte interface acting as a dissolved capacitor. This capacitor-like structure, when electrically charged, has interesting electrical properties which are mimicked by the accompanying optical changes.

Electro-optical shifts can be achieved by changing the optical absorption of metal nanoparticles by adding or removing electrical charge. In this study absorption changes were observed for larger spherical gold nanoparticles (d = 5, 10 nm) upon electrically charging, and the influence of charging was also studied with photoluminescence for small sized gold nanoparticles (d = 2, 5 nm).

The optical absorption of 10 nm gold nanoparticles has shown plasmon peak shifts upon electrical charging, while 5 nm sized gold nanoparticles gave no significant plasmon peak shift. For the 2 nm and 5 nm sized gold nanoparticles photoluminescence was observed. The 2 nm sized gold nanoparticles exhibit a clear dependence as a function of electrical potential: reduced photoluminescence at positive and increased photoluminescence at negative potentials, which can be explained by a reduced or increased transition probability. These changes might be even more pronounced for smaller nanoparticles.

# DFT MODELLING OF THE $In_{1-x}Ga_xAs$ SEMICONDUCTOR NANOCLUSTERS

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Recent advances in nanotechnology have lead to considerable success in creating and further development of semiconductor heterojunction devices. The further technological progress requires the development of adequate methods of study of nano-dimensional structures and thorough investigation of their properties. Due to the size confinement effect, quantum dots and quantum wells of the wetting layers effectively accumulate charge. Experimental methods that study the charge accumulation and tunneling processes usually deal with the ensembles of quantum dots rather than with a single QD [1, 2]. However, information about an individual quantum dot or a quantum well is crucial not only for understanding the physics of the processes but also for practical applications [3, 4]. Therefore it is important to study the properties of the heterolayers $In_{1-x}Ga_xAs$ with changing band gaps and other important characteristics.

For semiconductor systems, the calculations of energy structure are traditionally carried out by density functional theory (DFT) methods applied to bulk solids. However, quantum dots, as being intermediate between the two extreme cases of single atoms and the bulk, display many additional properties specific only to the so-called “quantum confined” structures. The most challenging problem in the cluster calculations is correct determination of their structure because of the existence of multiple local minima in their potential energy surfaces. Therefore the electronic and structural characterization of nanoclusters is one of the most intractable problems in theoretical material physics [5].

In the present project, the cluster approach to the description of fundamental properties of semiconductor nanostructures is consistently developed. This approach implies the search of the most energetically stable isolated nanoclusters depending on their elemental composition, size, and symmetry [6]. Modeling the semiconductor nanoclusters $In_{30}As_{29}$ and $In_{18}Ga_{12}As_{29}$ within the DFT method made it possible to obtain As-dimer surface structures $In_{12}As_{13}$ typical for the InAs/GaAs quantum dot β2(2×4)-surface reconstruction (Fig.1). These relaxed nanostructures can be regarded as a part of $In_{1-x}Ga_xAs$ heterolayers, playing an important role in the charge accumulation process. At this step of investigation, the anions of relaxed nanostructures were calculated by the restricted and spin-unrestricted local LSDA and gradient-corrected correlation functional HCTH methods with LANL2DZ pseudopotential; their electron and geometric structures as well as the charge and spin distribution were studied, and their electron affinity was estimated.

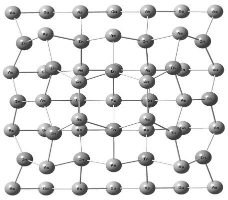

Fig.1. The geometry of the nanocluster $In_{18}Ga_{12}As_{29}$ (top view)

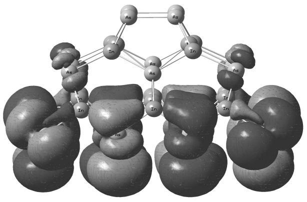

Fig.2. The spin density of the $In_{18}Ga_{12}As_{29}$ (side view)

Our calculations showed that the fully relaxed nanoclusters under study display a significant positive first and second electron affinity EA = 4.22 eV and EA = 2.73 eV, respectively, which points out their ability of negative charge accumulation. The calculations performed show that the additional electron charge is uniformly distributed over the entire volume of a nanocluster and the dipole moment decreases gradually but considerably as the charge of the anions increases. It is also found that the spin density is mostly localized on the Ga and As atoms in the bulk of the $In_{18}Ga_{12}As_{29}$ cluster. Besides, the spin density is partially localized on the periphery of the surface $In_{12}As_{13}$ structure (Fig.2).

Quantum-chemical calculations were carried out using the Gaussian 03 [7] program systems in St.Petersburg State University over a high-performance calculation Unix-cluster.

ACKNOWLEDGEMENTS
This work was supported by the Federal Agency of Science and Innovations, contract No. 02.740.11.0214 “Photonics and spintronics of low-dimensional condensed matter for Information Technologies”.

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# Electron-ion collision rates in noble gas clusters irradiated by femtosecond laser pulses

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## Abstract

Electron-ion collisions are studied for plasma conditions in atomic noble gas clusters irradiated by femtosecond laser pulses. We concentrate on the ponderomotive heating of the cluster. This heating is due to the acceleration of the electrons in the presence of multiply charged atomic ions inside the cluster. Moll et al [1] have calculated electron-ion collision frequency for xenon, krypton and argon ions in different charge states on the basis of classical momentum transport cross sections and compared their results with the corresponding collision frequency in the first Born approximation (FBA) . They have pointed out that in the wide parameter range met in typical experiments FBA is not satisfactory.

In the present investigation we have applied the eikonal approximation (EA) [2, 3] to calculate the electron-ion collision frequency using realistic model potentials. This frequency determines the absorption of laser energy in the plasma. It is worth stressing that the eikonal approximation has been found to be successful in a wide variety of collisions and has multiple scattering effects [4]. Preliminary first and second order eikonal results will be presented for xenon ions in different charge states. Comparisons will be made between the present collision frequencies and the corresponding results obtained in the FBA and the classical method. Details of the investigation will be reported at the symposium.

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# COLLISIONAL OXIDATION AND DISSOCIATION OF ISOMER-SEPARATED CARBON CLUSTER IONS

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Atomic clusters usually show structural transitions in their size growth. In the transient size range, contributions from two or more different isomers are involved in data of mass-selected experiments. In order to unveil isomer-dependent properties, we investigate dissociations and chemical reactions of each isomer ion spatially separated by ion mobility spectrometry. This spectrometry is one of the powerful techniques to obtain information on the geometric structures of gas-phase ions based on their collision cross sections in an ion-drift cell [1]. Electric field is applied in the drift cell, which is filled with a buffer gas, He. The injected ion velocity becomes constant by a balance between the collisional deceleration with He and the acceleration by the electric field. Then, ion drift time (arrival time) depends on the collision cross section with the buffer gas, and hence, isomers can be separated.

In this study, we have examined collision-induced dissociation, CID, and oxidation for carbon cluster cations, $C_n^+$, which show structural transition from linear to cyclic at $n$ = 7–10 [2]. The dissociation was induced by the collision of the ions with effused He from the drift cell after acceleration (1.3 keV). On the other hand, $C_n^+$ reacted with $O_2$ during the isomer separation in the drift cell, using a mixture gas of $O_2$ with He as a buffer gas in the cell.

From CID and oxidation, we have observed isomer-dependent reactivities. For the oxidation, intensity ratio of isomers changed after the reaction. Figure 1 shows $C_9^+$ ion intensity passed through the drift cell against the arrival time. In this figure faster and slower peaks correspond to cyclic and linear isomers, respectively. The decrease of the ratio of linear to cyclic isomers indicates that higher reactivity of linear isomers than that of cyclic ones. This result was already suggested to be ascribed to the high reactivity of lone-pair electrons in linear isomers [3].

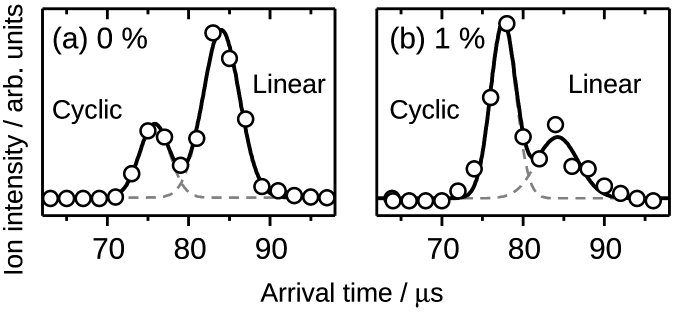

Fig. 1 Arrival time distribution of the linear and cyclic isomers of $C_9^+$
(a) before and (b) after reaction with 1 % of $O_2$ in He.

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# THE TEMPERATURE OF CLUSTERS

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Due to recent advances achieved both in the experimental precision [1] and in the analysis of supersonic beam velocity distributions [2] it is now possible to determine the aggregation state and the mean temperature of the clusters in the jet. Using accurate and comprehensive equations of state [3] this method is demonstrated for a pulsed, supersonic beam of pure $CO_2$.

Our systematic investigation of beam properties extends earlier studies [4], covering a wide parameter range, from medium to high pressures and sub- to supercritical temperatures. In general, our focus is on conditions close to the binodal and the vicinity of the critical point.

The detailed thermodynamic modeling also permits deciphering the ‘provocative’ velocity distributions of free-jet expansions of supercritical $CO_2$ reported earlier [5], confirming recent theoretical predictions of unusual properties of high density jet expansions [6].

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# MASS SPECTROMETRIC INVESTIGATION OF HELIUM DROPLETS DOPED WITH NEON AND KRYPTON

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In the present work rare gas cluster ions of neon and krypton ($Rg_N^+$) are studied. The neutral clusters are formed via pick-up in helium nanodroplets. The experimental setup consists of a helium cluster source, a pick-up chamber for the dopants and a high resolution time-of-flight mass spectrometer. The droplets are ionized with an electron ionization source. Most previous investigations of rare gases in helium focused mainly on one or few Rg dopant atoms plus attached helium atoms. In contrast the current setup has been used successfully in previous measurements to investigate Ar-clusters of various sizes [1]. The current measurements are designed to form large aggregates of neon and krypton. Cluster distributions are compared to data from conventional cluster sources where bare Rg-clusters are created. Solvation shells have been found for krypton embedded in helium [2]. Different expansion and pick-up conditions have been used to follow the evolution of cluster size distributions. In the case of neon different ionization conditions were found to have a clear impact on the cluster abundance at the second icosahedral shell closure around $N = 55$.

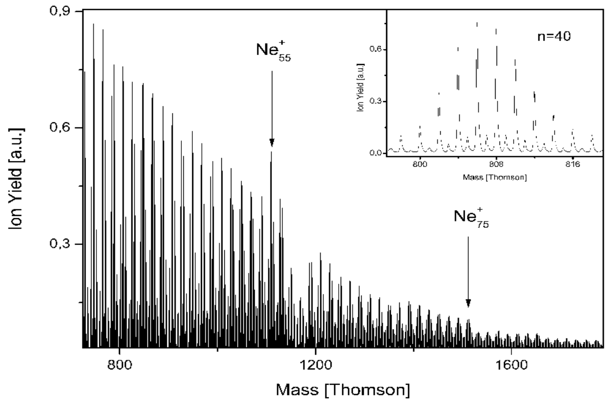

*Figure 1: NeN+ cluster size distribution; the inset shows Ne40+ isotopologues*

This work was supported in part by the FWF, Wien, Projects P19073 and L633

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# FRAGMENTATION OF TITANIUM CLUSTERS WITH COMPLEX NANOSTRUCTURE INDUCED BY INTENSE LASER FIELD

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Fragmentation of multicharged finite systems shows universal behaviour within a very broad size range, from femto-sized nuclei, through clusters, to millimetric droplets. Coulomb stability is generally well described by the liquid drop model, which predicts the fragmentation pattern on the basis of the size, the cohesive energy of the system, and the range of the interaction potential of the components [1]. The study of fragmentation processes in multicharged clusters is then identified as an effective tool for investigating their structural arrangement and phase [2]. In particular, the case of metal clusters is of great importance in the perspective of developing and optimizing functional nanostructured materials with technological relevance.

We present a momentum spectroscopy investigation of the photo-fragmentation of complex titanium clusters performed by coupling a pulsed vaporization cluster source to a femtosecond Ti:sapph laser through a momentum imaging mass spectrometer. Pulsed character of the source produces clusters with variable size distribution (avg. cluster size is 1500-2000 Ti atoms) and structural properties, according to different residence times in the source before supersonic expansion. Cluster fragmentation process has been investigated tuning the incident laser intensity over four orders of magnitude.

A competition between fission and explosion is observed in the fragmentation pattern by varying the incident photon flux, which clearly influences the cluster instability parameter. Most interestingly, the contribution from Coulomb explosion process consists of two distinct features arising from atomic fragments and from larger particles of high kinetic energy with an average size of few tens of atoms, a clear signature of the complex nanostructure of the clusters which are consisting of super-aggregates of primary particles [3]. The kinetic energy distribution of the exploding fragments is analyzed and modelled to get quantitative information on the structural arrangement at the different scales. The reported results provide a handle to a quantitative characterization of the complex nanostructure of transition metal clusters, highlighting the influence of a hierarchic structure on the relaxation processes after ionization induced by intense laser radiation.

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# TITANIUM CLUSTERS IONIZED BY INTENSE EUV RADIATION FROM A FREE ELECTRON LASER

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With the advent of short wavelength FEL sources, the issue of exploring experimentally the interaction of intense electromagnetic fields with condensed matter is experiencing a boost towards new directions and understanding [1]. Multi-coincidence techniques applied to rare gas clusters at photon fluxes in the range of $10^{13}$ W/cm$^2$ and above have shown strong potential for the investigation of physical processes in these extreme conditions [2] as well as for the understanding of spatial distribution of the elements in mixed clusters [3]; the application of these methods and physical conditions to metal clusters and clusters with higher degree of structural complexity has never been reported to date.

Here we report on the first investigation of the photoionization of complex titanium clusters by EUVFEL radiation, performed by coupling a pulsed vaporization cluster source to the SCSS FEL Test Facility at Spring-8. Pulsed character of the source produces clusters with variable size distribution (typically centred at 1500-2000 Ti atoms/cluster) and structural properties, according to different residence times in the source before supersonic expansion. Cluster ionisation process has been investigated tuning the incident FEL intensity over four orders of magnitude.

The evolution of photoionization with photon flux is markedly different from what reported from high field interaction of the same systems with IR or visible light and from the behavior of rare gas clusters under similar conditions. In particular, a frustration of cluster ionization is observed, which can not be explained by classical considerations on Coulomb interaction. An approach towards the physical interpretation of the observed phenomenology will be presented.

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# METAL CLUSTERS IN SUPERSONIC BEAMS: PROBING COMPLEX MORPHOLOGY BY ATOMIC COLLISIONS

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Clusters in the size range of few tens up to several hundreds atoms, are generally described in terms of compact spherical objects; nevertheless nanoparticles or colloids often come in the form of aggregates with fractal-like morphology and fractal description of their complex structure is often used to derive quantitatively their physical properties. This divide is to large extent of cultural origin, with limited role played by nature itself when transition metal clusters are of concern; as a matter of fact, for this class of objects sitting far away from thermodynamic equilibrium, the limiting size at which one picture should better leave the stage to the other depends significantly on the production method. Pulsed vaporization methods, as commonly applied to the production of refractory material clusters, easily lead to the production of soft aggregates from smaller primary particles yielded by the nucleation step.

The lack of experimental methods able to reveal complex morphology in the particle size range below a few nanometers is certainly a most relevant factor responsible for the general underrating of complex morphology for free metallic clusters. Atomic collisions occurring in the free jet expansion originating a seeded molecular beam can provide a powerful means to probe particle morphology with sub-nanometer length-scale. We recently proposed a method based on time of flight mass spectrometry with transverse velocity resolution, to perform a particle mobility analysis that could provide insight into cluster morphology descriptors on the time scale of particle growth [1].

Here we report on recent results obtained with this technique at the SCSS FEL test facility of SPring-8. We describe how the application of state of the art position sensitive ion detection and EUV pulsed light sources to this method can provide an accurate characterization of the sub-nanometer scale morphology of isolated nanoparticles, and discuss how this approach can open new ways in the investigation of photonic and electronic collisions with nanostructured objects with complex morphology.

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# THE NANOSTRUCTURE OF COMPLEX LEAD CLUSTERS PROBED BY X-RAY PHOTOEMISSION SPECTROSCOPY

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Understanding the role of metal clusters in complex nanophase systems is a key issue in the perspective of developing and optimizing functional nanostructured materials with technological relevance. The properties of isolated clusters are generally related to their size by scaling laws; yet, a multi-parametric approach involving, beyond the size, also morphology, composition stoichiometry, structural arrangement and spatial distribution of components is needed for a reliable description of systems grown with application-scale production technologies. XPS, due to its intrinsically local character, is a technique of choice for the investigation of electronic and geometric structure on a nanometer scale.

We present a XPS study of free lead clusters performed by coupling a pulsed vaporization cluster source to the I411 beamline at MAXLab. Pulsed character of the source produces clusters with variable size distribution and structural properties, according to different residence times in the source before supersonic expansion. The observed evolution with residence time of photoemission lines is discussed within the electrostatic shifts model for the binding energy in clusters [1]. The model is expanded relating the electrostatic radius to size distribution by means of a fractal dimension exponent parameter, so that the comparison with mass spectrometry data provides quantitative evaluation of the fractal character of the clusters.

Our results provide a generalization for a model previously provided for interpreting XPS spectra from free metal clusters [1], laying the ground for the establishment of an effective XPS-based approach to the characterization of complex nanoparticles.

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# METHANE AND DIMETHYLPROPANE CLUSTERS COMPLEXED WITH FULLERENES. A MASS SPECTROMETRIC STUDY.

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In this experiment we measured fullerenes $C_{60}$ and $C_{70}$, which are co-doped with methane / dimethylpropane. These fullerenes were picked up in helium nanodroplets, subsequently ionized by electron ionization and detected by high resolution time of flight mass spectrometry.

In the resulting mass spectra for methane distinctive intensity anomalies can be observed in the cluster distributions for $C_{60}(CH_4)_{32}^+$ and $C_{70}(CH_4)_{37}^+$ respectively. This can be explained by a face-centered solvation shell around the fullerene molecule. In addition, the isotopic correction reveals a protonated series $C_m(CH_5)(CH_4)_n^+$ and a series containing water from the background $C_m(H_2O)_k(CH_4)_n^+$ (m=60,70; k=1-3; n=0-40). The protonated series shows the same solvation shell as the unprotonated series at $C_{60}(CH_5)(CH_4)_{31}^+$ and $C_{70}(CH_5)(CH_4)_{36}^+$, with an ion yield of 15-20% respective to the unprotonated clusters. $C_2H_k$ (with k=2 to 6) molecules are formed inside the cluster complexes upon chemical reactions and replace one methane attached to the fullerene, as previously seen in pristine methane clusters [1], [2].

The multi-complex $C_{60}(H_2O)_k(CH_4)_n^+$ features solvation shells at (k,n) = (1,31); (2,31); (3,31), which suggests that the water molecules form a tight complex residing over one of the fullerene faces leaving the other 31 faces open for coverage with methane molecules.

The complexation of $C_{70}$ with dimethylpropane in helium droplets shows a different picture as far as the first solvation shell is concerned. A sudden drop in the ion yield is observed at $C_{70}(C_5H_{12})_{28}^+$ in contrast to the usual n=37 observed for $H_2$, $D_2$, He and methane complexed with $C_{70}$. We explain this with the larger dimensions of the dimethylpropane molecule. The most prominent fragmentation channel is the loss of a methyl group leading to complexes of the form $C_{70}(C_4H_9)(C_5H_{12})_n^+$.

This work was supported in part by the FWF P19073 and L633.

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# Clusters in magnetic fields: magnetic moments by XMCD

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The determination of spin and orbital magnetic moments from the free atom to the bulk phase is an intriguing challenge for nanoscience, in particular since most magnetic recording materials are based on nanostructures. We present temperature-dependent X-ray magnetic circular dichroism (XMCD) measurements of free $Co_N$-clusters ($N$=8-22) from which the *intrinsic* spin and orbital magnetic moments of small "ferromagnetic" particles have been deduced. The data provide information on the evolution of spin and orbital moment with cluster size and temperature. We experimentally verify an exceptionally strong orbital moment enhancement with respect to the bulk (4-6 times) in finite size magnetic particles not influenced by the interaction with any environment. The temperature-dependent measurements reveal that the spin orientation along the external magnetic field is nearly saturated at ~20 K and 7 T while the orbital orientation is clearly not. The comparison of the magnetic moments as deduced from XMCD and previous Stern-Gerlach measurements might help to reconcile divergent results of the total magnetic moments of small Co-clusters published earlier [1-3].

# NON-ADIABATIC DYNAMICS IN POLYATOMIC MOLECULES BY FEMTOSECOND PHOTOELECTRON IMAGGING

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Using femtosecond time-resolved mass spectrometry (fs-MS), photofragment imaging (fs-PFI), and photoelectron imaging (fs-PEI), we have studied the non-adabatic dynamics of some polyatomic molecules. Work focus on fs-PEI with the aim to track the temporal populations of relevant optically bright and dark states populated and depopulated by ultrafast non-radiative transitions via conical intersections. The followings are some examples of research works.

The laser induced predissociation dynamics of the *B* Rydberg state of $CH_3I$ following two-photon absorption of a pump pulse was studied. The predissociation lifetime was measured to be 1.55 ps induced by the crossing between the *B* state and the repulsive *A*-band. Two possible predissociation channels were observed originating from (a) direct coupling between the *B* state and the repulsive $^3Q_0$ state and (b) a second crossing between the $^3Q_0$ and $^1Q_1$ states after the coupling between the *B* and $^3Q_0$ states, respectively.

The electron dephasing mechanism of $S_1$ ($B_2$) state of *p*-bromofluorobenzene is determined to be the intersystem crossing (ISC) from the $S_1$ ($B_2$) to the $T_1$ ($B_2$) state and predissociation $S_1$ ($B_2$) *via* $T_1$ ($B_1$) state. The lifetime of $S_1$ ($B_2$) and $T_1$ ($B_2$) is determined to be 40ps and 33ps from the decay of the photoelectron signal.

The intramolecular vibrational energy redistribution (IVR) induced by a Fermi resonance in the $S_1$ low energy regime of *p*-difluorobenzene has been experimentally observed for the first time. The corresponding photoelectron angular distributions (PADs) clearly reflect each Fermi component character of the resonance $5^1 \cdots 6^2$. The oscillation period for the IVR is estimated to be less than 20 ps.

Nonadiabatic alignment of the asymmetric molecule on excited state by femtosecond laser pulse was observed on real time via time-resolved photoelectron angular distributions (TRPAD). Surprisingly, the molecular-axis alignment revival at as long as 296 ps of $S_1$ o-dichlorobenzene was observed.

# MBN EXPLORER - A FLEXIBLE PROGRAM FOR SIMULATING MOLECULAR AND NANOSTRUCTURED MATERIALS

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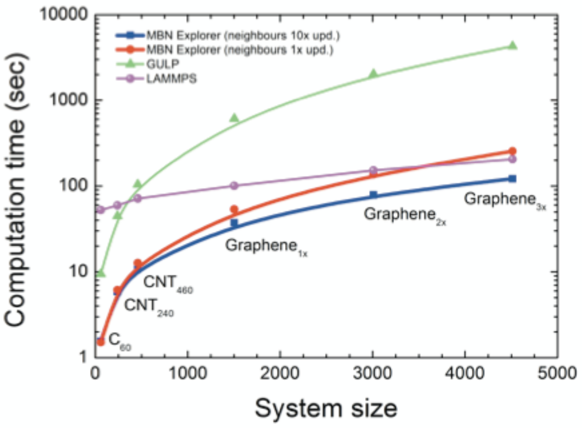
We present a multi-purpose computer code MBN Explorer. The developed package allows to model molecular systems of varied level of complexity. In particular, MBN Explorer is suited to compute the system's energy, to optimize structures, as well as to consider the molecular dynamics. MBN Explorer allows to use a broad variety of interatomic potentials, to model different molecular systems, such as atomic clusters [1], fullerenes, nanotubes [2], proteins, composite systems [3], nanofractals [4,5] etc. A distinct feature of the program, which makes it significantly different from the already existing codes, is its universality and applicability to a broad range of problems and molecular systems. Most of the existing codes are developed focusing on a particular class of molecular systems, and have severe limitations, while MBN Explorer goes beyond these drawbacks. On demand, MBN Explorer allows to group particles in the system into rigid blocks, thereby significantly reducing the number of degrees of freedom and simplifying the equations of motion. This algorithm is especially useful in studying of molecular dynamics of complex systems, consisting of large interacting building blocks, e.g. proteins or fullerene-based nanowires.



Despite the universality, the computational efficiency of MBN Explorer is comparable (and in some cases even higher) than the computational efficiency of the existing programs. The figure shows the computation time, needed to perform 1000 molecular dynamics simulation steps for a variety of carbon-based systems: $C_{60}$, carbon nanotubes (CNT) consisting of 240 and 460 atoms, graphene mono, di- and trilayers. The comparison shows that MBN Explorer is a promising alternative to the existing programs.

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# Vibrational Spectroscopy of Platinum Cluster Model Catalysts

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Isolated transition metal clusters in the gas phase and their complexes with small molecules are frequently suggested as model systems for the study of active sites of heterogeneous catalysts. In our experiments we combine resonant IR excitation with mass spectrometric detection to obtain detailed size-specific insights into the structure of the clusters and their gas-phase chemistry. The coverage of a wide frequency range from the mid-IR to below 100 cm-1 becomes possible by using the Free Electron Laser for Infrared eXperiments (FELIX) as an intense and tunable light source. Here we present vibrational spectra of small platinum clusters and their complexes with methane and hydrogen in the range from 100 to 2200 cm$^{-1}$. Comparison with spectra calculated using density functional theory allows the determination of the cluster structures and investigation of the effects of the cluster's structures on reactivity.

# LOCAL MAGNETIC AND ELECTRONIC STRUCTURE OF POST-SYNTHESIS OXIDIZED AND SURFACE-MODIFIED IRON OXIDE NANOPARTICLES FOR MAGNETIC RESONANCE IMAGING (MRI)
# (Times New Roman; bold; capital letters 14 dot)

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Iron oxide ($FeO_x$) nanoparticles are applied in medicine as contrast agents in magnetic resonance imaging (MRI) where they reduce the spin-spin relaxation time ($T_2$ time) of absorbing tissue. Hence, a control of their magnetic properties is essential for these applications. These properties strongly depend on the particle size, and shape, as well as the surface structure and the modification of the iron oxide core. Therefore, monodisperse, spherical iron oxide ($Fe_3O_4$/$Fe_2O_3$) nanoparticles were prepared by a high temperature approach in organic solvents using iron oleate as precursor. After the synthesis the particles are tempered in oxygen-free or oxygen rich environment to improve their crystalline order and to change their magnetite to maghemite ratio. NEXAFS (Near Edge X-Ray Absorption Fine Structure) and XMCD (X-Ray Magnetic Circular Dichroism) experiments are used to investigate local structural and electronic properties of the $FeO_x$ particles before and after post-synthetic oxidative and thermal treatment. The XMCD measurements show that both, the magnetization of the nanoparticles as well as their magnetite to maghemite ratio, are strongly increased after tempering in an oxidative environment which likely causes rearrangement of their crystalline order. The magnitude and the kinetics of this effect strongly depend on the particle size.

Further, we investigate if a functionalization of the nanoparticles with a polyethylene glycol bisphosphonate ligand also influences their local magnetic properties. This functionalization is relevant, as it renders the initially hydrophobic nanoparticles water dispersible which is mandatory for medical application. XMCD measurements show that the functionalization with these ligands has a similar effect as thermal oxidation, i. e. the magnetization and the maghemite content are increased. Subsequent transfer of the particles in aqueous media further increases these processes. However, after a transfer into physiological saline (0.90% w/v of NaCl) the magnetization of the $FeO_x$ nanoparticles is slightly decreased.

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| Time | Thursday, 21.07. | Friday, 22.07. | Saturday, 23.07. | Sunday, 24.07 | Monday, 25.07. |
|---|---|---|---|---|---|
| 09:15 | ***ISACC 2011 Opening***<br>Uwe Becker, Andrey Solov´yov | | | | |
| Morning session I | *Structure & Dynamics*<br>Chair: Solov´yov | *Systems of high complexity*<br>Chair: Wöste | *Clusters & biomol. in external fields*<br>Chair: Schlathölter | | *Structure & Dynamics of cl. & biom.*<br>Chair: Cederbaum |
| 09:30 | **Khanna**: at., elec. & magn. struct. of $Pd_n$ | **Brechignac**: nanoscale corrosion of $Ag_N$ | **Surdutovich**: damage in DNA | | **Cederquist**: biomole. & water attachment |
| 10:00 | **Jellinek**: DFT of Pt/Mo nanocatalysts | **Greiner**: clusters of matter & antimatter | **Yakubovich**: biom. at nanoscale stress | 10:00<br>-<br>21:00h<br>**Potsdam**<br>**castle**<br>**tour**<br>**&**<br>**lake**<br>**barbecue**<br>**nearby** | **Calvert**: fs-studies of biomolecules |
| 10:30 | **Nakajima**: self-assembled monolayers | **Siebert**: ultrafast supercontinuum spectr. | **Calvo**: modelling of cluster fragmentation | | **Wang**: shell effects of $C_{60}^+$ in He-droplets |
| 11:00 | Coffee | Coffee | Coffee | | Coffee |
| Morning session II | *Structure & Dynamics*<br>Chair: Jellinek | *Ion-cluster collisions*<br>Chair: Müller | $e^-$ & $\gamma$ *cluster collisions*<br>Chair: Ullrich | | *Collisions with clusters & biomole.*<br>Chair: Manson |
| 11:30 | **Dugourd**: ion-trap studies of $Ag_n$ & proteins | **Huber**: PAH & cluster ion interaction | **Broyer**: pump-probe on metal clusters | | **Schlathölter**: dissociation of peptides |
| 12:00 | **Suraud**: cluster + molecules in extreme light | **Korica**: plasmons in fullerenes | **Ivanov**: photoionisation by cluster anions | | **Fabrikant**: dissociative attachment |
| 12:30 | **Ferrando**: stability of AgCu nanoparticles | **Tribedi**: ionisation of fullerene & RNA | **Tiberiu**: el.-el.-coincidence methods | | **Avaldi**: (e,2e) exp. on $C_{60}$ |
| 13:00 | Lunch | 13:00 **Conference Photo**<br>13:15 Lunch | Lunch | | Lunch |
| Afternoon session I | $e^-$ & $\gamma$ *cluster collisions*<br>Chair: Becker | *Structure and dynamics on surfaces*<br>Chair: Brechignac | *Clusters & biom. studied with FEL*<br>Chair: Ueda | | *Clusters & biomol. in external fields*<br>Chair: Meiwes-Broer |
| 14:30 | **Korol**: Auger processes in endohedral atoms | **Lopez**: $Pd_N$ on graphene | **Ullrich**: FEL: fs & nm resolution | | **Ueda**: experiments at Spring-8-FEL |
| 15:00 | **Manson**: atoms confined in fullerenes | **Palma**: self-assembling & chirality | **Meiwes**: tailored strong field ionisation | | **Asmis**: IR of microhydrated conj. base ions |
| 15:30 | **Müller**: endohedral fullerenes | **Kowarik**: electron emission | **Kostyuk**: GAMMA laser: status & future | | **Fennel**: rare gas cl. in intense XUV light |
| 16:00 | Coffee | **Ismail**: theory AuPd on MgO (100) | Coffee | | **Rühl**: ultra short pulse excitation |
| Afternoon session II | $e^-$ & $\gamma$ *cluster collisions*<br>Chair: Neeb | 16:30-18:00<br>**Poster session & Coffee** | *Dynamics of clusters & biomolecul.*<br>Chair: Broyer | | *16:30-16:45 Closing remarks*<br><br>***The 5th International Symposium***<br>***“Atoms Cluster Collisions”***<br>***ISACC 2011, Berlin*** |
| 16:30 | **Reinhard**: laser excitation & elec. emission | | **Schoebel**: ions in doped He droplets | | |
| 17:00 | **Cederbaum**: interatomic Coulomb decay | | **Filsinger**: biomolecu. in liq. He-droplets | | |
| 17:30 | **Fielicke**: IR spectroscopy using FELIX | | **Ernst**: alkali atoms & molecu. in He-droplets | | |
| 18:00 | | | | | |
| 19:00 | | | 19:00-22:30h<br>**Conference banquet**<br>**@**<br>**Citadel Spandau** | | |
| 20:00 | | | | | |
| 21:00 | | | | | |
| 22.30 | | | | | |