

**ISACC 2009**

**International Symposium Atomic Cluster Collisions:  
structure and dynamics from the nuclear to the  
biological scale**

Ann Arbor, Michigan, USA, July 14 - 18, 2009

Editor: Andrey V. Solov'yov

**Abstracts**



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# Preface

**The Fourth International Symposium "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" (ISACC 2009)** will take place in July 14 – 18, 2009 in Ann Arbor, Michigan, USA. The venue of the meeting will be the hotel Four Points by Sheraton. The ISACC 2009 is organized by the Oakland University, Rochester, Michigan and the Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany.

ISACC started as an 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 fourth symposium will again be a satellite of the ICPEAC 2009, which will be held in Kalamazoo, Michigan soon after the ISACC 2009 (July 22-28).

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.

The ISACC 2009 will promote the growth and exchange of scientific information on the structure and properties of nuclear, atomic, molecular, biological and complex cluster systems studied by means of photonic, electronic, atomic and cluster collisions, high resolution mass spectroscopy, ion traps, versatile tunable lasers, new detectors and imaging techniques, NMR and atomic force spectroscopy. In the symposium, particular attention will be devoted to dynamical 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 and many more. 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 the subjects of the symposium.

## **Organizing Committee**

Andrey V. Solov'yov (Co-Chair) Frankfurt Institute for Advanced Studies  
Eugene Surdutovich (Co-Chair) Oakland University  
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# **Acknowledgements**

**The organizing committee gratefully acknowledges support by**

Frankfurt Institute for Advanced Studies (FIAS), Frankfurt am Main, Germany

Oakland University, Rochester, Michigan, USA

The European Commission within the Network of Excellence project EXCELL

We also acknowledge assistance from

Mrs. Veronika Dick, Mr. Alexander Yakubovich and Dr. Ilia Solov'yov

for their help in preparation of the book of abstracts



# Conference Program

Monday, 13 July 2009

16 <sup>00</sup> – 18 <sup>00</sup>	Participants registration
18 <sup>00</sup> – 21 <sup>00</sup>	Welcome party

Tuesday, 14 July 2009

9 <sup>20</sup> – 10 <sup>00</sup>		<b>ISACC-2009 Opening</b> Andrey V. Solov'yov - <i>Dynamics of bio-nano systems: clustering and self-organization</i>
10 <sup>00</sup> – 11 <sup>30</sup>	Tu-I	<b>Structure and properties of atomic clusters (part I) :</b> Julius Jellinek - <i>Finite systems: correlation between topographies of potential energy surfaces and structural and dynamical complexities</i> Junfeng Geng - <i>Exploring the structural complexities of metal-metalloid nanoparticles: a Ni-B case as catalyst</i> Pablo Villarreal - <i>Doped helium clusters: a quantum chemistry approach</i>
11 <sup>30</sup> – 12 <sup>00</sup>		Coffee break
12 <sup>00</sup> – 13 <sup>30</sup>	Tu-II	<b>Structure and properties of atomic clusters (part II)</b> Jean-Patrick Connerade - <i>A review of confined atoms</i> Andrey Lyalin - <i>Catalytic activity of gold clusters</i> Constantine Yannouleas - <i>Wigner molecules in semiconductor quantum dots and trapped ultracold bosonic clouds</i>
13 <sup>30</sup> – 13 <sup>40</sup>		Conference Photo
13 <sup>40</sup> – 15 <sup>00</sup>		Lunch
15 <sup>00</sup> – 16 <sup>30</sup>	Tu-III	<b>Clusters on surface (part I)</b> Nouari Kebaili – <i>Fragmentation of silver fractal islands grown from cluster deposition on graphite substrate</i> Veronika V. Dick - <i>Instability of silver fractals on graphite substrate</i> Dorin Poenaru - <i>Fission of deposited atomic clusters</i>
16 <sup>30</sup> – 17 <sup>00</sup>		Coffee break
17 <sup>00</sup> – 18 <sup>00</sup>	Tu-IV	<b>Clusters on surface (part II)</b> Richard E. Palmer - <i>Cluster deposition: from atomic structure to applications</i> Marie-Paule Delplancke-Ogletree - <i>Superlattices: preparation and characterization</i>

Wednesday, 15 July 2009

$9^{30} - 11^{00}$	We-I	<p><b><u>Clustering phenomena at subnuclear, nuclear and atomic scales</u></b></p> <p><b>Wolfgang Bauer</b> - <i>Non-equilibrium phase transition of non-trivial universality class in nuclear fragmentation</i></p> <p><b>Walter Greiner</b> - <i>Clusters in nuclear physics: superneutronic, superheavy, superstrange</i></p> <p><b>Jan-Peter Toennies</b> - <i>Microscopic superfluidity of He and para-H<sub>2</sub> clusters</i></p>
$11^{00} - 11^{30}$		Coffee break
$11^{30} - 13^{00}$	We-II	<p><b><u>Phase transitions, fusion, fission and fragmentation in finite systems (part I)</u></b></p> <p><b>A. Welford Castleman Jr.</b> - <i>Strong-field ionization and Coulomb explosion studies of small clusters</i></p> <p><b>Joshua Jortner</b> - <i>Extreme Coulomb explosion of clusters</i></p> <p><b>Adilah Hussien</b> - <i>Impurity effect on the melting of nickel clusters as seen via molecular dynamics simulations</i></p>
$13^{00} - 14^{30}$		Lunch
$14^{30} - 16^{00}$	We-III	<p><b><u>Clustering in nanosystems</u></b></p> <p><b>Shiv N. Khanna</b> - <i>Non-magnetic and magnetic superatoms and their assemblies towards novel nano-materials with precise control over properties</i></p> <p><b>Ilia A. Solov'yov</b> - <i>Towards understanding of C<sub>60</sub>-nanowire growth with anomalous anisotropy</i></p> <p><b>Octavio Roncero</b> - <i>H<sub>2</sub> reactivity on gold nano-structures: a cluster and embedding potential approach</i></p>
$16^{00} - 16^{30}$		Coffee break
$16^{30} - 18^{00}$		Poster session

Thursday, 16 July 2009

9 <sup>30</sup> – 11 <sup>00</sup>	Th-I	<b><u>Collision processes involving biomolecules</u></b> <b>Christophe Juvet</b> - <i>Photodissociation of protonated aromatic amino acid</i> <b>Paul Scheier</b> - <i>Ultracold cluster ions formed in doped helium droplets</i> <b>Ilya I. Fabrikant</b> - <i>Electron-induced bond breaking at low energies in biological molecules</i>
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Friday, 17 July 2009

$9^{00} - 10^{30}$	Fr-I	<p><b><u>Phase transitions, fusion, fission and fragmentation in finite systems (part II)</u></b></p> <p><b>Alexander V. Yakubovich</b> - <i>Statistical mechanics description of the process of polypeptide and protein folding</i></p> <p><b>Evgeniy Khain</b> - <i>Clustering instabilities in fluidized granular matter</i></p> <p><b>Eric Giglio</b> - <i>Charge instabilities of micro-droplets</i></p>
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$10^{50} - 12^{20}$	Fr-II	<p><b><u>Photon-cluster collisions and clusters in laser fields (part I)</u></b></p> <p><b>Charles K. Rhodes</b> - <i>Realization of the conceptual ideal for x-ray amplification at <math>\lambda \sim 2.9 \text{ \AA}</math> with xenon clusters</i></p> <p><b>Steven Manson</b> - <i>Theoretical studies of the ionization of endohedral atoms and fullerenes</i></p> <p><b>Alfred Müller</b> - <i>Fullerene-encapsulated atoms in the light of synchrotron radiation</i></p>
$12^{20} - 13^{40}$		Lunch
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Saturday, 18 July 2009

**Social program**

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## Tu-0

### **DYNAMICS OF BIO-NANO SYSTEMS: CLUSTERING AND SELF-ORGANIZATION**

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There are many examples of complex many-body systems of the micro- and nanometer scale size with very unique features, properties and functions. These systems can be of the very different nature and origin, e.g. atomic clusters, nanoobjects, nanostructures, mesoscopic and biomolecular systems. There is an increasing interest towards understanding of the principles of structure formation, clustering and self-organization dynamics in these Bio-Nano systems, as well as to the numerous applications of this knowledge in bio- and nanotechnology, and medicine [1]. The understanding of structure formation and dynamics of the Bio-Nano systems lies at the heart of a large variety of interdisciplinary problems at the forefront of physics, chemistry and biology, many of which will be presented at the IV<sup>th</sup> ISACC Conference. In this introductory talk I will try to overview some of the important directions in this fascinating field of research.

In this context there will be discussed self-organization processes in a number of Bio-Nano systems with the characteristic features of nanoscale phase transitions. A nanoscale phase transition is a common physical phenomenon manifesting itself in many nanoscale systems of both biological and non-biological nature, e.g. in protein folding process, or in fullerene fragmentation-reassembly dynamics.

Another important aspect of clustering and self-organization concerns the aggregation or coalescence dynamics in various complex many-body systems. Here the diffusion process of single atoms or nanoparticles plays the central role leading to the formation of various structures, like nanofractals, Bio-Nano superlattices, nanowires, nanotubes etc. This aspect of clustering and self-organization in Bio-Nano systems will be thoroughly addressed in the talk and a number of characteristic examples will be given.

Finally, the problem of monitoring, controlling and governing the Bio-Nano systems dynamics, their self-organization and growth with the use of various accessible parameters will be discussed. For these purposes atomic activators, plasmons excitations, nuclear magnetic resonance observables, quantum and geometrical shell effects, single molecule manipulations by means of atomic force field microscopy and optical tweezers, atomic confinement can be utilized.

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***Structure and  
properties of atomic  
clusters***



**FINITE SYSTEMS: CORRELATION BETWEEN TOPOGRAPHIES OF  
POTENTIAL ENERGY SURFACES AND STRUCTURAL AND  
DYNAMICAL COMPLEXITIES\***

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The quantity that underlies the specificities of structural forms and the peculiarities of dynamics of finite systems is their configurational (potential) energy. The topography of the potential energy surface is that single central element that is responsible for complexities of both the structures and the dynamics. How do we characterize the topographies of the surfaces? How do we correlate these topographies with the complexities of the structures and the dynamics? Is there a relationship between the structural and dynamical complexities? How do we probe all these?

I'll address these questions and will offer some answers. The discussion will include a way of probing the surface topography, in particular the catchment areas it is comprised of, through simulated dynamical cooling with various fixed cooling rates. A new algorithm for rapid and uniform in *temperature* cooling procedure within *constant-energy* molecular dynamics simulations will be presented. The illustrations and analyses will be given for atomic clusters of different sizes and compositions.

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\* This work was supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, U. S. Department of Energy under contract number DE-AC-02-06CH11357.

# EXPLORING THE STRUCTURAL COMPLEXITIES OF METAL-METALLOID NANOPARTICLES: A Ni·B CASE AS CATALYST

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The current development in catalysis by nanoparticles has stimulated a renewed interest in catalysts that display high catalytic activity and selectivity for hydrogenation or dehydrogenation reactions. Previously, the nickel boron nanomaterial (denoted as Ni·B catalyst), which was initially produced in the 1950s by chemical reduction of an appropriate nickel salt by alkali metal borohydrides, has been shown to have an exceedingly high catalytic activity for a wide range of hydrogenations and dehydrogenations. The catalyst has been demonstrated to be at least as active as standard Raney nickel but produces less double-bond migration than the latter in hydrogenations. Similar catalysts produced from alternative reduction media have been shown to be highly selective for certain hydrogenations of one double-bond in the presence of another. Importantly, these catalysts are known to be more easily prepared than Raney nickel, with a high degree of reproducibility and reliability.

The remarkable catalytic properties of the material have given rise to extensive studies that so far include the reaction kinetics, stoichiometric chemistry, chemical state of the surface and catalytic applications. In addition, studies on the Ni·B system have been widely extended to other similar metal-metalloid materials, involving transition metals and the elements of B and P to form Fe·B, Co·B, Pd·B, Ni·P, Fe·P, Fe·Ni·B, Ni·Fe·P, Fe·P·B, Ni·W·P, Pt·B, Ni·P·B, or Ni·Co·B. These studies have led to important applications not only in catalysis but also in other fields such as in deuterium exchange, selective desulfurizations, and for the preparation of magnetic recording materials, ferrofluids, and chemical composites.

Despite the important properties and applications, however, the precise nature of the nickel boron material itself has always remained unclear. It was originally thought that this material was a simple stoichiometric nickel boride compound, with a formula of Ni<sub>2</sub>B or Ni<sub>3</sub>B, but the boron content was later found to vary with the ratio of the reactants used in preparation. Studies on the structure using powder x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM), led to a view that the material is amorphous, and as a consequence, it is frequently referred as an “amorphous nickel boron alloy”.

Here we show our systematic investigations of the Ni·B catalyst prepared by the chemical reduction method. We are able to show that the material is not a simple nickel boride compound but a mixture of metallic nickel and a boron-containing substance. More importantly, we have found that rather than being amorphous, the material possesses a highly unusual nanostructure in which very small Ni nanoparticles (1-3 nm) form a cluster arrangement which serves as a host to guest B-containing species accommodated within their interstitial sites. In addition, we also show the formation of alternative Ni·B structures prepared under different conditions, and offer an explanation of their varying catalytic activity on the basis of their structural characteristics. The work has been further extended to the preparation and examination of colloidal Ni·B nanoparticles, which are substantially different from the original material. The results presented in this work are



## Tu-I-2

considered to represent a substantial progress toward a full understanding of the complexity of the nanoparticle structures for nickel boron chemistry.

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## DOPED HELIUM CLUSTERS: A QUANTUM CHEMISTRY APPROACH

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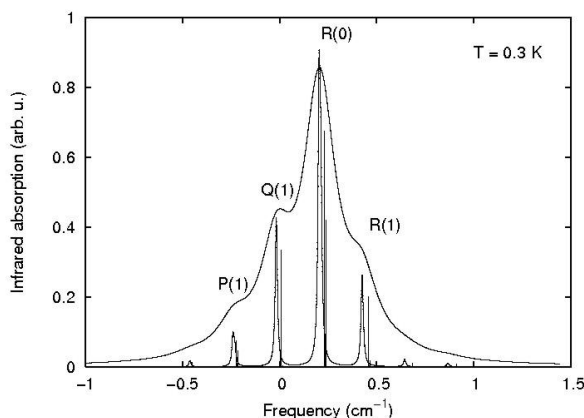
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Helium nanodroplets have proven to be a unique matrix in which to conduct high-resolution molecular spectroscopy. In particular, infrared (IR) spectra of OCS embedded in He droplets have provided direct evidence of microscopic superfluidity of boson <sup>4</sup>He environments [1]. Structures and binding energies of He clusters doped with different species are currently (and successfully) described by means of diffusion and path-integral Monte Carlo methods [2]. We outline here a different quantum chemistry (QC) approach [3] in which the He atoms are considered as “electrons” while the dopant plays the role of “nuclei” [4]. In addition to the above mentioned properties, the model furnishes wave functions thus enabling to perform spectral simulations which can be compared with the experiment. For instance, the figure depicts the simulated IR absorption profile of ICl(X) in <sup>3</sup>He: it bears a strong resemblance to the spectrum of the quasi-linear OCS molecule in such an environment [1].



Up to now, Hartree/Hartree-Fock approaches involving their own limitations have been used. It would be therefore desirable to implement more accurate *ab initio* methodologies. Encouraging “full interaction configuration” results, based on a Jacobi-Davidson diagonalization procedure, have been already obtained for small doped fermion clusters [5]. Extension to larger clusters also involving a boson solvent (or a boson/fermion mixture) is envisaged in the near future.

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## Tu-II-1

### A REVIEW OF CONFINED ATOMS

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A brief history of the Confined Atom problem will be presented. The hydrogen atom confined to the centre of an impenetrable sphere counts amongst the exactly soluble problems of physics, alongside much more noted exact solutions such as Black Body Radiation and the free Hydrogen atom in absence of any radiation field. It shares with them the disadvantage of being an idealisation, while at the same time encapsulating in a simple way particular aspects of physical reality. The problem was first formulated by Sommerfeld and Welker in connection with the behaviour of atoms at very high pressures, and the solution was published on the occasion of Pauli's 60<sup>th</sup> birthday celebration. At the time, it seemed that there was not much other connection with physical reality beyond a few simple aspects connected to the properties of atoms in solids, for which more appropriate models were soon developed. Thus, confined atoms attracted little attention until the advent of the metallofullerene, which provided the first example of a confined atom with properties quite closely related to those initially considered by Sommerfeld and Welker. Since then, the problem has received much more attention, and many more new features of quantum confinement, quantum compression, the quantum Faraday cage, electronic reorganisation, cavity resonances, etc have been described, which are relevant to real systems. Also, a number of other situations have been uncovered experimentally to which the problem is relevant. Thus, studies of the confined atom are now more numerous, and have been extended both in terms of the models used and the systems to which they can be applied.

## CATALYTIC ACTIVITY OF GOLD CLUSTERS

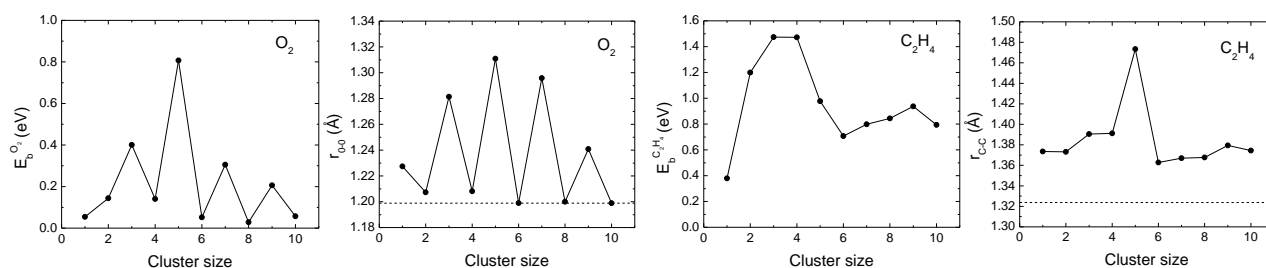
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The specific role played by small gold clusters in the process of catalytic oxidation of alkenes by dioxygen will be discussed in this talk. The emphasis is made on the catalytic oxidation of ethylene molecule,  $C_2H_4$ , which is the simplest alkene containing an isolated carbon-carbon double bond.

The unique catalytic activity of gold nanoparticles supported on transition-metal oxides had been discovered experimentally more than 20 years ago [1]. It was found that extraordinary catalytic properties of gold can be achieved by decreasing the size of the gold particles [2-4], in spite of the fact that the bulk gold does not possess any catalytic properties. The origin of this size-dependent catalytic activity remains poorly understood, see, e.g., [5] and references therein. It was believed that remarkable catalytic behavior of small gold clusters might arise from strong electronic interaction between gold nanoparticle and support material or special additives. However, recent experiments indicate that small gold clusters supported on inert materials are efficient catalyst for oxidation of alkenes by dioxygen [4]. Hence, even free gold clusters can be effective at catalysing the oxidation of hydrocarbons.

In the present work we report results of the theoretical investigation of the catalytic activity of small gold clusters consisting of up to 10 atoms in the process of oxidation of ethylene molecule by dioxygen. It is shown that adsorption of the  $O_2$  molecule on the gold clusters with odd number of atoms leads to a considerable weakening of the  $O=O$  bond. It is demonstrated that the odd-even oscillations in adsorption energy of  $O_2$  are governed by the electronic shell effects in the gold clusters. In addition, interaction of the ethylene molecule with the small gold clusters results in a weakening of the carbon-carbon double bond. Hence, activated dioxygen readily attacks loosened double bond in  $C_2H_4$ , oxidising ethylene molecule. It is demonstrated that simultaneous adsorption of  $O_2$  and  $C_2H_4$  molecules on free gold clusters considerably promotes the oxidation process. We suppose that similar scenarios can occur in the process of catalytic oxidation of various alkenes.



**Figure 1:** Adsorption energy and bond distance calculated for adsorbed  $O_2$  (left) and  $C_2H_4$  (right) molecules on free  $Au_n$  clusters with number of atoms  $n$  up to 10. Horizontal dashed lines indicate the equilibrium  $O=O$  and  $C=C$  bond distances in the free  $O_2$  and  $C_2H_4$  molecules, respectively.

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## Tu-II-3

### WIGNER MOLECULES IN SEMICONDUCTOR QUANTUM DOTS AND TRAPPED ULTRACOLD BOSONIC CLOUDS

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Strongly correlated phenomena associated with symmetry breaking in small finite-size systems will be reviewed [1], with a focus on the strongly correlated regime of electrons in two-dimensional semiconductor quantum dots (QDs; often referred to as artificial atoms and molecules) and trapped ultracold bosonic atoms in harmonic traps. The talk will emphasize universal aspects and similarities of symmetry breaking found in these systems, as well as in more traditional fields like nuclear physics and quantum chemistry.

A complete description of the strongly correlated regime requires approximations beyond the mean-field level. A unified description of strongly correlated phenomena infinite systems of repelling particles (whether fermions or bosons) has been achieved through a two-step method of symmetry breaking at the unrestricted Hartree-Fock (UHF) level and of subsequent symmetry restoration via post Hartree-Fock projection techniques [1]. The general principles of the two-step method can be traced to nuclear theory (Peierls and Yoccoz) and quantum chemistry (Löwdin). Quantitative and qualitative aspects of the two-step method are tested and validated by large-scale exact diagonalization calculations.

I will discuss how this method can describe a wide variety of novel strongly correlated phenomena. These include:

(I) Chemical bonding, dissociation, and entanglement in quantum dot molecules and in electron molecular dimers and trimers formed within a single elliptic QD, with potential technological applications to solid-state quantum computing.

(II) Electron crystallization along the vertices of concentric polygonal rings and formation of rotating Wigner molecules (RWMs) in circular QDs. At zero magnetic field ( $B$ ), the RWMs rotate rigidly; at high  $B$ , the RWMs exhibit a non-rigid rotational inertia, with the rings rotating independently of each other.

(III) At high  $B$ , the two-step method yields analytic many-body wave functions, which are an alternative to the composite-fermion and Jastrow-Laughlin approaches, offering a new point of view of the fractional quantum Hall regime in QDs.

(IV) Description of crystalline phases of strongly repelling ultracold bosons (impenetrable bosons/ Tonks-Girardeau regime) in 2D rotating harmonic and toroidal traps.

Recent applications concern: (1) symmetry-conserving rotating vortex clusters that incorporate quantum fluctuations beyond the broken-symmetry Gross-Pitaevskii vortex solutions [2]; (2) interpretation of non-universal phase lapses in electron transmission through a quantum dot [3]; (3) fractional-quantum-Hall-effect analogies and differences in graphene quantum dots at zero magnetic field [4].

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***Clusters on surface***





### FRAGMENTATION OF SILVER FRACTAL ISLANDS GROWN FROM CLUSTER DEPOSITION ON GRAPHITE SUBSTRATE

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Among recent progresses in the building of new architectures at the nanoscale, the use of preformed clusters, has demonstrated that their self assembly on a substrate, allows the control of the morphology of the obtained nanostructures.

One of the critical parameters driving the final morphologies is the size of the clusters. Small size clusters promotes compact shapes whereas large sizes are in favour of dendritic shapes, eventually fractal ones. This is an advantage in the use of clusters instead of atoms for the synthesis of nanostructures. Another major advantage lies in the possibility to include a small amount of impurities into the clusters.

The aim of this paper is to show how the deposition of clusters carrying impurities leads to completely new classes of morphologies. This study has been performed with silver clusters containing either oxygen or a mixture of oxygen and molybdenum oxide as a surfactant.

In our experiment heterogeneous clusters are produced by reactive nucleation process in a gas aggregation source. Their mean size and their stoichiometry are controlled by time of flight mass spectrometry. They are deposited at thermal energy on a HOPG surface. The samples are imaged with a scanning transmission electron microscope (STEM). A local probe of the chemical properties is done by electron energy loss spectroscopy (EELS). The main result is the drastic stoichiometry dependence of the final morphology: from fragmented islands with marked reminiscence of fractal structures to anisotropic growth promoting the building of quasi linear or folded chain-like islands, exhibiting pearled structure.

A 3D morphological phase diagram connecting the various characteristics of the nanostructured films to the stoichiometry of the clusters has been elaborated. It emphasizes the role played by the impurities not only on the final morphologies, but also on the cluster diffusion on the substrate. Comparison with thermal stability and perspectives on aging process are also discussed.

INSTABILITY OF SILVER FRACTALS ON GRAPHITE SUBSTRATE

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During the last years the formation of silver fractals on graphite substrate was extensively studied experimentally and theoretically [1- 3], but many important questions still remain open. For example, the influence of impurities and substrate roughness on stability of the fractal structure is not well understood.

Here we study the process of silver fractal formation on graphite substrate and its post growth relaxation by using the diffusion-limited aggregation (DLA) model [4]. For the study of the post growth relaxation process we developed a modified DLA model which accounts for the internal dynamics of the particles in the fractal and allows for their diffusion and detachment [6]. We consider different scenarios of the fractal relaxation and analyze the time evolution of the islands morphology. In Fig. 1 we illustrate several scenarios of fractal fragmentation.

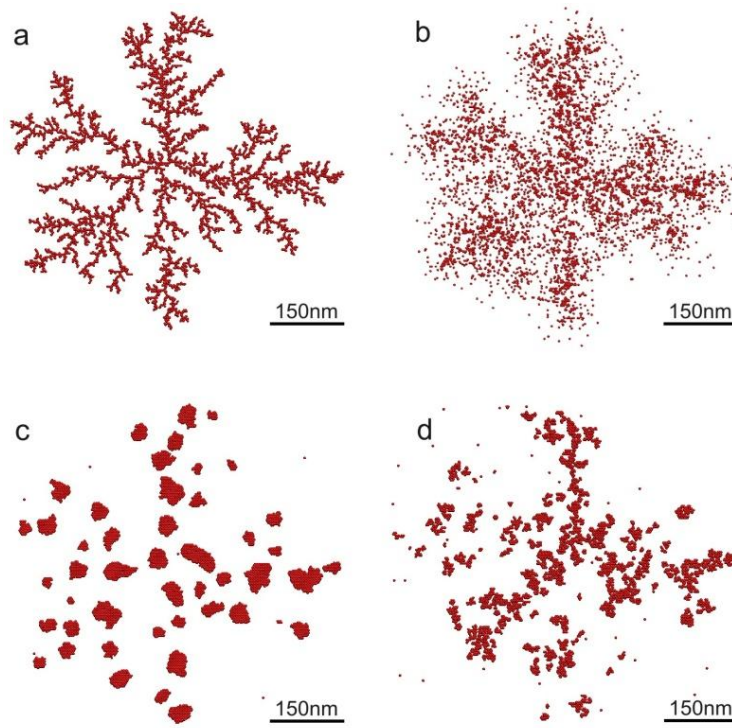


Figure 1: Evolution of the silver cluster fractal structure, calculated with the DLA model with accounting for the internal dynamics of the particles in the fractal. (a) Initial structure of the fractal; Plots (b) – (d) show snapshots of the fractal structure after different time periods: (b)  $t = 3s$ , the bonding energy between two silver clusters is weak ( $1 kT$ ), resulting in a rapid fragmentation of the a fractal; (c)  $t = 20s$ , the diffusion of a clusters along the fractal branch is a more preferable process, fractal fragments on group of compact droplets; (d)  $t = 20s$  slow diffusion of clusters along the branch, the fractal fragments into a group of non-compact islands;

## Tu-III-2

We demonstrate that stability of the fractal structure depends strongly on several factors, such as the concentration of impurities and temperature. Using the developed model we study various scenarios of the fractal defragmentation and compare them with those reported in experiment [1-3].

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### FISSION OF DEPOSITED ATOMIC CLUSTERS

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The similarity between atomic nuclei and metallic atomic clusters is based on the fact that both systems consists of fermions moving freely in a confined space. The idea was exploited by adapting the nuclear liquid drop model (LDM) and the the shell correction method, for neutral atomic clusters as well as charged ones. A rich variety of experimental and theoretical work is available (see e.g. [1-3] and the references therein).

We used the macroscopic{microscopic method to investigate neutral hemispheroidal atomic clusters deposited on a surface. Such shapes were observed in experiments using atomic force microscope [4]. Analytical relationships for the deformation-dependent LDM energies of oblate and prolate hemispheroidal atomic clusters have been obtained. A superdeformed prolate hemispheroid was found to be the most stable shape within LDM. It is also the shape with maximum degeneracy of quantum states of the hemispheroidal harmonic oscillator used to compute the shell and pairing corrections [5].

It is interesting to investigate the stable deformations as well as the fission process of charged metallic hemispheroidal drops and of other shapes under the influence of Coulomb energy. Compared to nuclei, in which the electric charge of protons is assumed to be homogeneously distributed in the volume, in metallic atomic clusters the excess charge of electrons produced by ionization is concentrated on the (equipotential) surface. The self Coulomb energy of a nuclear spherical drop,  $E_C^0 = 0.6Z^2e^2/R_0$ , became  $E_C^0 = 0.5Z^2e^2/R_0$  for a spherical metallic cluster. As a consequence, the calculations performed for nuclei should be tested before they are applied to clusters. Fortunately, at least for some particular shapes (e.g. spheroids), apart for this factor independent of deformation, one has the same deformation dependence in the two cases. The stability against fission of deposited charged clusters increases due to the decrease of Coulomb energy and the increase of the surface one.

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# CLUSTER DEPOSITION: FROM ATOMIC STRUCTURE TO APPLICATIONS

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The controlled deposition of size-selected clusters creates new possibilities for the fabrication of both biochips and model catalysts [1]. Knowledge and control of the 3D atomic structure of the cluster is relevant to these applications, and also to the fundamental physics and chemistry of the clusters. Direct structural measurements of clusters in the gas phase are very challenging, so surface measurements after (gentle) deposition may also shed new and valuable light on the intrinsic cluster structure. Here we demonstrate that measurement of the incoherently scattered electron intensity - the high angle annular dark field (HAADF) signal - in the scanning transmission electron microscope (STEM) allows us (a) to count the number of atoms in a cluster on the surface and (b) to determine a 3D atom-density map of the cluster when an aberration-corrected STEM is used [2]. Moreover, size-selected clusters can also be used as a mass standard to "weigh", for example, metal nanoparticles produced by other less precise (but sometimes more practical) methods as well as non-spherical, mass-selected clusters: this is mass spectrometry on the surface [3].

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## Tu-IV-2

### SUPERLATTICES: PREPARATION AND CHARACTERIZATION

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Nanoparticles superlattices can be prepared by self assembly, under strict synthetic control, of hybrid nanoparticles composed of a metallic bulk (from a few to hundreds of nanometers in diameter) surrounded by an organic passivating layer. The nanoparticles are arranged with long-range crystalline order.

These superlattices are promising materials for applications in various fields such as recording media, light-emitting devices, biological tags, catalysts, solar cells, and sensors. The characterization and elucidation of the size-evolutionary patterns of the properties of these finite size assemblies are among the major challenges in modern materials science.

The different methods available for preparing nanoparticles superlattices will be summarized in this talk. Emphasis will be put on the role of ligands in the control of the particle size and in the formation of the lattices. We wish, in particular, to investigate the influence of non-covalent interactions between ligands on the mechanical properties of the superlattices. The structural, electronic, magnetic, optical, spectroscopic and chemical properties of isolated nanoparticles and their assemblies are intensively investigated but relatively few studies have been devoted to their mechanical properties.

As single-crystal nanoparticle superlattices can be prepared with lateral dimensions of ten or more microns and thicknesses of at least several hundred nanometers, nanoindentation can be used to characterize these systems. The observation by atomic force and scanning electron microscopies of the superlattices before and after indentation provides quantitative data on the elastic modulus, plastic deformation (hardness) and fracture properties of the material. Proof-of-principle experiments indenting on superlattices have recently been carried out. We hope, by systematically varying the nature of the nanoparticle ligands, the conditions under which the nanoparticles are assembled (pH, solvent, etc), and the indentation environment (temperature, humidity) to be able to rationalise the effect of the ligand-ligand interactions on the mechanical properties of the superlattices.

***Clustering  
phenomena at  
subnuclear, nuclear  
and atomic scales***





**NON-EQUILIBRIUM PHASE TRANSITION OF NON-TRIVIAL  
UNIVERSALITY CLASS IN NUCLEAR FRAGMENTATION**

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The conventional picture of atomic and sub-atomic multifragmentation reactions is that of a thermodynamic equilibrium phase transition or first order, terminating at a critical point. However, I will argue that nuclear and molecular fragmentation reactions do not allow enough time for this picture to be valid in the traditional sense, and that these systems undergo non-equilibrium phase transitions. Non-equilibrium phase transitions in condensed matter and atomic physics have exhibited critical exponents in the mean field universality class. In nuclear and molecular fragmentation, however, evidence based on models and experimental data suggests that this non-equilibrium transition falls into the percolation universality class.

## We-I-2

### CLUSTERS IN NUCLEAR PHYSICS: SUPERNEUTRONIC, SUPERHEAVY, SUPERSTRANGE

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The extension of the Periodic System into various areas will be discussed:

- a) Nuclei with extraordinary number of neutrons - outside the neutron dripline; for example  $^{42}\text{O}$ ,  $^{120}\text{Zr}$ ,  $^{260}\text{Pb}$ .
- b) Superheavy nuclei around proton numbers  $Z=114$  and  $Z=120$ . Possible reaction mechanisms for introducing more neutrons.
- c) Nuclei with strangeness: Many hyperons like  $\Lambda$ ,  $\Xi$ , etc. and the generalisation of the Bethe-Weizsäcker mass formula are theoretically possible.
- d) Antinuclei

For all these possibilities possible ways for their creation will be indicated. Also the possibilities of the creation of such exotic nuclei in supernova-explosions and on the surface of neutron stars will be discussed, if time permits.

# MICROSCOPIC SUPERFLUIDITY OF He AND PARA-H<sub>2</sub> CLUSTERS

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Even now the statement “the explicit connection between superfluidity and BEC is not trivial...” still hold 70 years after the discovery of superfluidity in <sup>4</sup>He<sup>1</sup>. Today insight into new unexpected microscopic manifestations of superfluidity in finite sized systems comes from high resolution spectra of single molecules embedded in the interior of <sup>4</sup>He and <sup>3</sup>He liquid droplets<sup>2</sup> with more than 10<sup>3</sup> atoms as well as from sophisticated scattering experiments. From chromophore spectroscopy it is now established that the <sup>4</sup>He droplets are superfluid<sup>3, 4</sup> and therefore the unexpected sharp infrared features which indicate that the chromophore molecules rotate freely is now recognized as an indication for superfluidity. The phenomenon of free rotations has since been used to establish that about 6 - 8 <sup>4</sup>He atoms attached to a chromophore suffice for microscopic superfluidity<sup>5</sup>. Scattering experiments from and within <sup>4</sup>He droplets using either <sup>3</sup>He atoms<sup>6</sup>, photodissociated Ag atoms<sup>7</sup>, or electrons<sup>8</sup> also confirm their superfluidity.

These extensive spectroscopic experiments have established an He droplet as the most gentle and coldest (0.38 K (<sup>4</sup>He), 0.15 K (<sup>3</sup>He)) matrix, making it ideal for dynamical and structural studies of even large biomolecules<sup>2</sup>. Presently, for example, several groups are preparing to use droplets as nanocryostats to cool and laser orient *single* bio-molecules in preparation for X-ray or electron diffraction structural investigations<sup>9</sup>.

The inherent complexity of chromophore containing large droplets makes the theoretical interpretation difficult. For this reason recent experiments are directed at understanding the *pure* small He clusters ( $N \leq 10^2$ ). Nondestructive matter wave diffraction experiments, which are ideally suited for such fragile species, have exposed unexpected magic numbers in jet expanded small <sup>4</sup>He clusters. Since magic stabilities are ruled out by numerous theoretical studies the magic sizes are now thought to be related to the quantized elementary excitation levels<sup>10</sup>. Each time a specific sized cluster acquires an additional level either the growth (in one theory<sup>10</sup>) or the destruction (in another theory<sup>11</sup>) is enhanced. In either case the experiments confirm the calculated excitation energies and

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## We-I-3

provide deep insight into the internal dynamics and superfluid fractions of the small pure  $^4\text{He}$  clusters.

Small clusters of pure bosonic para- $\text{H}_2(j=0)$  provide even greater challenges to theory and experiment. Theory predicts that small clusters ( $N \leq 26$ ) are superfluid in apparent contradiction to the predicted magic number *stabilities* and structured radial density distributions, both of which are properties of solid clusters<sup>12</sup>. Of the very few experiments two confirm the existence of at least one magic number but an experimental test of their superfluidity has so far not been possible<sup>13 14</sup>. Today the only evidence comes from the spectroscopy of a chromophore molecule with  $N \geq 11 - 16$  para- $\text{H}_2$  molecules inside  $^4\text{He}$  droplets<sup>15</sup>. Presently efforts are directed at understanding what properties of  $\text{H}_2$  govern its unusual behaviour<sup>16</sup> and to devise experiments to detect superfluidity in the bulk<sup>17</sup>.

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***Phase transitions,  
fusion, fission and  
fragmentation in  
finite systems  
(part I)***



## We-II-1

### STRONG-FIELD IONIZATION AND COULOMB EXPLOSION STUDIES OF SMALL CLUSTERS

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With the advent of the ultrashort laser pulse, scientists gained an incredible tool for use in their investigations of light-matter interactions. Nearly 15 years ago [1,2], research began in earnest on the studies of strong-field interactions with clusters and the field has rapidly gained momentum ever since. Here, we present experiments investigating the strong-field ionization behavior of small homo- and hetero-nuclear clusters. Specifically, neutral clusters typically containing fewer than 40 atoms which are composed of Group Vb transition metals (V, Nb, Ta), either pure or clustered with oxygen or carbon, were irradiated with 100-350fs pulses of focused 624nm light resulting in intensities between  $10^{14}$  and  $10^{15}$  W/cm<sup>2</sup>. The highly charged cations resulting from the strong-field ionization are investigated for a variety of experimental conditions and target species. Ion detection was performed using a home-built dual-stage Wiley-McLaren time-of-flight mass spectrometer. A laser vaporization source was used for the production of our neutral cluster distributions and a colliding-pulse, mode-locked dye laser provided our ultrashort pulses.

It has been shown previously that the ionization ignition mechanism (IIM) and the charge-resonance enhanced ionization (CREI), or enhanced ionization (ENIO), mechanism play key roles in the strong-field ionization of dimers, molecules, and small clusters (<30 atoms) and result in ionic states beyond those which are attainable via field ionization alone [3]. Further, collective electron effects leading to enhanced ionization in small (~22 atoms) metal clusters have also been reported [4] which are attributed to cluster plasmon enhanced ionization (sometimes referred to as the coherent electron motion mechanism); a similar phenomenon to the nanoplasma model applied to larger cluster systems. We have conducted the present series of experiments with the intention of contributing to the relatively limited collection of physical data in which small clusters are ionized via strong-field radiation and we present observations regarding maximum observable charge states in relation to cluster composition as well as the influence of incident laser pulse width. This size regime may represent the range in which the transition from one ionization enhancement mechanism to another begins to occur, and thus it is of significant interest in the field.

Interestingly, we observe no pulse width dependence (100fs vs 350fs) on the ionization behavior of any of our target clusters. Since cluster expansion in longer pulse widths leads to the manifestation of coherent electron motion, we verify that our clusters are expanding to a greater extent in our long pulse experiments by measuring the relative kinetic energy release (KER) observed following Coulomb explosion. This lack of further ionization enhancement can be attributed to the fact that collective effects are relatively unlikely in clusters of this size, or possibly due to the expected inhomogeneity of the electric field created within the cluster during ionization. Further, based on previously reported experiments [see ref. 5 for a recent review], the CREI mechanism is expected to dominate the ionization enhancement process in systems of this size. These findings may be especially significant for the pure niobium and tantalum cluster ionization experiments, as they appear to undergo CREI ionization but are too small to exhibit collective electron effects, contrary to the behavior reported from slightly larger pure metal clusters [4].

## We-II-1

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## We-II-2

### EXTREME COULOMB EXPLOSION OF CLUSTERS

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The exploration of photoinduced ultrafast response, dynamics, reactivity and function in ubiquitous molecular, nanoscale macroscopic and biological systems pertains to the interrogation and control of the phenomena of energy acquisition, storage and disposal, as explored from the microscopic point of view. We shall focus on recent theoretical, computational and experimental studies of finite systems dynamics under extreme energetic and temporal conditions. Ultrafast and ultrahigh phenomena pertain to extreme cluster ionization in ultraintense laser fields (peak intensities  $I_M = 10^{15} - 10^{21} \text{ Wcm}^{-2}$ , with  $I_M = 10^{21} \text{ Wcm}^{-2}$  constituting the highest light intensity on earth), ultrafast femtosecond dynamics on the time scale of nuclear motion, attosecond–femtosecond electron dynamics, the production of ultrahigh charges in completely ionized molecular or elemental clusters, and the attainment of ultrahigh energies (keV–MeV) in Coulomb explosion of multicharged clusters and nanostructures. Coulomb explosion of clusters and nanostructures transcends chemical–physical dynamics towards the driving of nuclear reactions involving table-top nuclear fusion and nucleosynthesis of astrophysical interest.

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## We-II-3

### IMPURITY EFFECT ON THE MELTING OF NICKEL CLUSTERS AS SEEN VIA MOLECULAR DYNAMICS SIMULATIONS

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We demonstrate [1] that the addition of a carbon impurity leads to significant changes in the thermodynamic properties of a Ni<sub>147</sub> cluster. The magnitude of the change induced is dependent on the parameters of the Ni-C interaction. Hence, thermodynamic properties of Ni clusters can be effectively tuned by the addition of a particular type of impurity. We also show that the presence of a carbon impurity considerably changes the mobility and diffusion of atoms in the Ni cluster at temperatures close to its melting point. The calculated diffusion coefficients of the carbon impurity in the Ni cluster can be used as a reliable estimate of the growth rate of carbon nanotubes.

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# ***Clustering in nanosystems***



## We-III-1

# NON-MAGNETIC AND MAGNETIC SUPERATOMS AND THEIR ASSEMBLIES TOWARDS NOVEL NANO-MATERIALS WITH PRECISE CONTROL OVER PROPERTIES

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The quantum states in metal clusters are grouped into bunches of close lying eigenvalues, termed electronic shells, similar to atoms. Filling of the electronic shells with paired electrons results in local minima in energy; leading to stable species called magic clusters. This led to the realization that selected clusters can mimic chemical properties of elemental atoms on the periodic table and can be classified as superatoms. So far, the work on superatoms has focused on non-magnetic species. We have recently propose a framework for magnetic superatoms by invoking systems having both localized and delocalized electron states, where localized electrons stabilize magnetic moments while filled nearly free electron shells lead to stable species. I will outline these developments and show that an isolated  $\text{VCs}_8$  and a ligated  $\text{MnAu}_{24}(\text{SH})_{18}$  are such magnetic superatoms. The magnetic superatoms assemblies could be ideal for molecular electronic devices, as the coupling could be altered by charging or weak fields. I will discuss our recent findings that show that the magnetic superatom assemblies offer the prospect of spin polarized currents as well as high magneto resistance.

I will also briefly outline our efforts in developing cluster assembled materials. In particular, we have established selected arsenic-alkali cluster as a potential building block via gas phase molecular beam experiments. Employing the idea that the particular species identified in the gas phase is a uniquely stable Zintl entity that could effect self-assembly, we report success in synthesizing several assemblies of  $\text{As}_7^{3-}$  clusters with alkali metal counter-cations and those linked with covalent linkers. I will present our recent striking finding combining optical measurements and first principles theory that indicate that the band gaps in assemblies based on the same polyvalent anion can vary over a wide range. Theoretical studies reveal that the variations in the band gap are linked to the energy levels of the counter-cation, the degree of charge transfer, with additional tuning through covalent linkers. The findings offer a novel protocol for synthesis of nanoassemblies with tunable electronics.

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## TOWARDS UNDERSTANDING OF C<sub>60</sub>-BASED NANOWIRE GROWTH WITH ANOMALOUS ANISOTROPY

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The growth of one-dimensional (1D) nanocrystals is an important research topic in crystal engineering for nanotechnology because of the properties associated with the low-dimensionality, quantum confinement effect, and potential magnetic and photonic applications.

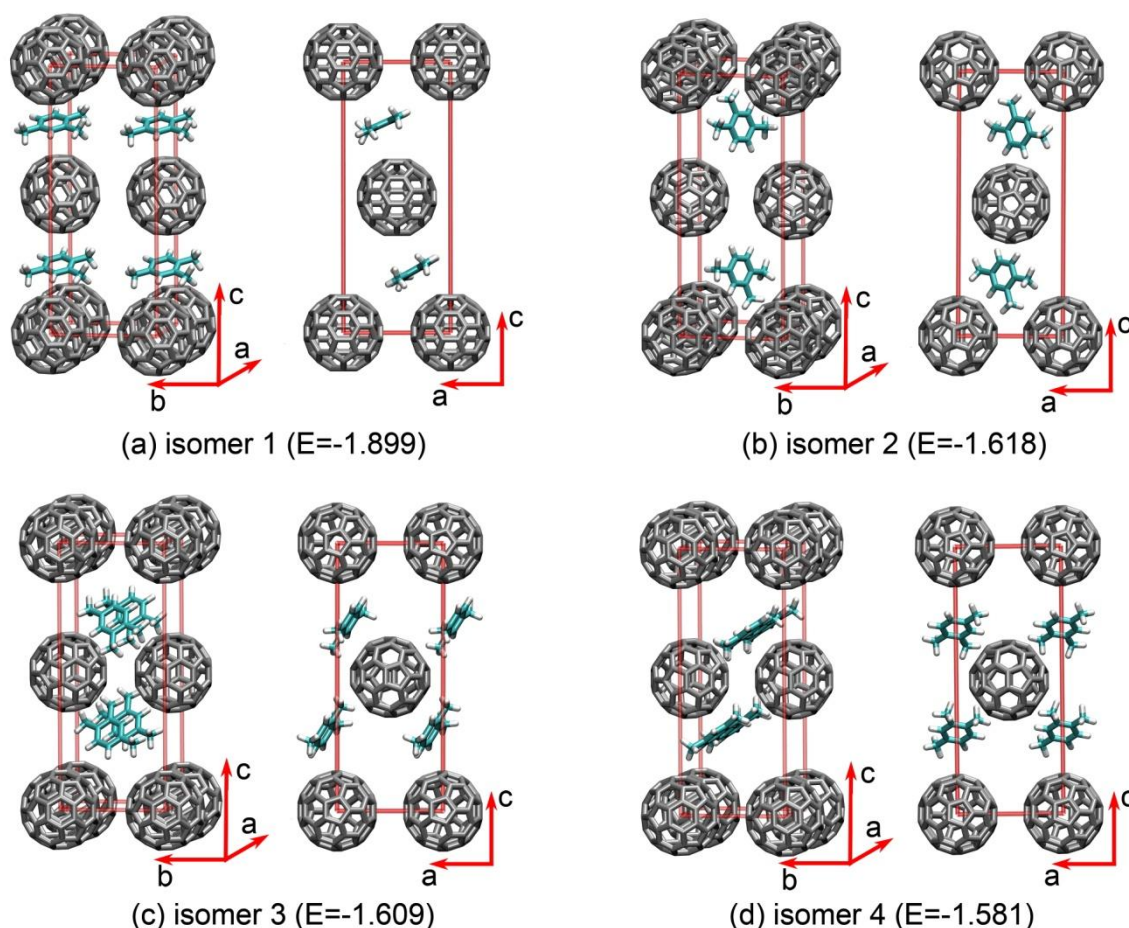


Figure 1. Optimized isomeric states in the C<sub>60</sub>-TMB nanowire unit cell as derived from the calculations. The number in the brackets below each image shows the energy of the structure (in eV).

In a recent study [1], it was demonstrated that exceptionally long fullerene nanowires, with a length-to-width aspect ratio as large as ~3000-5000, can be grown from 1,2,4-trimethylbenzene solution of C<sub>60</sub>.

## We-III-2

We have performed a thorough theoretical analysis, aiming at gaining an in-depth understanding of to explain the exceptionally large aspect ratio of C<sub>60</sub>-based nanowires. By accounting for different interactions in the system we have calculated the structures of the unit cell and determined the role of the fullerene and of the solvent molecules in the crystallization process of the nanowires [2]. The structures of four energetically favorable isomers of the unit cell are shown in the Fig. 1. We have also calculated the adhesion energy of C<sub>60</sub> molecules to the nanowire surface, and on the basis of this explained the growth anisotropy of the crystal.

To get a more profound understanding of the nanowire growth mechanism we have also considered the influence of electron polarization on the growth anisotropy [3] and studied the possible polymerization reactions occurred between the C<sub>60</sub> and the solvent molecules [4].

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## We-III-3

### H<sub>2</sub> REACTIVITY ON GOLD NANO-STRUCTURES: A CLUSTER AND EMBEDDING POTENTIAL APPROACH

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Gold is the noblest of the transition metals and presents a very low catalytic activity in bulk. However, small gold nano-structures lower down the reaction barriers of many reactions, and there is a recent increasing interest in determining their catalytic properties because their possible industrial impact [1]. The dissociation of H<sub>2</sub> on nanowires [2] and clusters [3] have been studied recently, showing no barrier for the reaction. In order to understand in detail the factors determining such high reactivity and the transition from clusters to bulk, here we present a study for different coordinations of gold atoms on model systems, paying special attention to their fluxionality [4]. To simplify the study of larger clusters an extension of a recently developed embedding potential method [5] is used.

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***Collision processes  
involving  
biomolecules***



# Th-I-1

## PHOTODISSOCIATION OF PROTONATED AROMATIC AMINO ACID

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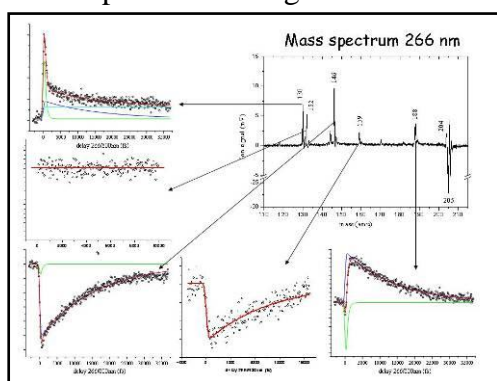
The photofragmentation of protonated tryptophan and aromatic containing peptides has been investigated in a combination of experimental and theoretical means.

The excited state evolution is followed with pump/probe femtosecond techniques and the fragmentation paths may be controlled through time selected re-excitation.

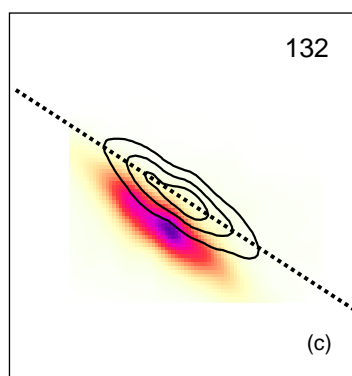
In a second experimental setup, the ion and neutral(s) issued from the photofragmentation are detected in coincidence, in time and in position. From these data are extracted the kinetic energy, the number of neutral fragments associated with an ion, their masses and the order of the fragmentation steps. Moreover, fragmentation time scales ranging from tens of nanoseconds to milliseconds can be obtained.

Ab-initio calculations and in particular excited state optimizations (ri-cc2 level) give some insights of the processes involved after optical excitation.

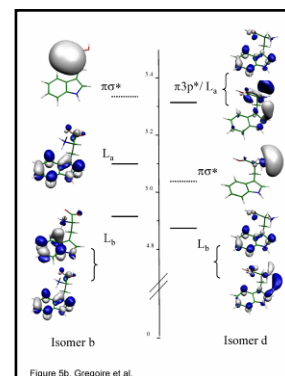
The comparison between experimental data and excited state calculations results in a comprehensive fragmentation mechanism.



protonated tryptophan femtosecond dynamics



ZZ correlation for the m/z=132 fragment



protonated tryptophan excited states

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## Th-I-1

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## Th-I-2

### ULTRACOLD CLUSTER IONS FORMED IN DOPED HELIUM DROPLETS

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Positively [1] and negatively charged cluster ions [2,3] are formed upon collisions of free electrons with doped He nanodroplets. The ions are analyzed by mass spectrometry and their stability is probed via MS-MS techniques. The dominant ionization process for cations is charge transfer from an initially formed He<sup>+</sup> to the embedded cluster. On the one hand, the large ionization energy of He provides efficient double ionization for molecules with low appearance energies that subsequently leads to Coulomb explosion and characteristic product ion distributions. On the other hand, efficient heat dissipation into the surrounding He droplet quenches rapidly vibrational excitation and thereby freezes many intermediate reaction products. Attachment of electrons to doped He droplets initiates a unique sequence of processes. The penetration of the electron into the droplet requires 1.15 eV and for very low-energy electrons a vacuum bubble is formed around the electron prior to the attachment to the embedded molecular aggregate, which requires another 350meV energy. First results on negatively charged CO<sub>2</sub> clusters with improved electron energy resolution ( $\Delta E \sim 100\text{meV}$ ) indicate that the position of the electron attachment resonances does not depend on the droplet size. However, low-energy resonances are suppressed for larger droplet sizes (see Figure 1, lower panel, blue line). In the case of CO<sub>2</sub> clusters the ultra-low temperature inside the He droplet (0.38K) quenches all vibrational excitations and thus has a pronounced effect on the formation of CO<sub>2</sub><sup>-</sup> since the anion is bent and its formation requires an excitation of the bending mode of the neutral precursor. The presence of weakly bound complexes of ions with He atoms attached indicates that ultra-cold ions can be formed. Thus doped He droplets may be utilized to form ions in single quantum states.

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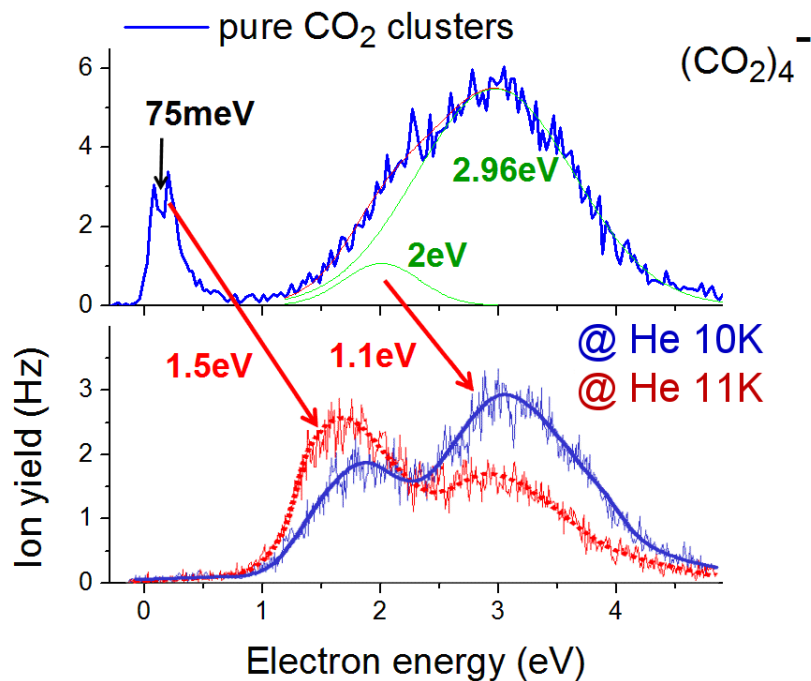


Figure 1: Ion efficiency curves for  $(\text{CO}_2)_4^-$  formed upon free electron attachment to pristine  $\text{CO}_2$  clusters (upper panel) and  $\text{CO}_2$  doped He droplets at two different temperatures of the He cluster source (lower panel). He pressure: 20bar, nozzle diameter: 5 $\mu\text{m}$ .

Acknowledgements: This work has been supported by the FWF, Wien, Austria and the European Commission, Brussels. S.D. gratefully acknowledges an APART grant from the Austrian Academy of Sciences.

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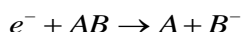
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## Th-I-3

### ELECTRON-INDUCED BOND BREAKING AT LOW ENERGIES IN BIOLOGICAL MOLECULES

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Low energy electron interactions with biological molecules in the gas phase have proved to be a challenge for experimentalists and theorists alike. Although the field has been highly motivated by applications to radiation damage [1], it warrants fundamental interest because of the remarkable variety of bond-breaking reactions produced through the dissociative electron attachment (DEA) process



where the fragments  $A$  and  $B^-$  are not necessarily atomic. This arises not only from the properties of the initially formed temporary anion states, e.g., their symmetries, energies, lifetimes and antibonding sites, but from the range of neutral bond energies, dipole moments and fragment electron affinities found in complex molecules. In addition, from a chemistry point of view, the theory of DEA produces insight into the fundamental electrochemical reduction process producing ions and radicals.

Progress in understanding interactions with large systems such as DNA strands and proteins must be grounded on an accurate analysis of the DEA process in the simplest components of these systems. Surprisingly, in the case of the amino acids and closely related molecules such as formic acid (HCOOH), there is not yet a consensus on the mechanism by which electrons with energies near 1.2 eV produce the sole fragment  $(M-H)^-$ , where  $(M-H)$  represents the target molecule minus an H atom. In this work, we present a theoretical treatment of this process in the two compounds that have been studied most extensively, namely, HCOOH and glycine, the simplest of the amino acids. We show that the existing experimental results can be explained by invoking a single  $\sigma^*$  valence anion state in which the additional electron is largely located on the OH bond [2]. The calculated properties of this resonance in HCOOH are extreme, in that the resonance energy and width are very large, 5.3 eV and 5.8 eV, respectively. Such a short-lived anion state located at this energy would not a priori be expected to play a direct or substantial role in the low energy DEA process. Indeed, almost all of the experimental studies have attributed the DEA process to initial electron attachment into the COOH  $\pi^*$  orbital followed by out of plane distortions that couple this orbital to  $\sigma^*$  (OH), ultimately producing the  $(M-H)^-$  fragment. This interpretation was also put forth in a theoretical study by Rescigno et al. [3].

The primary significance of the present work is thus to call attention to this class of very short-lived high-lying resonances whose large widths preclude their direct observation in the total electron scattering cross section but which are clearly manifested in the DEA and vibrational excitation cross sections at much lower energies. Secondly, we show that in HCOOH and glycine, and by implication the other amino acids, capture into the  $\pi^*$  orbital followed by  $\pi^*/\sigma^*$  coupling is not required to account for the bond breaking.

## Th-I-3

To calculate DEA cross sections for formic acid and glycine, we use the resonant R-matrix theory essentially in the same way as it was done before for hydrogen halides [4, 5]. A model with one effective reaction coordinate close to the O-H stretch motion is employed. The choice of the anion R-matrix pole and the surface amplitude as functions of the reaction coordinate for formic acid are based on scattering phase shift calculations using the finite element discrete model [6]. For glycine the input parameters are adjusted to reproduce experimental data. The results show that the mechanism of DEA in these molecules is similar to that for the hydrogen halides. Nonlocal effects play an important role for both molecules. In particular, pronounced steps and cusps are seen at the vibrational excitation thresholds.

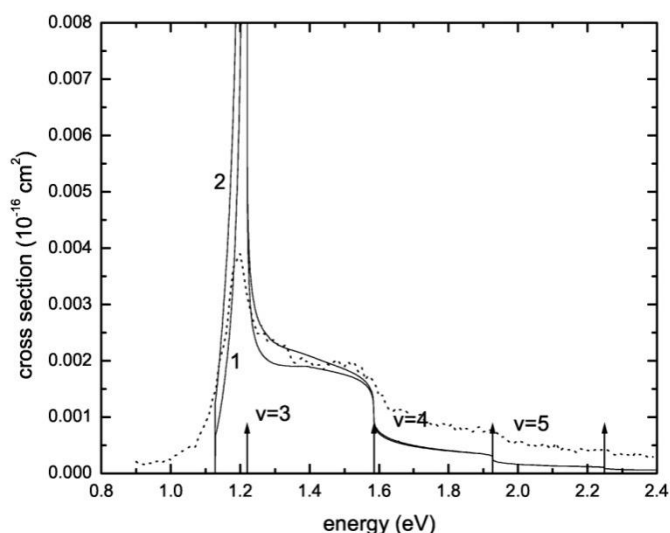


Figure 1: Dissociative electron attachment cross section for glycine. Solid curves marked 1 and 2 are calculations with two different sets of R-matrix parameters. Dotted curve: experimental results [7] normalized to  $0.002 \text{ \AA}^2$  at 1.4 eV. Thresholds for vibrational excitation of O-H vibrations are indicated by arrows.

These results are illustrated in Fig. 1 where DEA cross sections for glycine are shown. A sharp threshold peak in glycine is interpreted as a vibrational Feshbach resonance.

This work was supported by the US National Science Foundation, Grant PHY-0652866.

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***Molecular  
mechanisms of  
radiation damage in  
biomolecular  
systems***



## Th-II-1

### RADICAL FORMATION AND CHEMICAL TRACK STRUCTURE IN ION-BEAM IRRADIATED DNA: ELECTRON SPIN RESONANCE INVESTIGATIONS

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Ion-beam irradiation[1] of hydrated DNA results in formation of the three base radicals, the guanine cation radicals  $G^+$ , the thymine anion radical  $T^-$ , and the reversibly protonated cytosine anion radical,  $C(N3)H^\bullet$ . [2] At 77 K, the shapes of the dose-response curves for these radicals, that is, the curves that give the trapped radical yield as a function of dose, are very similar to the dose response curves for the same radicals in  $\gamma$ -irradiated samples, although the absolute yields of the radicals, expressed as G-values in  $\mu\text{mol/J}$ , are substantially lower than those found in  $\gamma$ -irradiated samples. From these results, we have formulated a radiation-chemical model of the track structure for these samples.[3] The model starts with a standard physical track structure model, in which there is present in ion-beam irradiated matter a high energy density track core and a penumbra of high energy electrons ( $\delta$ -rays) emitted from the core. The model for chemical behavior posits that the base radicals, which are trapped as ion radicals or as reversibly protonated ion radicals, are formed almost entirely by the shower of electrons emitted from the core. The electrons cause radical formation in spurs, similar to the spurs formed from  $\gamma$ -irradiation. The lower yields observed in ion-beam irradiated samples results from the fact that only part of the energy deposited by the ion beam ends up in this  $\gamma$ -like region (Figure 1.)

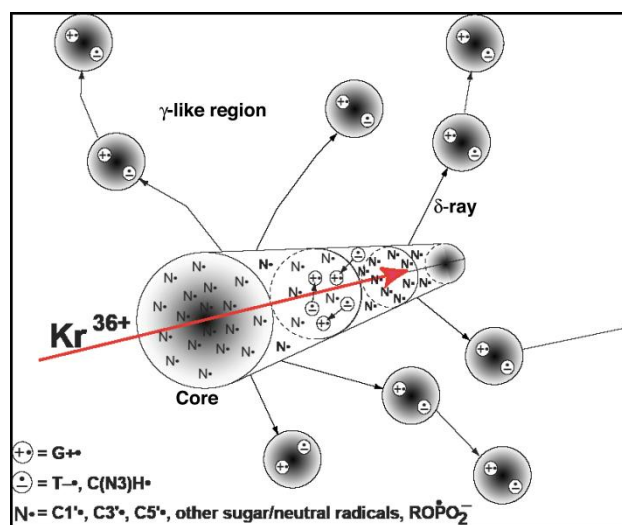
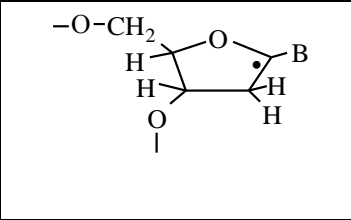
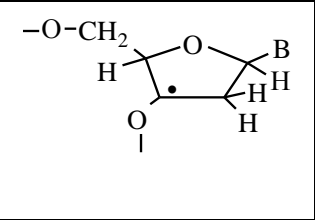
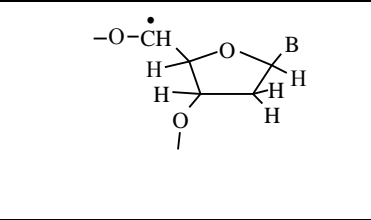
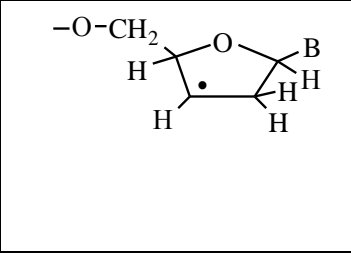
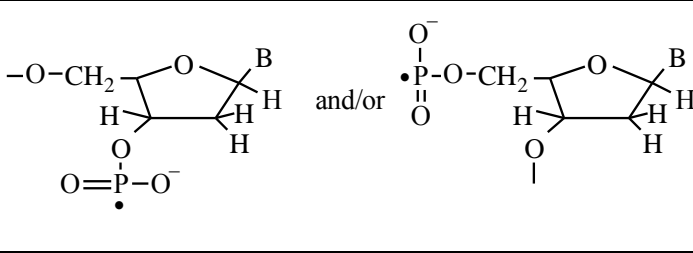


Figure 1. Radiation chemical track structure model for ion beam irradiated samples.

The remainder of the energy is deposited in the core. The proximity of ion-radical formation in the core results in fast recombination of oppositely charged radicals, so it is hypothesized that few or no ion radicals survive in the core at 77 K. However, a second group of radicals found in ion beam irradiated samples are presumed to form almost entirely in the core. These are neutral radicals, which are not as susceptible to recombination as are ion radicals, so they can survive after formation in the core. They include the  $C1^\bullet$ ,  $C3^\bullet$ , and  $C5^\bullet$  sugar radicals, formed from oxidative processes, and  $C3'_{\text{dephos}}^\bullet$ , an immediate strand break radical thought to result from low energy electrons (LEE.)

## Th-II-1

**Table. Structures of Core Radicals**

		
C1'•	C3'•	C5'•
		
C3'•dephos	ROPO <sub>2</sub> <sup>-</sup> •	

These core radicals show a linear dose response up to very high doses, a dose response which is very different from those of the ion base radicals. Because they are neutral, they do not recombine easily and are insensitive to radiation destruction; their relatively high yields lead in ion beam irradiated samples supports the conclusion that they are formed in the core, perhaps through excited state processes.[4] Two phosphorus radicals are also found in ion-beam irradiated DNA; they likely from well established dissociative electron attachment mechanisms, and are therefore thought to originate with LEE. One, RO<sub>2</sub>PO•<sup>-</sup>, is an immediate strand break radical. A new, as yet unidentified phosphorus radical has been observed in Krypton ion beam samples. One or both of these phosphorus radicals appear to show an LET dependent yield.

The spatial characteristics of the radicals formed in DNA after irradiation are critical to the biological effects of the radiation. A critical lesion that results from irradiation is the double strand break (dsb.) If a dsb is accompanied by nearby base or sugar damage, or base deletions, (a cluster of damage) biological repair becomes very difficult and the lesion may be lethal. In a pulsed electron double resonance (PELDOR) experiment, the radical density in a track core cluster of radicals (18 radicals per cluster) and the radius of the cluster (6.8 nm), which is the same as the radius of the core, was determined for Argon ion beam irradiated samples.[5] Further PELDOR experiments are contemplated for ion beam irradiated samples.

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## Th-II-2

### A QUEST FOR COMPARISON OF DIFFERENT PATHWAYS OF DNA DAMAGE IN ION-BEAM CANCER THERAPY

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For more than ten years, heavy-ion-beam cancer therapy has been successfully used clinically in Germany and Japan. Proton-beam therapy is performed in many more centers around the globe and even more are under construction. These therapies appear to be a more favorable alternative to the conventional photon therapy due to a number of advantages [1].

It is understood that projectiles losing energy due to ionization of a medium produce secondary electrons and radicals that cause the main damage to DNA. Some of that damage is irreparable and causes cell death. One of the main advantages of the ion-beam therapy is related to the type of effects that cause DNA damage. The proton/ion beam therapies are characterized by a high linear energy transfer (LET), which means that the production of agents of damage is highly concentrated and the direct and quasi-direct effects as well as effects caused by secondary electrons dominate over indirect effects due to free radicals, which are characteristic for the low-LET radiotherapy. The high concentration or clustering of damage impedes the capability of cells to repair damaged DNA. The prevalence of direct and quasi-direct effects along with secondary electrons over the effects of radicals reduces the importance of the radical-related chemistry.

The main type of irreparable damage, discussed in the literature, is double strand breaking (DSB). One DSB can still be repaired, but if the DSB's are clustered enough then the damage is lethal. However, even if clustered DSB's are the predominant cause of cell death, there is still a debate about pathways leading to DSB's. Direct and quasi-direct effects, secondary-electron effects, thermal effects, etc., are claimed to be important pathways alone and in relation to each other, but they are not yet quantified sufficiently. Effects of multiple single strand breaks (SSB's) coupled with thermal stress and base damage may also comprise a significant fraction of irreparable damage. The main obstacle to understanding a scenario leading to DNA damage is that microscopic events happen on many spatial, temporal, and energetic scales.

We are developing a multiscale inclusive approach to the physics relevant to ion-beam cancer therapy aimed at presenting a clear physical picture of the events starting from an ion entering tissue leading to DNA damage aimed at theoretical calculation of the rate of cell death in irradiated regions [2-4].

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## Th-II-3

### DNA DAMAGE INDUCED BY ENERGETIC IONS AT A MOLECULAR LEVEL

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Presently, ambitious space and therapy projects are devoting great interest in the analysis of DNA damage induced by energetic ions: From one side, encouraging results arising from ion beam cancer therapy have triggered a tremendous development of new medical facilities for cancer treatment[1]. On the other side, radiation damage by ion beams is becoming a major topic of research for shielding of human space missions by ESA and NASA. In fact these ions, not experienced on the earth, are present in the Galactic Cosmic Rays (GCR) and, even with small density, are able to produce tremendous damaging effects to human tissues as their Relative Biological Efficiency (RBE) is huge[2].

Both curing and shielding purposes have the aim to understand and control as much as possible the clustered damage, i.e. the simultaneous occurrence of several damaging events on closeby regions of a DNA molecule, increasing drastically the probability of an irreparable break. More, the two phenomena involve similar initial ion energies (hundreds of MeV).

In the space contest, as any single cell will have negligible probability to be traversed by more than one single ion, this clustering effect is emphasized

A key step in this understanding is in the initial abundance and energy distribution of secondary electrons formed in the process of ionization, as it is commonly accepted that they are mostly responsible for DNA damage, either by directly breaking the DNA strands, or by reacting with water molecules producing more secondary electrons and free radicals, which can also damage DNA. These quantities are then used as input for Monte Carlo track structure codes or other diffusion methods, to evaluate the propagation of secondaries and their damaging impact on DNA elements at a given distance from the track.

More, as the ionization of the medium is the major source of energy loss of the ion projectile, this microscopic quantity can be linked to a macroscopic one as the penetration depth, through the stopping of the ion.

Following one recent work of ours [3], where we started to input a new approach to such a complicate series of phenomena, we will overview the state of the art in research on ion-beam induced electron production that is mostly abundant in proton beams studies.

Then we will focus on an ion that is much relevant both in therapy and space protection issues, C6+, reporting our results [4-6]: we analysed liquid and vapour water as the tissue like media, with different approaches according to the validity ranges of the Born approximation, and thus the applicability of dielectric response approaches, and availability of experimental data. We produce Singly Differential Ionization Cross Sections (SDCS) that, after integration are consistent with a macroscopic calculation by Monte Carlo transport Code (GEANT4), returning a Bragg Peak position within 1% of deviation, and provide electron spectra for the whole energy range.

Finally, we will attempt to report with a similar accuracy the subsequent damaging effects on the biological target.

## Th-II-3

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***Structure and  
dynamics of atomic  
clusters and  
biomolecules***



## Th-III-1

# FROM THE ELECTROPHILIC PROPERTIES OF DNA'S SUB-UNITS, TO ELECTRON-INDUCED ACID-BASE CHEMISTRY, TO ALUMINUM HYDRIDE CLUSTERS: ANION PHOTOELECTRON SPECTROSCOPIC STUDIES

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This talk focuses on anion photoelectron spectroscopic studies of the negative ions of (1) DNA's sub-units, (2) acid-base pairs, and (3) aluminum hydride clusters.

(1) Low energy electrons have been shown to induce single and double strand breaks in DNA. While the mechanism is still under debate, it is clear that the electrophilic properties of DNA's sub-units play a role. Using a novel ion source for bringing parent negative ions of DNA's sub-units into the gas phase, we have measured electrophilic properties of a variety DNA sub-units and combinations thereof, including nucleic acid base pairs, nucleosides, nucleotides, nucleoside-base dimers, nucleoside-nucleotide dimers, and hydrated versions thereof. We have enjoyed theoretical support and collaboration in this work with M. Gutowski and from J. Rak.

(2) When ammonia and hydrogen chloride vapors mix, they form a white cloud due to the formation of ammonium chloride microcrystals. However, when single molecules of ammonia and hydrogen chloride form neutral hetero-dimers, they do not proton transfer (they do not react). We explored the ability of an excess electron to induce proton transfer in these systems by forming the negative dimer anions,  $[(\text{NH}_3)(\text{HCl})]^-$ , and we found that a single electron is sufficient to induce proton transfer and thus salt formation in these systems. The specific mechanism for electron induced, proton transfer involves the formation of dipole bound states and Rydberg molecules. We have enjoyed theoretical support and collaboration in this work with M. Gutowski.

(3) While boron forms many hydrides, aluminum has been thought to form only a few. Using a pulsed arc discharge source, we found that aluminum can form many hydrides. Using anion photoelectron spectroscopy to measure their HOMO-LUMO gaps, we found that some of these species display the hallmarks of significant stability. Calculations and electron counting rules implied specific structures. The bulk synthesis of derivatives of the  $\text{Al}_4\text{H}_6$  stoichiometry permitted x-ray crystallographic analysis which found the same structure implied by theory. This work follows a path from discovery of previously unknown molecules in the gas phase to the bulk synthesis of their analogs. These studies have implications to hydrogen storage materials and to propulsion. We have enjoyed support and collaborations in this work with G. Gantefoer, P. Jena, and H. Schnoekel

## Th-III-2

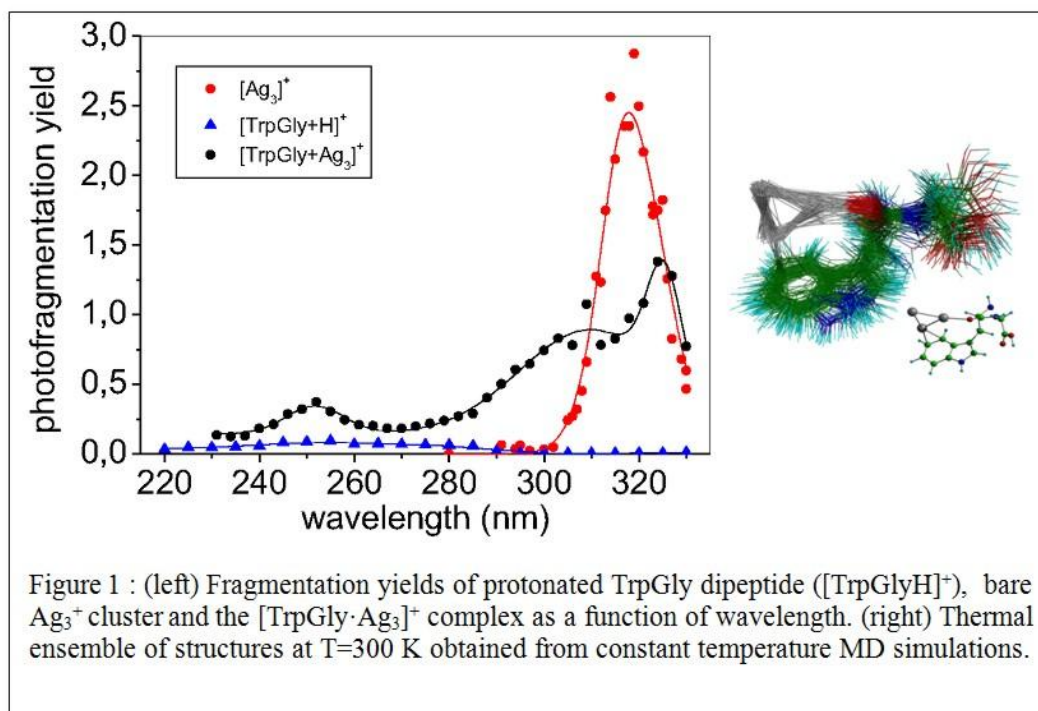
### STRUCTURAL AND OPTICAL PROPERTIES OF GAS PHASE METAL CLUSTER– BIOMOLECULE HYBRID SYSTEMS

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Roland Mitrić<sup>2</sup>, Jens Petersen<sup>2</sup>, Alexander Kulesza<sup>2</sup> and Vlasta Bonačić-Koutecký<sup>2</sup>

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The coupling of the unique electronic and optical properties of metallic nanoparticles to biomolecules is an exciting field of basic and applied research. In particular, a remarkable enhancement of photoabsorption and emission processes occurs in biomolecules near to a metal surface or nanoparticle. These effects are generally interpreted as resulting from a local amplification of the electromagnetic field of the biomolecule due to coupling with the metal surface plasmon. This phenomenon enables fluorescence labeling, imaging, and Raman scattering of single molecules. The photoabsorption characteristics of nanoparticles are strongly size and shape dependent, which allows the synthesis of hybrid systems with tailored optical properties.



Despite the attraction of the gas phase approach, few works were devoted to isolated nanohybrids until now. Recently, we were able to form and to store in an ion trap, model hybrid systems made of a noble metal cluster and a peptide. We studied, by photodissociation experiments, the optical properties of silver cluster-peptide complex cations. The metallic moiety induces a strong enhancement of the optical absorption of the peptide (see Figure 1). We also show that its binding to a peptide can reduce the conformational flexibility and induce transitions between secondary structures.

## Th-III-2

Recent results obtained on the structural and optical properties of gold-tryptophan complexes will also be presented.

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## Th-III-3

### NON-ADIABATIC EXCITED STATES DYNAMICS SIMULATIONS OF ATOMIC AND MOLECULAR CHROMOPHORES ON INERT CLUSTERS

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The photodynamics of alkali earth atoms or molecules deposited on inert clusters is investigated in several groups. From the experimental point of view, a particularly interesting technique is the Cluster Isolated Chemical Reaction technique (CICR) developed in the group of Saclay by J.-M. Mestdagh and coworkers [1]. In these experiments rare gas clusters are generated in a supersonic expansion, a controlled number of atoms are deposited on the cluster through pick-up technique, the atoms eventually associate and form a molecule or an aggregate. The atomic and/or molecular chromophore can be photoexcited and subsequent processes (relaxation, photodissociation) can be monitored via fluorescence or action spectra. Pump-probe femtosecond spectroscopy experiments (excitation + ionization) can also provide insight into the excited states dynamics via the time dependence of the photo-electron or photo-ion spectra.

However, the excited state pattern and the coupled electron-nuclei dynamics of the chromophore/rare gas cluster system can be rather involved, yielding several different competing processes such as fluorescence, non-radiative relaxation, chromophore photodissociation, evaporation. Theory is needed to provide detailed insight in the electronic structure and dynamical processes.

The present contribution reports a modelling of the electronic excited states of alkali earth (atoms or molecules) deposited on rare gas (Rg) cluster systems and of their dynamics. The electronic states are determined using ab initio calculations to design Diatomics-in-Molecules modeling of the excited states potential energy surfaces. The behaviour of the photoelectron spectrum of  $Ca/Ar_{55}$  in a pump-probe type experiment (the first pulse excites the system in the vicinity of the  $4s4p$  line of  $Ca$ , the second pulse ionizes the system) is simulated [2]. This involves surface-hopping non-adiabatic dynamics in the excited states, and the determination of the photoelectron energy as a function of the pump-probe delay. The time-oscillating dependence of the spectrum occurs to be a nice signature of the geometric motion of the chromophore atom at the cluster surface, finally quenched through non-adiabatic relaxation and energy transfer to the cluster. The simulations provide insight into the relaxation mechanisms and the relative importance of intra-cluster relaxation versus the competing chromophore evaporation process.

In addition to the case of a single calcium atom, preliminary results describing more complex situations, like population of higher excited states ( $Ba/Ar_n$  in the vicinity of the  $6s9p$  line), or photoexciting molecules involving molecular doubly excited ( $Ca_2/Ar_n$ ), states will be presented and discussed [3].

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## Th-IV-1

# ELECTRONIC PROPERTIES OF NANOSCALE ORGANOMETALLIC AND BIOLOGICAL CLUSTERS

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Organic molecular clusters, consisting of 2-1000 molecules, are finite aggregates, providing a microscopic model to investigate the chemical and physical properties of molecular assemblies in organic nanomaterials or at interface. A unique nature of organic molecular clusters is originated from weak intermolecular van der Waals interactions, which results in narrow electronic bandwidths, and electron (or hole) charge carriers in organic molecular aggregates are often strongly localized on individual molecules, where molecular ions are formed. Such a molecular ion is instantaneously stabilized by the electronic polarization of its neutral neighbors, which significantly affects charge-transport energy levels in organic molecular aggregates. Since the number of constituent molecules can be tuned accurately in combination with mass spectrometry, size-selective investigations on a broad size range of organic molecular clusters can provide a deep understanding on the evolution of the electronic and geometric properties. In particular, oligoacenes such as tetracene and pentacene are classical examples for the study of charge carrier localization and transport.

We have recently realized an efficient formation of large oligoacene molecular nanoclusters up to more than 200 constituent molecules; naphthalene (Nph), anthracene (Ac), tetracene (Tc), and so on. By adding a single excess electron, the corresponding nanocluster anions were produced in the gas-phase, and the size-selective properties could be revealed by photoelectron spectroscopy. In particular, two types of anion states are shown to coexist in nanometer-scale cluster anions of oligoacene of Nph, Ac, and Tc. The photoelectron spectra of size-selected cluster anions containing 2 to 100 molecules revealed that rigid “crystal-like” cluster anions emerge, greater than ~2 nanometers in size, and coexist with the “disordered” cluster anion in which the surrounding neutral molecules are reorganizing around the charge core. For Tc clusters, surprisingly, only 14 tetracene molecules within a 2D herringbone-type layer including an excess charge can provide the charge stabilization energy corresponding to ca. 80 % of that of the crystal and the rest of the energy is provided by polarization of neutral molecules in adjacent layers.

Similarly, the electronic structures of biological cluster anions consisting of amino-acid molecules have been investigated by using anion photoelectron spectroscopy and theoretical calculations. Spectral features in the photoelectron spectra exhibited two components for isomers, and the anionic core switching along the cluster size evolution was identified.

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## Th-IV-2

# HIGH-SENSITIVITY SPECTROSCOPY OF MASS-SELECTED ATOMIC AND CLUSTER IONS STORED IN AN ION TRAP

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A novel experimental technique is presented for photoabsorption spectroscopy, magneto-optics, and spin polarization of atomic and cluster ions. The technique employs a mass spectrometer, an ion trap, and an optical cavity; mass-selected ions stored in an ion trap interact with photons trapped in a cavity. The storage lifetime of photons in the cavity provides extremely high sensitivity in absorption and polarization-rotation measurements (photon-trap spectroscopy: a generalized scheme of cavity ring-down spectroscopy). This experiment is motivated by studies of magnetic clusters, such as  $\text{Mn}_2^+$  and  $\text{Mn}_3^+$ , of which responses to a magnetic field are to be investigated through magneto-optical effects to understand their electronic and magnetic structures specific to these clusters; the small Mn cluster ions are presumed to be ferromagnetic in contrast to antiferromagnetic solids [1].

The main part of the experimental setup is shown in Fig. 1. The first experiment was performed on atomic ions of manganese,  $\text{Mn}^+$  ( $^7\text{S}_3$ ) [2]. Figure 2(a) shows one of the three absorption lines of spin-allowed electronic transitions  $^7\text{P}_J \leftarrow ^7\text{S}_3$  ( $J = 2, 3, \text{ and } 4$ ) observed in the UV region. The spectrum was split under a magnetic field by the Zeeman effect as shown in Fig. 2(b). The Zeeman splitting is associated with the Faraday effect causing polarization rotation; the spectrum is shown in Fig. 2(c). Furthermore, the stored  $\text{Mn}^+$  ions were spin-polarized by a circularly polarized nanosecond laser pulse, where an optical cavity stretches the laser pulse sufficiently long for completing spin polarization (cavity-assisted optical pumping) [3]. These results were simulated on the basis of the quantum theory, which could explain all the details of the measured spectra. The electronic structure of  $\text{Mn}^+$  in a magnetic field is presented along with the procedures of analyses of the spectra.

The experiment has been extended to cluster ions. It is unique to the present technique that an absorption spectrum of size-selected cluster ions is measured "directly" without relying on "indirect" action spectroscopy of laser-induced fluorescence (LIF) or photo-depletion/dissociation. It is known that clusters, particularly of large sizes, neither fluoresce due to fast internal conversion from electronic to vibrational energy nor dissociate readily due to a slow statistical rate of dissociation; these "indirect" techniques hardly work in such cases [1].

We present the first cluster experiment on  $\text{Ag}_9^+$  [4]. The absorption spectra measured at ion-trap temperatures of 300 and 10 K are shown in Fig. 3; the use of an ion trap instead of an ordinary ion beam allows experiments under a controlled temperature as well. The spectra exhibited blue-shift and/or sharpening as the temperature was lowered. Although the photon-energy range of the measurement is limited by the reflectivity of the cavity mirrors, it is clear that the spectrum consists of single-electron transitions between molecular orbitals inherent to relatively cold clusters showing a *molecular* nature. The present spectrum should be contrasted with those assigned to surface-plasmon resonance due to collective excitation of electrons in hot silver clusters showing a *metallic* behavior [5].



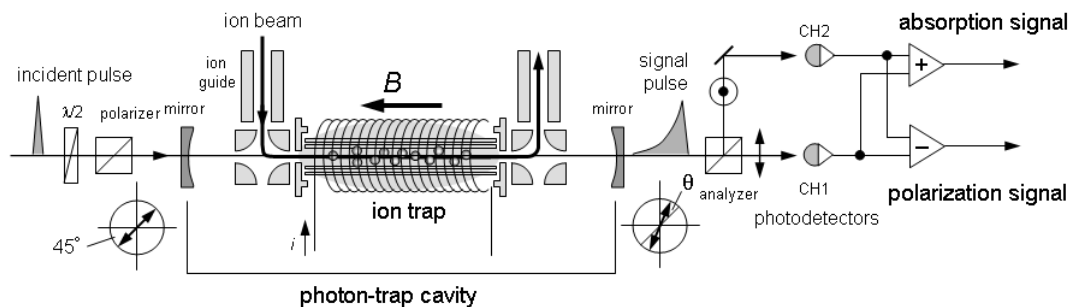
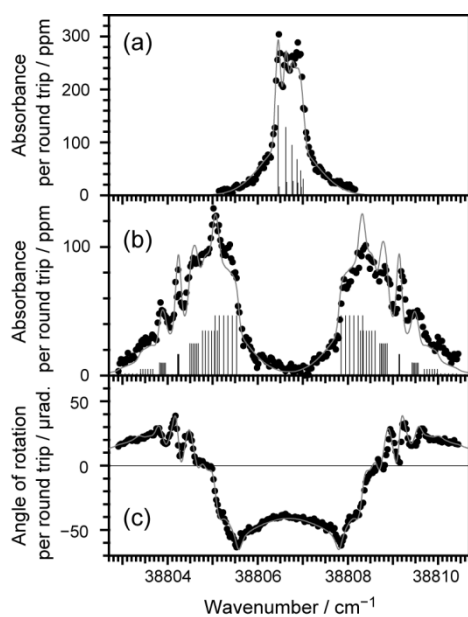
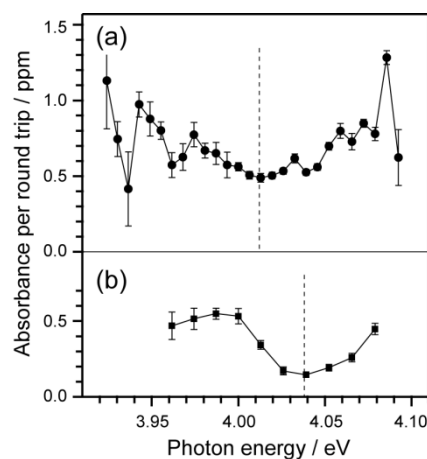


Figure 1: A schematic of the experimental setup.

Figure 2: Spectra of (a) field-free absorption, (b) Zeeman splitting, and (c) Faraday rotation at  $B = 3$  T measured for  $\text{Mn}^+ 7P_4 \leftarrow 7S_3$  transition.Figure 3: Absorption spectrum of  $\text{Ag}_9^+$  measured by photon-trap spectroscopy. The temperature of the ion trap were (a) 300 and (b) 10 K.

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## Th-IV-3

# CRYSTALLIZATION AND MELTING OF ION CLUSTERS CONFINED IN HIGH-ORDER ELECTROSTATIC TRAPS

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Large sets of atomic ions cooled in quadrupolar traps provide a finite realization of Wigner crystals, with well defined structures and a first-order like melting transition. In this talk, we examine ion clouds stored in isotropic octupolar traps. Using a combination of simple semi-analytical models, global Monte Carlo optimization and molecular dynamics simulations, the stable structures and melting temperatures of the ion clouds are investigated with a particular emphasis at the finite size scaling effects. The stable structures of small-size clouds containing less than a few thousands ions are found to be hollow and arranged in shells corresponding approximately to the solutions of the Thomson problem. Above this size, the loss of the shell structure proceeds from the core, the inner parts of the cloud being soft and amorphous. At finite temperature, melting is first initiated in the inner shells, and eventually extends toward outer layers. However, and even though the ion clouds resemble more a two-dimensional thick film, the melting transition is found to follow the expected rule for three-dimensional dense particles, with a depression scaling linearly with the inverse radius. The broad distributions obtained at very high temperatures are in agreement with the predictions of simple mean-field models. Finally, some aspects of the chaotic dynamics are discussed, highlighting again the special status of quadrupolar confinement.

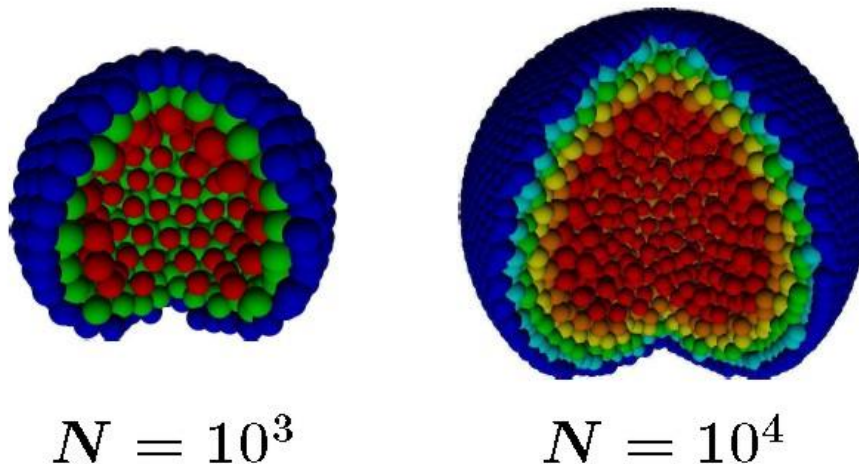


Figure 1: Snapshots of stable conformations obtained for ion clusters in octupolar confinement, containing  $10^3$  and  $10^4$  particles, respectively

***Phase transitions,  
fusion, fission and  
fragmentation in  
finite systems  
(part II)***



## STATISTICAL MECHANICS DESCRIPTION OF THE PROCESS OF POLYPEPTIDE AND PROTEIN FOLDING

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The conformational transitions in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state or vice versa (also known as (un)folding process) occur or can be expected in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes [1]. We suggest a theoretical method based on the statistical mechanics for treating the helix $\leftrightarrow$ random coil transition in polypeptides. This method describes essential thermodynamical properties of the system such as heat capacity, the phase transition temperature and others from the analysis of the polypeptide potential energy surface calculated as a function of two dihedral angles, responsible for the polypeptide twisting [2]. We perform thorough comparison of the predictions of the statistical model with the results of molecular dynamics simulations [3]. Two methods of calculation of heat capacity of the system are analyzed, namely method based on differentiation of energy on temperature dependence and method based energy fluctuations. We also investigate the influence of side chain radicals on the thermodynamic properties of the system [4]. The developed formalism is extended for the description of the helix $\leftrightarrow$ coil transition in water environment [5].

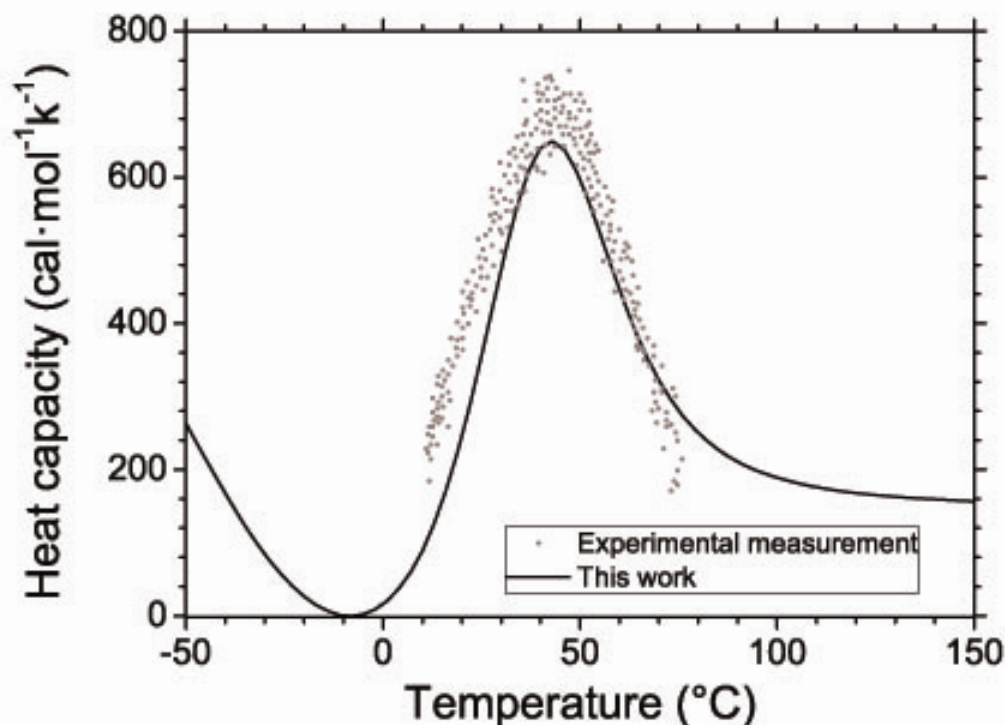


Figure 1. Dependencies of the heat capacity on temperature calculated for the alanine-rich polypeptide consisting of 50 amino acids. The results obtained using the statistical mechanics model are shown by thick solid line, while the results of experimental measurements from Ref [6] are presented by dots.

## Fr-I-1

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# CLUSTERING INSTABILITIES IN FLUIDIZED GRANULAR MATTER

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Fluidized granular matter (matter composed of macroscopic particles) exhibit a plethora of fascinating symmetry-breaking instabilities and pattern-formation phenomena. Their understanding is needed for developing quantitative models of granular flow. I will focus on two recently discovered clustering instabilities, which result from the inelasticity of particle collisions.

I consider an ensemble of macroscopic particles in a box where the particles move and collide inelastically with each other. The system is driven, at zero gravity, by one or two rapidly vibrating side wall(s). This setting represents a paradigmatic driven granular system. An immediate consequence of the inelasticity of the particle collisions is the formation of a cluster of particles away from the driving wall(s). This static (laterally uniform) clustering state can become unstable. The first instability occurs in the lateral direction parallel to the thermal (vibrating) walls. This spontaneous symmetry-breaking instability leads to the development of strongly localized "droplets" of granulate. These predictions were obtained in the framework of a hydrodynamic description. We performed a detailed linear stability analysis of the equations of granular hydrodynamics and obtained the marginal stability curves. Surprisingly, the instability in this far-from-equilibrium system resembles the van der Waals phase-separation.

We found that static (laterally uniform) clustering state can also become oscillatorily unstable. The instability, predicted by a linear stability analysis of the equations of granular hydrodynamics, occurs when the inelasticity of particle collisions exceeds a critical value that depends on the rest of the parameters of the system. Molecular dynamic simulations support the theory and show a stripe-shaped cluster moving back and forth in the middle of the box away from the driving walls. The oscillations are irregular but have a single dominating frequency that is close to the frequency at the instability onset, predicted from hydrodynamics.

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### CHARGE INSTABILITIES OF MICRO-DROPLETS<sup>a</sup>

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Coulomb instabilities have been studied in the past for a variety of finite size systems, from nuclei to large clusters. Already in 1882 Lord Rayleigh established the so-called Rayleigh limit for liquid incompressible, surface-charged droplets [1]. At this limit, the electrostatic pressure compensates the cohesive force acting between the water molecules, and the system becomes unstable and deforms spontaneously. In recent experiments, we took snapshots of levitated metallic (Hg) micro droplets. We used a Paul trap in a controlled atmosphere to avoid the oxidation of the mercury surface. We followed the ultra-fast deformation pathway of the droplets towards the formation of 2 fine jets at opposite ends and back to the stable spherical shape. We focused on mercury droplets, for they behave like perfect conductors and ideal liquids, having a negligible kinematic viscosity. The observed shape deformation is compared to that of other liquids (water, glycol) [2] which differ by ion mobility and viscosity and to home-made simulations based on fluid dynamics of ideal liquids [3]. We highlight the role of the charge mobility and viscosity on the deformation pathway and jet formation. For super-critical charged droplets (above the Rayleigh limit), the model foresees that the oblate deformation competes with the already observed prolate deformation. Interestingly, the deformation energy of super-critically charged oblate droplets has a minimum and may be observed experimentally (part of this project). We discuss the deformation limit of such droplets.

<sup>a</sup> Thanks to CNRS (ANR project) for financial support.

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***Photon-cluster  
collisions and  
clusters in laser  
fields***



## Fr-II-1

# REALIZATION OF THE CONCEPTUAL IDEAL FOR X-RAY AMPLIFICATION AT $\lambda \sim 2.9 \text{ \AA}$ WITH XENON CLUSTERS

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The Xe(L) system that operates on hollow-atom transition arrays produced by the excitation of  $(\text{Xe})_n$  clusters is an amplifier with fundamentally different dynamic characteristics from all previously developed laser amplifiers; it represents the conceptual ideal through full utilization of the Kramers-Kronig relations that fundamentally couple the dispersive and absorptive components. The dispersive response of the system, through optimal governance of the power compression, rules the amplification and establishes a minimum value of the dispersion to be surpassed; the corresponding gain follows automatically. As a leading consequence, since this minimum gain is sufficiently high, the key experimental observation is the uniform presence of saturated amplification signaled by strong spectral hole-burning on all transitions exhibiting amplification, including double-vacancy lines. This cardinal signature demonstrates that the amplification is legislated by the saturated gain  $g_s$ , not the corresponding small signal value  $g_o$ . The chief outcome is that explosive dispersion yields perforce explosive amplification and the efficient generation of maximally bright coherent power.

## Fr-II-2

### THEORETICAL STUDIES OF THE IONIZATION OF ENDOHEDRAL ATOMS AND FULLERENES

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Atoms confined in hollow fullerenes, endohedral atoms, were discovered some time ago. The situations where the atom is at the center of the fullerene, held there by very weak van der Waals forces, in a sense represents a new kind of dimer-like structure, a van der Waals molecule with an atom inside a molecule. The surrounding molecule interacts with the trapped atom, thereby altering its properties; among these properties is the response of the caged atom to ionizing radiation. This is of interest as a basic process of nature, as well as because of the many possible technological and biomedical applications of such structures. This is the impetus for the research program aimed at understanding the nature and cause of the alteration of the properties of atoms when they are confined. In particular, we are involved with the theoretical study of the ionization of an atom A confined in a hollow fullerene  $C_n$ , generally referred to a  $A@C_n$ , with particular emphasis on  $A@C_{60}$ .

Two general types of theoretical methodologies are used to treat the  $A@C_{60}$  system. The simpler is to treat the confined atom in an external potential arising from the surrounding fullerene. This potential takes the form of a radial square well with parameters obtained from experimental studies on free fullerenes.

Using this approximation, much has been learned about the photoionization of atoms caged in  $C_{60}$ . Oscillations in the cross section of the caged atom about the free atom cross section, termed confinement resonances have been found and explained in terms of the interference between the photoelectron wave emitted directly, and the waves scattered off the inner and outer edges of the confining potential [1]. And, since this affects the matrix elements themselves, these confinement resonances are seen in the photoelectron angular distribution parameters as well, both dipole and nondipole [2]. We have also found that correlation in the form of interchannel coupling can transfer the confinement resonances from one atomic subshell to another, leading to correlation confinement resonances. This has been found in  $Xe@C_{60}$  in the 5s cross section owing to the coupling with the 4d photoionization channels [3]. In addition, it has been found that these confinement resonances

## Fr-II-2

are significantly enhanced by when the  $C_{60}$  confining cage is negatively charged [4]. Further, atoms confined in  $C_{240}$  and  $C_{540}$  have been investigated, along with atoms confined in nested buckyballs known as buckyonions, e.g.,  $A@C_{60}@C_{240}$ , and significant enhance of the confinement resonances occurs in certain cases [5].

In the more complex theoretical methodology, the  $C_{60}$  cage is considered to be 240 delocalized valence electrons of the carbon atoms, in the field generated by the 60  $C^{+4}$  centers smeared out in a jellium potential which is adjusted to give the correct ionization potential of the free  $C_{60}$  molecule. To this the atomic potential is added and the wave functions of the 240 delocalized electrons along with the atomic electrons are found by solving the Kohn-Sham equations. Then the random-phase-approximation-like time-dependent-local-density-approximation (TDLDA) is used to include correlation. The major advantage that this has over the simpler method is that it includes correlation between the cage electrons and atomic electrons, which can have a very significant effect on the atomic photoionization [6,7]. Using this theoretical methodology and the example of  $Xe@C_{60}$ , we have found hybridization of the wave functions between localized atomic states and delocalized cage states. Owing to this hybridization, the cross sections for the states affected are altered radically from the free atom and pristine cage values [8].

Using both approximations, we have just begun to investigate the ionization of fullerenes and atoms confined in fullerenes by charged particle impact at the Born approximation level. Our results indicate the existence of confinement resonances in the spectrum of secondary electrons and in the generalized oscillator strengths, using  $He@C_{60}$  and  $Ne@C_{60}$  targets as examples [9]. We have also looked at charged particle impact ionization of pristine  $C_{60}$  and preliminary results suggest the possibility of nondipole plasmon excitations in the process.

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## Fr-II-3

### FULLERENE-ENCAPSULATED ATOMS IN THE LIGHT OF SYNCHROTRON RADIATION

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The concept of an atom trapped inside a fullerene molecule has fascinated both chemists and physicists for the past two decades. Numerous theoretical studies have explored the response of atoms encapsulated in fullerene cages to ionizing electromagnetic radiation. In a first successful series of experiments at the ALS on single and double photoionization of endohedral Ce@C<sub>82</sub><sup>+</sup> ions it has been possible to extract the contributions of cerium 4d photoexcitation to the single and double ionization channels of the endohedral molecule [1]. For this purpose, single and double photoionization of free atomic Ce<sup>q+</sup> ions (q=2,3,4), of empty C<sub>82</sub><sup>+</sup> ions and of endohedral Ce@C<sub>82</sub><sup>+</sup> ions was measured as a function of the photon energy. The experiment yielded information about the charge state (q=3) of the cerium atom residing within the fullerene shell.

Free Ce<sup>3+</sup> ions absorb photons with energies between 100 eV and about 170 eV almost exclusively via photoexcitation of the 4d subshell with subsequent single or double Auger decay. By that, they fully exhaust the available absorption oscillator strength  $f_a=10$  through the net single and double ionization channels. In contrast, the encapsulated Ce<sup>3+</sup> ion might be expected to mediate preferentially multiple ionization of Ce@C<sub>82</sub><sup>+</sup> complex where the most loosely bound electrons can be removed with much less energy than that required by the free Ce<sup>3+</sup> ion. Clearly, the presence of the fullerene shell opens additional opportunities for a 4d vacancy to decay. One such process is the Inter-Atomic Coulomb Decay, where, in a molecule, one atom's inner-shell vacancy is filled while an electron is released from an outer shell of a second atom (or the whole fullerene sphere). This should evidently lead to increased ionization in the endohedral fullerene. Surprisingly, the experiments with the endohedral Ce@C<sub>82</sub><sup>+</sup> ions revealed even less 4d oscillator strength in the ionization channels than free atomic Ce<sup>3+</sup> ions. The sum of the integrated oscillator strengths of single and double ionization of Ce@C<sub>82</sub><sup>+</sup> in the energy range of primary cerium 4d excitations was found to be only 3.4.

Beside electron emission channels the presence of the cage around the absorbing Ce<sup>3+</sup> ion can give rise to a large number of additional decay mechanisms involving fragmentation of the fullerene sphere. It is likely, that the oscillator strength missing in single and double photoionization of endohedral Ce@C<sub>82</sub><sup>+</sup> ions is transferred to the channels of fragmentation with and without additional ionization.

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## Fr-III-1

# DIRECT OBSERVATION OF FULLERENE PLASMON OSCILLATIONS IN MOMENTUM SPACE

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Oscillatory behavior of particle breakup processes is the result of quantum interference between different emission pathways. Prominent examples are the partial cross section oscillations in the ionization of fullerenes [1] and homonuclear diatomic molecules [2]. This behavior may be described in the simplest way by a 'ripple tank' simulation. Such a simulation predicts a cosine-like behavior from threshold to the asymptotic limit. New near threshold measurements of the photoionization of  $N_2$  corroborate these predictions. They are, however, in contrast to the original predictions by Cohen and Fano [3] who derived a  $\sin(kR)/kR$  behavior for partial cross section oscillations. The result of the ripple tank simulation should apply more adequately to the photoionization probability for fixed in space molecules along the molecular axis. The corresponding measurements and calculations using the relaxed core Hartree-Fock method for  $N_2$  support this assumption. This includes the non-declining character of the sinusoidal function in contrast to the behavior of the integrated partial cross sections. The difference between the two kinds of measurements is well reproduced by the corresponding ripple tank simulations. Cohen and Fano's early predictions are based on a hydrogenic model for two emitter atoms sharing a joint centre. The result is a kind of standing wave model.

An extended spherical object which gives rise to standing wave oscillations is  $C_{60}$ . We performed new near threshold measurements for  $C_{60}$  in order to reveal the corresponding threshold behavior. The result was a surprise. The extension of the high energetic sinusoidal behavior to lower energies uncovers a phase jump of  $\pi/2$  in the plasmon excitation region [4]. By subtraction of the extended regular oscillation from the experimental data we could unfold the oscillatory behavior of the plasmon excitations directly in momentum space for the first time. In addition, after subtraction of the plasmon oscillation the shell thickness dependent beating behavior of the partial cross sections was exhibited much more clearly than demonstrated before.

The corrected partial cross section follows a  $\sin(kR)/kR$  function as predicted. Only the very near threshold behavior is experimentally still uncovered. These new results point to the conclusion, that Cohen and Fano's ingenious work should be regarded more as a general prediction for sinusoidal behavior of ionization cross sections of mirror symmetric systems, rather than providing a specific formula. However, it provides a very good measure for determining the large scale coherent photoionization behavior as prerequisite for the derivation of energetically more restricted kind's of behavior such as the plasmon oscillations exhibited directly in momentum space for the first time here.

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## Fr-III-2

### PHOTOIONIZATION OF FREE AND ENDOHEDRAL C<sub>60</sub>: COLLECTIVE, REFLECTIVE, AND COLLATERAL EMISSIONS

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Fullerenes are a family of carbon allotropes that show extraordinary stability even at the room temperature. Owing to their special structure these nanoparticles have been the subject of intense research activities. The buckyball fullerene, C<sub>60</sub>, attracts prime attentions in theoretical studies due to its near-spherical symmetry. Some of our recent studies on C<sub>60</sub> and its derivatives, as outlined below, will be reviewed in the talk.

We have performed a detailed theoretical investigation of the collective resonance phenomenon in the photoionization of C<sub>60</sub> [1]. The time-dependent density functional theory is used to calculate the total and subshell-differential cross sections. The calculation reveals two plasmon resonances in the total cross section in agreement with the experiment. It is found that a phase-coherent superposition of amplitudes leading to enhancements in the ionization from various C<sub>60</sub> subshells in two distinct energy regions essentially build the plasmons.

It is known that the interference between electron waves from inner- and outer-wall of C<sub>60</sub> produces oscillations in the photoionization cross section of the molecule. However, these oscillatory structures from various C<sub>60</sub> subshells do not show a universal spectral "morphology". We have predicted that the oscillations evolve with the orbital angular momentum of the bound electrons such that the structures of the highest and the lowest angular momentum subshell cross sections differ dramatically [2]. A Fourier analysis of the cross sections at energies below the carbon K-shell continuum indicates that the effect can be observed by photoelectron spectroscopy.

Synthesis of endohedral fullerene compounds by trapping an atom inside a fullerene cage is now well-established by experiment. Such entrapments are easier to sustain than the traditional field-entrapments, like laser cooling or magneto-optical trap. Technologically, endohedral fullerenes show the potential of fascinating applications. In the realm of fundamental science, with a robustly stable shell fullerenes are natural laboratories for testing traditional physics of free atoms in confinement. The confined atom is free from significant interactions with the outer environment, thereby allowing the new quantum mechanical effects from the atom-fullerene mutual interactions to be explored. Therefore, theoretical studies of the photoionization of these compounds, both for the confined atom and the conning shell, from low energies up to the carbon K-shell threshold are valuable.



## Fr-III-2

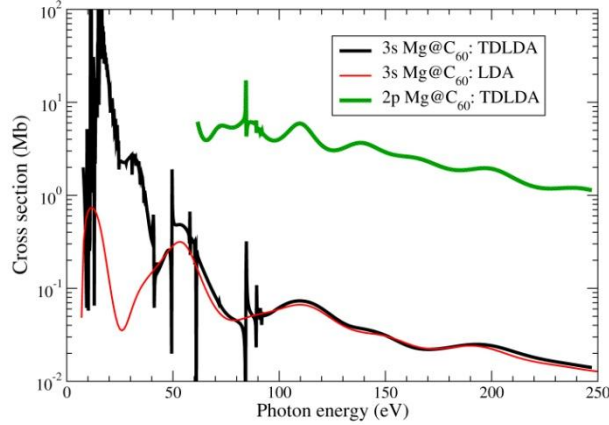


Figure 1: Mg  $2p$  cross sections of Mg@C<sub>60</sub> calculated in the independent particle LDA and the many-body TDLDA method. The TDLDA result for Mg  $2s$  is also displayed.

Considering an Ar atom endohedrally sequestered in C<sub>60</sub>, we have found a phenomenal increase in the photoionization cross section of the confined atom through the dominant outer  $3p$  channel [3]. A more spectacular enhancement is obtained for the Mg  $2p$  ionization in Mg@C<sub>60</sub> [4], as shown in Fig. 1. The effect occurs owing to a powerful coherent interchannel coupling between the atomic and the cage ionization channels which re-directs the bulk of oscillator strength from the giant surface plasmon to the atomic ionization channel. Recent studies on Xe@C<sub>60</sub> unravel further new phenomena [5], indicating rich physics that can be extracted.

At energies above the plasmon region the photoionization cross section of the confined atom is known to oscillate; this is seen in Fig. 1. As for the origin of the oscillation, the interference of the photoelectron emanating directly from the atom with the one reected from the cage is previously suggested. Indeed, for any general atomic subshell the confinement-induced reflective ionization amplitude interferes with the direct ionization amplitude to induce oscillations in the cross section. However, the complete picture extends far beyond that. For the outermost atomic level, the collateral ionization of the atomic electron from the cage engenders strong further interferences with the direct emission. This is evidenced in very different oscillation patterns in Mg  $2p$  and  $2s$  in Fig. 1. Both the reective and the collateral amplitudes, oscillating in the momentum space with frequencies determined by their path differences from the direct amplitude, uniquely measure the geometry of the confinement which can be determined from the reciprocal spectrum [6]. Although the effect is illustrated for an encapsulated atom, it must exist for the confined molecules, clusters, and even for the cylindrical entrapments like nano-peapods, pointing to a generic implication of the Fourier photo-spectroscopy.

The research is partly supported by the NSF.

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## TOWARDS THE DYNAMICAL SCREENING OF AN ENDOHEDRAL MOLECULE

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The fullerene cage screens the endohedral atom from external electromagnetic fields. Recent theoretical studies [1-3], using semi-classical methods, show that this effect is strongly dependent on the photon energy. In the vicinity of the plasmon resonances of the fullerene, the photoabsorption of the confined atom is strongly enhanced from that of the free atom. A dynamical screening factor may be defined to relate the two photoabsorption cross sections. A more elaborated investigation into the centrally confined atom is performed and compared with time dependent local density approximation (TDLDA) calculations for dynamical screening factor of Ar@C<sub>60</sub> [4] and Mg@C<sub>60</sub> [5]. The  $\pi$  and  $\sigma$  plasmons of the fullerene are accounted for in a modified screening factor to improve correspondence with the quantum calculations, see figure 1.

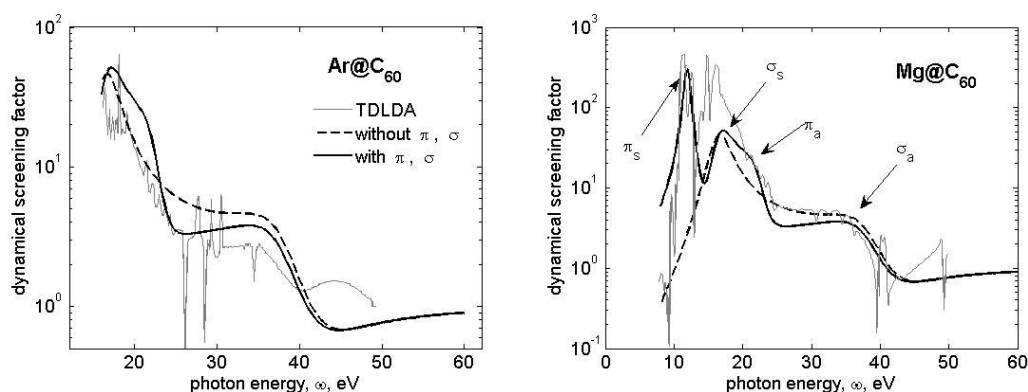


Figure 1: The dynamical screening factor with and without accounting for the  $\pi$  and  $\sigma$  plasmons are shown for Ar@C<sub>60</sub> and Mg@C<sub>60</sub>. The features due to the symmetric (s) and antisymmetric (a) modes of the  $\pi$  and  $\sigma$  plasmons are indicated on the right panel. These factors are compared with the TDLDA calculations of [4] and [5], respectively.

The photoionization cross section of Sc<sub>3</sub>N@C<sub>80</sub><sup>+</sup> was recently measured by Schippers et al [6]. The extension of this semi-classical model to consider endohedral molecules/clusters will be discussed. A comparison with the experimental results will be performed, to understand the effect of confinement and of dynamical screening.

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# ***Electron and ion cluster collisions***



# LASER- AND COLLISION-INDUCED COLLECTIVE DYNAMICS IN FULLERENES

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During the last decade, fullerene reactions became an exciting new field of collision physics and experiments involving photons, electrons, atoms, molecules, clusters, surfaces, ions, and highly charged ions have been performed. In this contribution, we will show that collective VIBRATIONAL excitations play a central role in the reaction mechanism of high-energetic ion-fullerene reactions, low-energetic fullerene-fullerene collisions and femtosecond laser-fullerene interactions. The investigations are based on the so-called nonadiabatic quantum molecular dynamics (NA-QMD) [1]. In this approach, electronic and vibrational degrees of freedom are treated simultaneously and self-consistently by combining time-dependent density functional theory in basis expansion with classical molecular dynamics. This universal theory has been successfully used, e.g., to describe conformational changes (cis-trans isomerization) in organic molecules induced by ultrashort laser pulses [2,3]. First indications on the existence of collective vibrational excitations in fullerenes has been already observed in high-energetic ion-fullerene collisions [4]. Here we will discuss the following phenomena:

## 1. Excitation of the radial symmetric breathing mode $A_g(1)$ in fs-laser pulses (fig.1)

It will be shown that in  $C_{60}$ , exposed to fs-laser pulses, the breathing mode will be excited due to multielectron excitation and subsequent electron-vibration coupling. The theoretical calculations explain consistently experimental results obtained in recent pump-probe experiments [5].

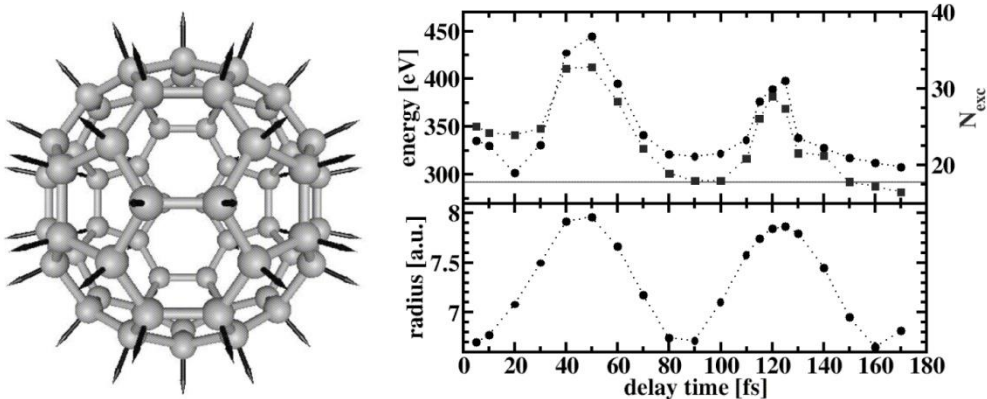


Figure 1: (Left) The breathing mode  $A_g(1)$  of  $C_{60}$ . (Right) Pump-probe setup: (top) Absorbed energy (circles) and number of excited electrons (squares) of  $C_{60}$  after excitation with pump ( $\lambda = 370$  nm,  $I = 3.3 \cdot 10^{13}$  W/cm<sup>2</sup>,  $\tau = 27$  fs) and probe pulses ( $\lambda = 800$  nm,  $I = 7.3 \cdot 10^{13}$  W/cm<sup>2</sup>,  $\tau = 27$  fs) as a function of time delay. The horizontal line indicates the absorbed energy after the pump pulse alone (292 eV). (down)  $C_{60}$  radius at the maximum of the probe pulse as a function of delay time.

## Fr-IV-1

### 2. Dominating role of collective vibrational excitations in the reaction mechanism of fullerene-fullerene collisions (fig.2)

We reanalyzed the reaction mechanism in fullerene-fullerene collisions at energies around 100 eV where fusion and inelastic scattering occur. It will be shown that the DIRECT excitation of collective vibrational modes (in particular the prolate-oblate mode  $H_g(1)$ ) represent the keypoint for the understanding of the reaction mechanism. In particular, it explains the existence and the large absolute values of fusion barriers observed in fullerene-fullerene collisions [6], which represents one of the still outstanding questions in the field. In addition, we present a one-dimensional classical trajectory model which reproduces the gross features of the 360 - dimensional microscopic NA-QMD calculations and provides a clear and transparent physical picture from the underlying reaction mechanism [7].

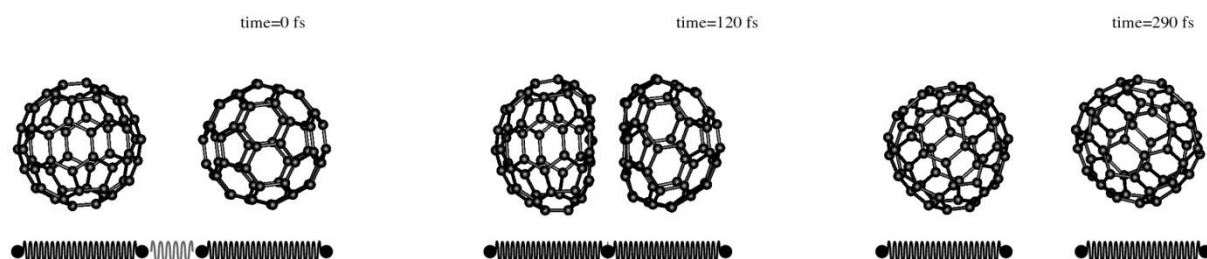


Figure 2: Snapshots of a  $C_{60}+C_{60}$  inelastic scattering event for an impact energy of 40 eV. From left to right: before collision, point of closest approach and after collision.

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## Fr-IV-2

### PHOTOABSORPTION BY VOLUME PLASMONS IN METAL CLUSTERS

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Clusters of simple metals, such as the alkalis, exhibit strong photoabsorption resonances in the visible part of the spectrum. These are collective “surface plasmon” excitations which have been extensively investigated. However, the ultraviolet part of the spectrum has remained rather unexplored up to now. A number of theoretical calculations have predicted that a measurable portion of the delocalized valence electrons’ dipole oscillator strength should be located in this region. This predicted absorption feature has been ascribed to a volume-plasmon type of excitation.

It is well known that plasmons in bulk metals cannot be excited by direct photoabsorption, that is, by coupling of volume plasmons to light. However, the selection rules in finite systems are different, and as a result the optical spectroscopy of nanoclusters can explore a greater variety of elementary excitations. Analogous effects have been explored in nuclear physics and in fullerenes.

We have carried out a measurement of the photodepletion cross sections for a pair of prototypical simple-metal nanoclusters,  $\text{Na}_{20}$  and  $\text{Na}_{92}$ , finding that these systems indeed possess a broad volume-plasmon absorption peak centered at  $\approx 4$  eV and having an oscillator strength contents of  $\approx 15$ - $20\%$  of the total, in good agreement with theoretical calculations. We will discuss this finding, together with the implications of the oscillator strength contents of the resonance peaks.

## Fr-IV-3

### GIANT DIPOLE PLASMON RESONANCE IN C<sub>60</sub> PROBED BY FAST ION COLLISIONS

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The energy and angular distributions of the double differential cross sections of low energy electrons emitted in a collision are used to explore the ionization mechanisms. Highly charged fast ions has been proved to be a useful tool, besides photons and electrons, to investigate the structural aspects and ionization-mechanisms in collisions with atoms and molecules. In case of collisions with C<sub>60</sub>-fullerene the mechanisms of electron emission are governed by even more complicated processes. The fullerenes are “small” particles with diameter  $\sim 10\text{\AA}$  over which a large electron density similar to that of a solid foil, is sampled. Fullerenes are known to exhibit collective excitation known as *Giant Dipole Plasmon Resonance* (GDPR), as observed in photo-ionization studies [1-3]. The influence of the GDPR on single or double ionization of fullerene [4-8] and on x-ray emission following electron capture from fullerene [9] under fast heavy ion impact have been reported. The earlier experimental investigations on photo-ionization of C<sub>60</sub> are predominantly carried out by detecting the photo-ions. However, plasmon excitation tend to de-excite through emission of electrons with energy characteristic of the plasmon frequency. A direct observation of this process in low energy electron double differential spectrum (induced by fast ions) is awaited. In addition, it has an additional advantage of measuring the angular distributions of these electrons. The electron energy due to the decay of GDPR-excited state is expected at  $\sim 10$  eV (i.e.  $20$  eV -  $I_p$ ,  $I_p$ =ionization potential).

We have measured the low energy (1-300 eV)  $e^-$  - DDCS from C<sub>60</sub> in collisions with 4 MeV/u bare F ions at various angles. The well collimated fully stripped ion-beams from the 14 MV BARC-TIFR Pelletron accelerator was made to interact with C<sub>60</sub> vapour obtained from an oven heated to about  $\sim 500^\circ$  C. We observe a broad hump like structure near the expected GDPR peak position in all the electron spectra. The C<sub>60</sub> DDCS spectra are also very different from the DDCS spectra of other atomic gaseous targets like Ne and He and there is marked contrast with the CDW-EIS model for carbon atom as well. We have measured the angular distribution of GDPR electrons, as well as other high energy electrons. The electrons emission (at  $\sim 10$  eV i.e. at GDPR peak) is maximum in forward and backward direction w.r.t. to the projectile beam and a dip is observed at  $90^\circ$ . This distribution is in sharp contrast to the expected behaviour for atomic targets, He and Ne, for which the maximum appears around  $75^\circ$ - $85^\circ$ . The angular distribution indicates that the dipole oscillations are induced preferably along the projectile beam direction in this energy range. The angular distributions of electrons at higher energies ( $>40$  eV), however, show similarity with the behavior observed for the He and Ne targets.

We also measured the K-LL Auger electron emission from C<sub>60</sub> and other gaseous targets under heavy ion and fast electron impact. The K-LL Auger electron emission from C<sub>60</sub> is found to be anisotropic w.r.t the beam direction showing a dip at  $90^\circ$ , whereas a purely atomic target like Ne shows an isotropic distribution. This anisotropy in K-LL auger electron emissions w.r.t. beam direction could be due to the molecular nature of the target and beam induced polarization. The angular distribution of auger electrons for various targets like Ne, CH<sub>4</sub> or N<sub>2</sub>, was seen to be isotropic under fast electron impact.

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# Posters



**ELECTRON ATTACHMENT EXPERIMENTS TO CARBON  
DIOXIDE CLUSTERS IN GAS PHASE AND HELIUM DROPLETS**

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Superfluid helium droplets evolved into a widely and extensively used technique for studying fundamental properties of atoms, molecules or clusters of molecules at low temperatures [1]. A very important property of these aggregates is, due to the loss of heat via evaporation, that the temperature of the helium system is extremely cold (approx. 0.37K). At this temperature the helium is even in the superfluid state (He II). Dopants can either move to the center of the He droplet or stay on the surface, depending on their own electronic structure. In a pickup cell gaseous atoms or molecules are crossed with the beam of He droplets and collisions introduce or attach the dopants to the droplet. If more than one dopand collides with the droplet, clusters of these can be formed. Due to the ultra-cold temperatures, the embedded particles are cooled to the vibrational groundstate. This allows the investigation of the (temperature wise unperturbated) physical properties in a very precise manner. In the present experiment the emphasis lies on the attachment of electrons to the dopants in the He clusters [2, 3]. These electrons are generated via thermal emission from a filament, are energy selected with a hemispherical energy analyzer (electron monochromator) and guided to the collision chamber with electrostatic lenses.

In the present contribution recent highlights of our electron attachment studies with  $CO_2$  molecules and clusters embedded in helium droplets will be presented. The yield of the carbon dioxide cluster anions  $(CO_2)_n^-$  is determined as a function of the electron energy for different helium droplet sizes. Compared to the free electron capture by molecules and clusters in gas phase the resonant attachment process to embedded species is strongly altered. Electrons require an energy of at least 1.15eV to enter the conduction band of He. Furthermore, at low electron energies the captured electron forms a metastable bubble inside the helium droplet which requires another few 100meV energy. Thus low energy features (vibrational Feshbach resoances [4]) observed for free molecules and clusters are shifted up by about 1.6eV. In contrast, a feature of the  $(CO_2)_4^-$  anion yield that is located at 2eV is shifted only by 1.1eV to higher energies and thus indicating that at this energy no bubble formation is happening. Finally a third feature at 3eV is completely missing in the He droplet and can be explained by the complete absence of vibrationally excited molecules in He droplets. This complete freezing of the  $CO_2$  bending mode also explains the absence of the  $CO_2^-$  anion upon electron attachment to  $CO_2$  doped He droplets. In a large range of different droplet sizes we observed no shift of the anion efficiency curves for  $CO_2$  cluster anions, however, the relative abundance of the two features exhibits a strong size dependence.

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## BORON BRIDGED MOLECULAR COMPLEXES

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The density functional theory (DFT) with B3LYP functional and 6-311+G basis set [1] has been carried out for the analysis of geometries, stabilities, and energetics of boron bridged molecular complexes. The series of  $BH_m(C_6H_5)_n$  and  $BH_mC_n(C_6H_5)_n$ , up to  $m$  and  $n=4$ , complexes have been studied in detail. Arrangements of the atoms and molecules in the various structures of selected complexes,  $C_n(C_5H_4)_n$ ,  $C_n(C_6H_5)_n$  and  $C_n(C_7H_6)_n$ , containing small boron clusters ( $B_2$ - $B_7$ ) have been investigated too. Results are compared with the previous studies [2,3].

**Acknowledgment.** This work was supported by TUBITAK (Grand No. 108T466).

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### PHASE TRANSITION AS A MECHANISM OF FULLERENE FORMATION

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Phase transition in fullerenes  $C_{60}$  and  $C_{240}$  are investigated by means of constant-temperature molecular dynamics simulations [1]. In the phase transition region, the assembly (and fragmentation) of the  $C_{60}$  cage from (and to) the gaseous state is demonstrated via the dynamical coexistence of two phases. In this critical region, the fullerene system is seen to continuously oscillate between the carbon cage (the solid phase) and the state of carbon dimers and short chains (the gas phase). These oscillations correspond to consecutive disintegration and formation of the fullerene. Furthermore, the temperature-dependent heat capacity of the fullerene features a prominent peak, signifying the finite system analogue of a first-order phase transition. The simulations were conducted for 500 ns using a topologically-constrained pairwise force field which was developed for this work. Results of the simulations were supplemented by a statistical mechanics analysis to account for entropy and pressure corrections, corresponding to experimental conditions. These corrections lead to a phase transition temperature of 3800-4200 K for pressure 10-100 kPa, in good agreement with available experimental values.

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### IONIZATION AND FRAGMENTATION OF CLUSTERED DNA BASES

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This poster reports on the development of a new experiment to investigate radiation-induced inter-molecular processes within molecular clusters as simple models for biological material. The system is based upon the application of REMPI-TOF (resonance-enhanced multi-photon ionisation – time of flight) mass spectrometry to characterise mixed beams of monomers and clusters formed by rapid expansion in an inert buffer gas. Initial experiments will probe the effects of associated water molecules on the electronic excited states of DNA bases, building upon previous experimental [1] and theoretical work [2]. On a longer timescale, the group aims to combine REMPI-TOF beam characterisation studies with electron- and ion-impact experiments in order to investigate neutral hydration effects upon the fragmentation patterns of DNA bases and other key biological building blocks.

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## LASER-INDUCED DISSOCIATION OF STORED DYE IONS PRODUCED BY LASER DESORPTION

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Matrix-assisted laser desorption ionization (MALDI) is widely employed in producing organic molecular ions and biomolecular ions for mass analyses. Recently, this method is also applied to spectroscopy and collision experiments of the molecular ions.

In the present study, we carried out spectroscopic studies of methylene blue cations (hereafter MB<sup>+</sup>, the molecular structure is shown in fig. 1.) with an electrostatic ion storage ring [1]. The MB<sup>+</sup> formed by the MALDI method with a nitrogen laser were stored in the ring and irradiated by a pulsed tunable laser, leading to evaporation of neutral species from the cations. Based on the assumption that the reaction yield only depends on photo-absorption cross sections of the cations, the plot of the neutral yield against the excitation wavelength corresponds to the absorption spectrum. A preliminary excitation spectrum is shown in fig. 2, together with the absorption spectrum of the MB<sup>+</sup> in water [2]. Although the data points are rather sparse, the absorption band of the cations in gas phase is clearly observed in the same wavelength region for solution, indicating that the MALDI process does not seriously damage the structure shown in fig. 1. The relatively large blue shift of the peak position is consistent with the theoretical prediction [3].

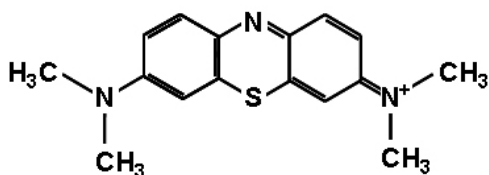


Figure 1. Molecular structure of MB<sup>+</sup> in solution.

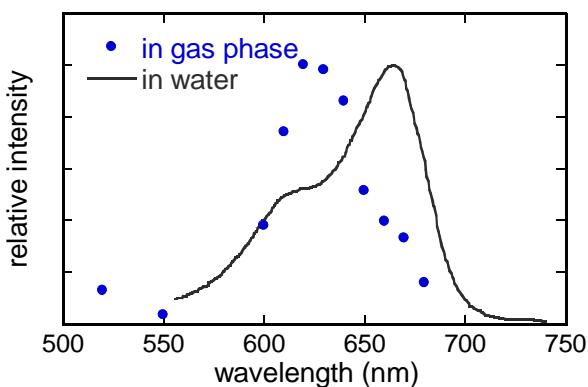


Figure 2. (Circle) The excitation spectrum of MB<sup>+</sup> in gas phase obtained in the present study. (Line) The absorption spectrum of the cations in water [2]. The hump at 610 nm is due to the dimer coexisting in the solution.

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**COLLISIONAL AND RADIATIVE PROCESSES INVOLVING  
STRONGLY POLARIZABLE CLUSTER TARGETS**

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Specific role played by various plasmon excitations in collisional and radiative processes involving strongly polarizable targets will be discussed in this talk. The emphasis is made on the photoionization and electron scattering from metal clusters and fullerenes.

In support of the results of recent experiments [1], we demonstrate that the angular distribution of photoelectrons from a strongly polarizable target exposed to a laser field can deviate noticeably from the prediction of conventional theory. Even within the dipole-photon approximation the profile of distribution is modified due to the action of the field of alternating dipole moment induced at the residue by the laser field:

$$I + \beta(\omega) P_2(\cos \theta) \rightarrow I + a_2(\omega) P_2(\cos \theta) + a_4(\omega) P_4(\cos \theta), \quad (1)$$

where the coefficients  $a_2(\omega)$  and  $a_4(\omega)$ , being quite sensitive to the dynamic polarizability of the residue and to its geometry, depends also on the intensity and frequency of the laser field. Numerical results, presented for sodium cluster anions [2], demonstrate that dramatic changes to the profile occur for the photon energies in vicinities of the Plasmon resonances, where the effect is enhanced due to the increase in the residue polarizability. Strong modifications of the characteristics of a single-photon ionization process can be achieved by applying laser fields of comparatively low intensities  $I_0 \sim 10^{10} - 10^{11} \text{ W/cm}^2$ .

The processes of elastic and inelastic electron scattering from clusters and fullerenes are also strongly dependent on the dynamic response of the target. However, in contrast to the photoionization, which is governed solely by the contribution of a dipole surface plasmon, the collisional processes allow for the multipolar surface and volume plasmon excitations. In our work we elucidate the role of plasmon excitations in the formation of electron energy loss spectra as well as in the total inelastic scattering cross section. Special attention is paid to the interplay of various plasmon modes and to their manifestation in the profile of the cross section.

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PLATINUM CLUSTERS COLLISIONS WITH SINGLE WALL CARBON NANOTUBES

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The carbon nanotubes are usually assumed as perfect species in most of the studies. In practice, even high-quality Single-Wall Carbon Nano Tubes (SWCNTs) contain on average one structural defect per 4  $\mu\text{m}$  [1].

In the present study we compare the perfect (10,0) and (20,0) and defective SWCNTs in collisions with platinum clusters  $\text{Pt}_n$ ,  $n = 2, 9, 13$  of various kinetic energies (50 - 100 eV/atom) in order to understand the melting and disintegration of small clusters and, also, the hardness of the SWCNT when imposed upon heavy ion irradiation. Platinum clusters (cationic and anionic) containing up to 24 Pt atoms can be formed by laser vaporization [2] and ion irradiation of SWCNT is feasible in the modern experiments [3]. Thus, computations can be compared with experimental data once available.

Molecular dynamics simulations with a mixture of empirical and semi-empirical potentials [4] have been performed to study the result of collisions of Pt clusters with perfect and defective single-walled carbon nanotubes with open ends. Carbon-carbon interactions in the nanotube have been modeled with a semi-empirical potential due to Brenner [5]:

$$E_{CNT} = \sum_i \sum_{j < i} [V^R(r_{ij}) - \bar{B}_{ij} V^A(r_{ij})] \quad (1)$$

Carbon-platinum interactions have been described with the 12-6 Lennard-Jones potential:

$$E_{C-Pt}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (2)$$

with  $\sigma = 2.905 \text{ \AA}$  and  $\epsilon = 256\text{K}$ .

Metallic bonding in the Pt cluster was computed with the n-m Sutton-Chen potential [6] that implemented the basic model of Finnis and Sinclair [7]. For the platinum clusters  $n=10 / m=8$ :

$$E_{Pt_N} = \epsilon \sum_i \left[ \frac{1}{2} \sum_{j \neq i} \left( \frac{a}{r_{ij}} \right)^{10} - c \sqrt{\rho_i} \right] \quad (3)$$

$$\rho_i = \sum_{i \neq j} \left( \frac{a}{r_{ij}} \right)^8$$

$\rho_i$  is the local density;  $\epsilon = 11605\text{K}$ ,  $a = 3.9242 \text{ \AA}$  and  $c = 34.408$ .

For the case of initially perfect SWCNTs when  $\text{Pt}_9$  clusters hit the tubes perpendicular to their axis, the following results have been obtained. Depending on the tube length (400 C atoms or

## PS-07

3000 C atoms), SWCNT diameter, fixed or free SWCNT ends we observe: (a) short CNTs with fixed ends reflect the clusters; (b) both short and long CNTs generate shock waves and twist in collisions if the ends are free; (c) energetic clusters (above 70 eV/atom) penetrate the tubes (for both lengths and diameters) producing holes on the front and rear surfaces of the tube and disintegrate into two or more fragments; (d) medium energy clusters produce holes in the front surface and being captured inside the tube.

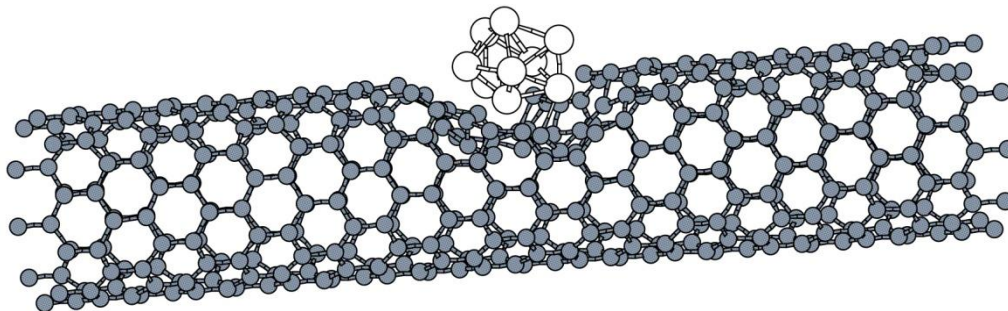


Figure 1: Collision of a Pt<sub>9</sub> with a (10,0) SWCNT with fixed ends - the cluster is reflected.

The dimers, Pt<sub>2</sub>, are extremely robust, however it is very difficult experimentally to conduct an experiment with them.

The most amazing result is the shock wave transmission along the tubes when hit with energetic clusters. Research on collisions of graphene with metallic clusters will be reported soon.

**Acknowledgments** The computations have been performed on the PhysOn cluster funded by the National Science Fund under the contract No. WU F05/06. and the contract DO02-136/08.

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**IMPORTANCE OF POLARIZATION POTENTIAL AND PCI IN THE ( e, 2e) PROCESSES ON ALKALI AND ALKALI EARTH TARGETS AT LOW ENERGIES**

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The study of electron impact ionization of atoms and molecules has been of interest, since the early days of atomic and molecular physics, since the kinematics of this process are easily controlled, and the electrons or ions resulting from the reaction can be observed with relative ease. The electron impact ionization of atoms is a three body problem governed by the Coulomb force acting between incident electron, target electron and residual ion. Fundamentally an (e, 2e) process is one where an electron of well defined energy and momentum is incident on a target, ionizes it and the outgoing electrons are detected in coincidence with their energies and angles resolved. Ionization is a technique which is used as a tool to probe target wave functions. Study of ionization process in different geometrical arrangements offers a help to understand the reaction mechanism better. Through the careful choice of geometrical arrangement and the energies of incoming and exiting electrons one can predict the physics which will dominate the shape and magnitude of the triple differential cross section. The calculation of triple differential cross section opens up a whole new area of theoretical study and offers a direct insight into the subtleties of spin-dependence and other purely relativistic effects etc. Since the first coincident measurement of (e, 2e) process on atoms by Erhardt et al[1] and Amaldi et al [2] extensive theoretical and experimental investigations have been done to measure the TDCS.

There has been recent interest to study (e, 2e) processes on alkali and alkali earth atoms initiated by measurements of Murray [3]. Recently U Hitawala et al [4], Srivastava et al. [5] and Bray et al. [6] have reported the results of (e, 2e) triple differential cross sections for alkali atom Na and K. We present in this communication the results of our distorted wave Born approximation (DWBA) calculations of TDCS for the ionization of alkali atoms Na and K and alkali earth atoms Mg and Ca. We also include correlation-polarization potential in DWBA formalism as a function of density function. We discuss the salient features of our DWBA results which are different from the results of earlier workers. We will also discuss the effects of incident electron energy, distortion, nuclear charge, correlation-polarization, post collision interaction etc. on the trend of TDCS for alkali and alkali earth targets.

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## ELECTRON ATTACHMENT TO TRINITROTOLUOENE EMBEDDED IN HELIUM DROPLETS

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Helium nano-droplets provide a powerful experimental tool to investigate molecules, molecular complexes and molecular clusters. Atoms and molecules that collide with a droplet are picked up, cooled down and transferred in most cases to its center. The temperature inside the He droplet is 0.37K, at which the droplet is superfluid [1]. Negative ion formation in doped He droplets via electron attachment is studied in our group. Small molecules such as  $SF_6$  or  $CCl_4$  were used as dopants as well as biomolecules like thymine or adenine and explosives like dinitrobenzene or trinitrotoluene (TNT) [2,3]. TNT is a prototype explosive known since more than hundred years and its essential characteristic is the presence of the elements *H*, *N*, *C* and *O* within the molecule. The rate of chemical reactions is strongly dependent on the temperature and a second important aspect, which can affect the rate and the nature of the intrinsic reaction, is solvation.

Electron attachment to TNT embedded in Helium droplets generates the non-decomposed complexes  $(TNT)_n^-$ , but no fragment ions in the entire energy range 0-12 eV. This strongly contrasts the behaviour of single TNT molecules in the gas phase at ambient temperatures, where electron capture leads to a variety of different fragmentation products via different dissociative electron attachment (DEA) reactions. Single TNT molecules decompose already by attachment of an electron at virtually no extra energy reflecting the explosive nature of the compound. The complete freezing of dissociation intermediates in TNT embedded in the droplet is explained by the particular mechanisms of DEA in nitro-aromatic compounds which is characterised by complex rearrangement processes in the transitory negative ion (TNI) prior to decomposition. Due to this rearrangement process the dissociation process is slowed down and sometimes extended to the metastable ( $\mu$ s) time scale. Such metastable decay reactions of negative TNT ions in gas phase can be seen in our measurements. These DEA mechanisms provide the condition for effective energy withdrawal from the TNI into the dissipative environment thereby completely suppressing its decomposition [4].

## PS-09

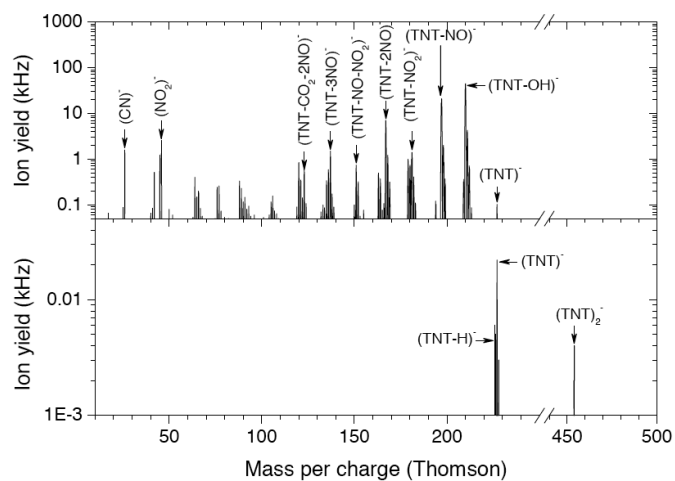


Figure 1: Negative ion mass spectrum from gas phase TNT (upper panel) and TNT embedded in He droplets (lower panel). Both spectra are recorded at the lowest possible electron energy (near zero eV for the gas phase and about 1.6eV for doped He droplets).

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# IRRADIATION OF CLUSTERS AND MOLECULES IN CONTACT WITH AN ENVIRONMENT

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We present a hierarchical approach for the description of the dynamics of clusters or molecules in contact with an environment. Typical applications of this formalism concern the deposit of metal clusters on inert surfaces, the response of an embedded cluster to an intense short laser pulse or the irradiation by ions of molecules of biological interest.

We treat the cluster/molecule by means of explicit time dependent Density Functional Theory (DFT) for the electrons, classical molecular dynamics for the cluster's ions and we use a classical treatment of matrix/environment constituents (including an account of dynamical polarizabilities of the constituents of the environment). Such an approach bears some similarities with standard QM/MM (Quantum Mechanics/Molecular Mechanics) methods of quantum chemistry used in the context of biological systems, but now with an explicit time dependent account of the polarizabilities of the constituents of the environment, which is a crucial aspect in truly dynamical scenarios.

We apply this modelling to gentle situations (soft deposition, photoelectron spectroscopy, photoelectron angular distributions of deposited clusters) and to more violent scenarios (hindered Coulomb explosion of embedded clusters) following both electronic, ionic (cluster) and atomic degrees of freedom explicitly. We also consider the case of the irradiation of small organic molecules to a bypassing ion.

The deposition cases show the influence of net charges in the capability of the cluster to strongly attach to the surface. We discuss the possibility to observe, as a dynamical process, the sticking or the inclusion of single Na in Ar substrate. Effects of Na charge, initial kinetic energy given to the Na and size of the Ar substrate are explored. We show that neutral Na sticks or is reflected on the Ar surface, while Na<sup>+</sup> always penetrates the Ar substrate. The impact of surface on photoelectron spectra is also discussed especially in the case of Na deposited on MgO.

The case of short and intense laser excitation of embedded clusters allows to explore various (possibly violent) dynamical scenarios. We discuss microscopic mechanisms of laser induced dynamics, taking as test case Na<sub>8</sub>@Ar<sub>434</sub>. We analyze both electronic, ionic (cluster ions) and atomic (matrix atoms, matrix polarizability) dynamics and show how the matrix accommodates the, initially electronic, excitation of the embedded metal cluster which acts under such conditions as a chromophore. We discuss the results in relation to recent experiments dedicated to shaping of embedded metal clusters.

Both situations (gentle deposition, violent irradiation) show the crucial importance of a proper inclusion of electronic degrees of freedom of the surface/matrix in this demanding domain of embedded/deposited clusters. To the best of our knowledge, such a modelling including a non adiabatic treatment of cluster electrons, coupled to electronic excitations of the surface/matrix, is the first theoretical attempt to account for such intricate irradiation scenarios in the non linear domain.



## PS-10

The extension of the above described formalism to the case of irradiated organic molecules reveals intriguing difficulties on the time dependent treatment of the self interaction corrections to be included in the DFT approach. This is compulsory to attain acceptable ionization potentials and thus develop a proper access to low energy irradiation phenomena. We propose a method to overcome such difficulties. Examples of applications are presented on small model molecules.

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## FRAGMENTATION OF THIN WIRES UNDER HIGH VOLTAGE PULSES AND BIPOLAR FUSION

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In the proposed paper we will present an alternative explanation of the phenomenon of wire fragmentation under high voltage pulses based on classical electromagnetism.

For this phenomenon several explanations have been proposed (see [1,2,3,4,5]) that to our opinion are inadequate.

As it will be shown by the proposed analysis the high transient currents produced by these high voltage pulses can form transient steady waves on the wires, acting as transient antennas, the basic harmonic of which is creating excess bipolar Coulombic forces between its opposite pulsating parts.

We also explain how this phenomenon can be utilized as a primitive example of low energy-high power disruptive phenomena that can affect even nuclear matter. The produced fusion effects have already been experimentally realized by many researchers see [6,7,8,9] however due to lack of proper explanation of the origin of the high forces they could not be used for fusion applications of practical importance.

We strongly believe that the proper electromagnetic explanation of these phenomena due to high bipolar forces arising by the transient steady currents on the wire under extreme voltage pulses can lead to fine tuning of proper electromagnetic devices that could use this type of “bipolar fusion” in energy and thrust applications of major importance.

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## PS-12

# MICROMAGNETIC INSIGHT INTO A MAGNETORECEPTOR IN BIRDS: ON THE EXISTENCE OF MAGNETIC FIELD AMPLIFIERS IN THE BEAK

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The Earth's magnetic field provides an important source of directional information for many living organisms, especially birds, but the sensory receptor responsible for magnetic field detection still has to be identified. Recently, magnetic iron oxide particles were detected in dendritic endings of the ophthalmic nerves in the skin of the upper beak of homing pigeons, and were shown to fulfill the special prerequisites of a biological receptor. Here we study the proposed receptor theoretically and formulate the criteria for which it becomes operational and can be used for registering the weak magnetic fields as, e.g. the geomagnetic field, by a bird.

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