

International Conference
"Dynamics of Systems on the Nanoscale"

DySoN Conference 2012

Courtyard by Marriott Vasilievsky Hotel,
Saint Petersburg, Russia
September 30 – October 4, 2012



DYSON
2012

Book of Abstracts

Editor: Andrey V. Solov'yov

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Preface

The Second International Conference "Dynamics of Systems on the Nanoscale" (DySoN 2012) will take place in Saint Petersburg, Russia during September 30 – October 4, 2012. The venue will be the Courtyard by Marriott St. Petersburg Vasilievsky Hotel, 2nd line of Vasilievsky Island 61/30A, 199178. The conference is organized by the Frankfurt Institute for Advanced Studies – Goethe University, A.F. Ioffe Physical-Technical Institute and Saint Petersburg State Polytechnic University.

This DySoN conference has been built upon a series of International Symposia "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" (ISACC 2003, ISACC 2007, ISACC 2008, ISACC 2009). During these meetings it has become clear that there is a need for an interdisciplinary conference covering a broader range of topics than just atomic cluster collisions, related to the Dynamics of Systems on a Nanoscale. Therefore, in 2010 it was decided to launch a new conference series under the title "Dynamics of Systems on the Nanoscale". The first DySoN conference took place in National Research Council, Rome, Italy in 2010. The DySoN 2012 is the second conference in this series.

The DySoN 2012 Conference will promote the growth and exchange of scientific information on the structure formation and dynamics of animate and inanimate matter on the nanometer scale. There are many examples of complex many-body systems of micro- and nanometer scale size exhibiting unique features, properties and functions. These systems may have very different nature and origin, e.g. atomic and molecular clusters, nanoobjects, ensembles of nanoparticles, nanostructures, biomolecules, biomolecular and mesoscopic systems. A detailed understanding of the structure and dynamics of these systems on the nanometer scale is a difficult and fundamental task, the solution of which is necessary in numerous applications of nano- and biotechnology, material science and medicine.

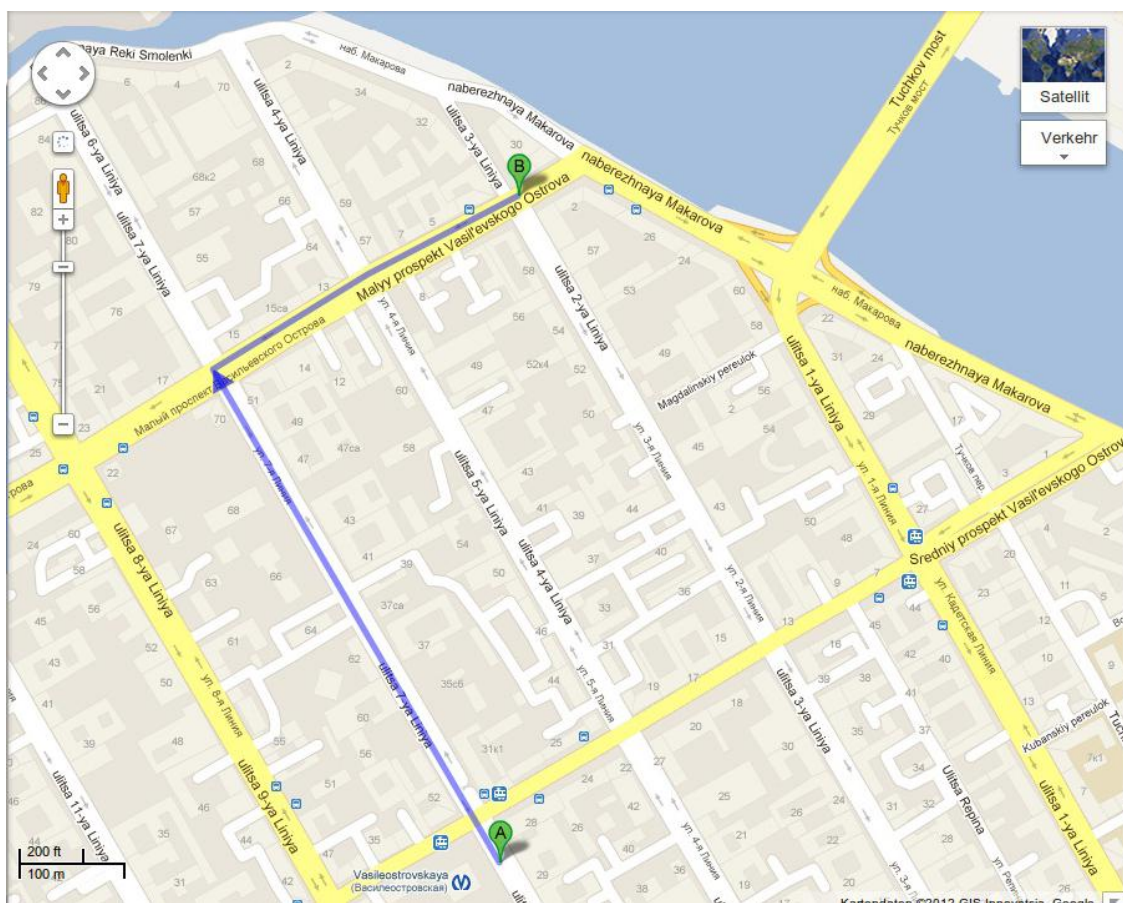
Although mesoscopic, nano- and biomolecular systems differ in their nature and origin, a number of fundamental problems are common to all of them: What are the underlying principles of self-organization and self-assembly of matter on the micro- and nanoscale? Are these principles classical or quantum? How does function emerge on the nano- and the mesoscale in systems of different origin? What criteria govern the stability of these systems? How do their properties change as a function of size and composition? How are their properties altered by their environment? Seeking answers to these questions is at the core of a new interdisciplinary field that lies at the intersection of physics, chemistry and biology, a field now called Meso-Bio-Nano (MBN) Science.

Experimental and theoretical aspects of these problems will be discussed at the DySoN 2012 Conference. Particular attention will be devoted to dynamical phenomena and many-body effects taking place in various MBN systems, which include problems of structure formation, fusion and fission, collision and fragmentation, collective electron excitations, reactivity, nanoscale phase transitions, nanoscale insights into biodamage, channeling phenomena and many more. The hope is that all participants will be enriched and further motivated by the session topics and the ensuing general discussions. Have a memorable Meeting!

Conference Venue

The Conference will be hosted by Courtyard by Marriott St. Petersburg Vasilievsky Hotel, 2nd line of Vasilievsky Island 61/30A, St. Petersburg, Russia 199178.

The photo (right) shows the main building of the hotel. The map below shows the route from “Vasileovstrovskaya” (A), the nearest metro station, to the conference site (B). The walking distance is about 1 km.



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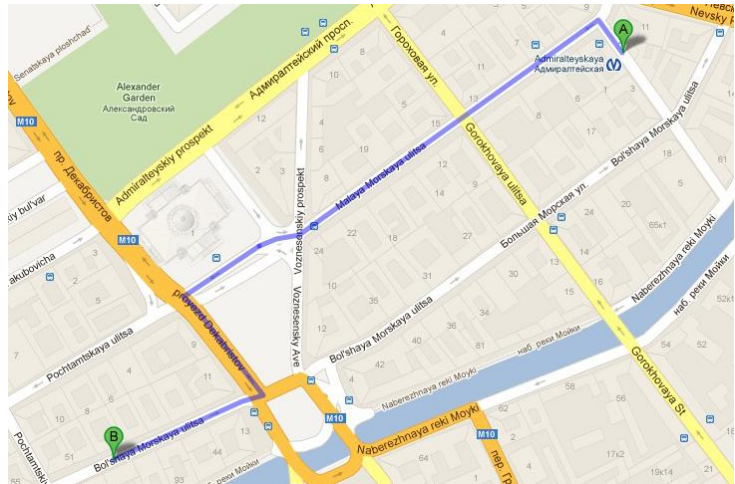
Conference Reception

The conference reception will be take place at the hotel, 30 September, 2012, 18.00 - 21.00

Conference Dinner

The Conference Dinner will take place in the Restaurant Polovtsev Mansion (Bolshaya Morskaya st. 52).

The map shows the route from Admiralteyskaya, the nearest metro station, to the venue.



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Conference Tour

On October, 4 there will be a bus excursion to the famous suburb of Saint Petersburg, the summer residence of Russian tzars, the town “Pushkin” (also known as Tsarskoe selo). There you will have the opportunity to visit the Catherine the Great Palace - a splendid example of the Russian Baroque, and see the well-known Amber room, to enjoy the parks during the beautiful time of golden autumn. More information about Pushkin can be found via the following link: <http://eng.tzar.ru/>.



The tour will start at 9.30 from the conference hotel and end at 16.00.

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DySoN Conference web page

Updated information on the conference is available at the following Internet address:
<http://fias.uni-frankfurt.de/dyson>

Conference e-mail

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

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A.F. Ioffe Physical-Technical Institute, St. Petersburg, Russia

European Commission

We also acknowledge assistance from Mr. Alexey Verkhovtsev and Dr. Alexander Yakubovich for their help in preparation of the book of abstracts.

Conference Program

Sunday, 30 September 2012

16 ⁰⁰ – 18 ⁰⁰	Participants registration
18 ⁰⁰ – 21 ⁰⁰	Conference reception

Monday, 1 October 2012

9 ⁰⁰ – 9 ³⁰	<p>DySoN 2012 Opening Andrey V. Solov'yov, Frankfurt Institute for Advanced Studies, Germany <i>Dynamics of systems on the nanoscale: challenges for theory and experiment</i></p>
9 ³⁰ – 11 ⁰⁰	<p><u><i>Morning session I: Structure and dynamics of clusters, nanoparticles and biomolecules</i></u> Chair: Jean-Patrick Connerade, Imperial College, UK Julius Jellinek, Argonne National Laboratory, USA <i>Novel analysis of dynamics at the nanoscale</i> Philippe Bréchnac, Université Paris Sud, Orsay, France <i>New investigations of coronene clusters</i> Eric Suraud, Université Paul Sabatier, France <i>On electronic emission from irradiated clusters and nano structures</i></p>
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<p><u><i>Morning session II: Nanoscale dynamical transitions and transformations</i></u> Chair: Julius Jellinek, Argonne National Laboratory, USA Shiv N. Khanna, Virginia Commonwealth University, USA <i>Spin accommodation and geometric effects in catalysis: breaking polar covalent bonds via complementary active sites</i> Jerry Bernholc, North Carolina State University, USA <i>Structural transformations in ferroelectric polymers and metal-protein complexes</i> Andrey Lyalin, Hokkaido University, Japan <i>Role of the active and inert supports in enhanced catalytic activity of gold clusters</i></p>
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<p><u><i>Afternoon Session I: Nanoscale insights in biodamage</i></u> Chair: Bernd Huber, CEA-CIMAP, France Ilia I. Fabrikant, University of Nebraska-Lincoln, USA</p>

	<p><i>Electron attachment to molecules in a cluster environment</i> Pablo de Vera, Universitat d'Alacant, Spain <i>Ionization of biomolecular targets by ion impact: Input data for radiobiological applications</i></p> <p>Oral presentation of posters, 10 min each: Presentation 1 Presentation 2 Presentation 3</p>
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	<p><u><i>Afternoon Session II: Clustering and self-organization on the nanoscale</i></u> Chair: Catherine Bréchnac, CNRS, France</p> <p>Kit Bowen, Johns Hopkins University, Baltimore, USA <i>(PbS)₃₂: a baby crystal</i></p> <p>Michael Wilkinson, The Open University, Milton Keynes, UK <i>Ostwald ripening and a test-tube model for rainfall</i></p> <p>Sergiy Perepelytsya, Bogolyubov Institut for Theoretical Physics, Ukraine <i>Dynamic ordering of ions around DNA helix</i></p>

Tuesday, 2 October 2012

9 ³⁰ – 11 ⁰⁰	<p><u><i>Morning session I: Collision processes involving nanosystems</i></u> Chair: Eric Suraud, Universite Paul Sabatier, France</p> <p>Bernd Huber, CEA-CIMAP, France <i>Ion-induced chemical reactions in finite size systems</i></p> <p>Rafael Garcia Molina, Universidad de Murcia, Spain <i>Interaction of proton beams with carbon nanotubes</i></p> <p>Bing Zhang, Wuhan Institute of Physics and Mathematics, China <i>Non-adiabatic dynamics in polyatomic molecules by femtosecond photoelectron imaging</i></p>
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<p><u><i>Morning session II: Thermo-mechanical, optical and magnetic properties of nanosystems</i></u> Chair: Shiv N. Khanna, Virginia Commonwealth University, USA</p> <p>Florent Calvo, Université de Lyon 1, France <i>Assessing quantum thermal baths for finite systems</i></p> <p>Alexander Yakubovich, Frankfurt Institute for Advanced Studies, Germany <i>Diffusion and nanoindentation processes in titanium and nickel materials</i></p> <p>Mikhail Petrzhhik, National University of Science and Technology “MISIS”, Moscow, Russia</p>

	<i>Dynamics of martensitic structure at TiNb-based quenched alloys under heating and loading</i>
13 ⁰⁰ – 13 ¹⁵	Conference photo
13 ¹⁵ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<p><u>Afternoon session I: Clustering and self-organization on the nanoscale</u> Chair: Kit Bowen, Johns Hopkins University, Baltimore, USA</p> <p>Catherine Bréchnac, CNRS, France <i>Atmospheric degradation of silver nanofractal by trace amount of chlorine</i></p> <p>Artur Böttcher, Karlsruhe Institute of Technology, Germany <i>Supported mass-selected carbon clusters: thermally and chemically driven surface modifications</i></p> <p>Ilya A. Solov'yov, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, USA <i>Dynamics of nanofractal formation and fragmentation</i></p>
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ¹⁰	<p>Oral presentation of posters, 10 min each Chair: Gustavo Garcia, Instituto de Fisica Fundamental, Spain</p> <p>Presentation 4 Presentation 5 Presentation 6 Presentation 7 Presentation 8 Presentation 9 Presentation 10</p> <p>Open Discussion, 30 min Interdisciplinary DySoN conference: current status and perspectives</p>

Wednesday, 3 October 2012

9 ³⁰ – 11 ⁰⁰	<p><u>Morning session I: Nanoscale insights in biodamage</u> Chair: Rafael Garcia Molina, Universidad de Murcia, Spain</p> <p>Eugene Surdutovich, Oakland University, USA <i>Multiscale physics of ion induced radiation damage</i></p> <p>Sandrine Lacombe, Universite Paris Sud, Orsay, France <i>Lanthanide nanoparticles: toward theranostic in hadrontherapy</i></p> <p>Gustavo Garcia, Instituto de Fisica Fundamental, Spain <i>Electron and positron scattering with nanostructures (atomic clusters and macromolecules)</i></p>
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11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<p><u><i>Morning session II: Collision processes involving nanosystems</i></u> Chair: Andrei Korol, Frankfurt Institute for Advanced Studies, Germany</p> <p>Vadim Ivanov, St. Petersburg State Polytechnic University, Russia <i>Photoionization of clusters and fullerenes</i></p> <p>Alexey Verkhovtsev, Frankfurt Institute for Advanced Studies, Germany <i>Study of collective electron excitations in fullerenes</i></p> <p>Andrej Grubisic, JILA, University of Colorado, Boulder, USA <i>Coherent multiphoton photoelectron emission from individual, supported metallic nanoparticles</i></p>
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16 ³⁰ – 17 ³⁰	<p><u><i>Afternoon session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i></u> Chair: Andrey V. Solov'yov, Frankfurt Institute for Advanced Studies, Germany</p> <p>Yurii Lozovik, Institute of Spectroscopy, Russia <i>Mesoscopic supersolid of dipole clusters</i></p> <p>Jean-Patrick Connerade, Imperial College, UK <i>From Pauli's birthday to confinement resonances - a potted history of quantum confinement</i></p>
17 ³⁰ – 18 ⁰⁰	<p>Open Discussion Interdisciplinary DySoN conference: current status and perspectives</p> <p>Conference Closing</p>
19 ⁰⁰ - 22 ³⁰	Conference Dinner

Thursday, 4 October 2012

9 ³⁰ – 15 ³⁰	Conference Tour
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Talks

Opening

DYNAMICS OF SYSTEMS ON THE NANOSCALE: CHALLENGES FOR THEORY AND EXPERIMENT

Andrey V. Solov'yov

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There are many complex molecular systems exhibiting rather unique features, properties and functions. These systems may have very different nature and origin. The concrete examples include atomic and molecular clusters, nanoobjects (fullerenes, endohedrals, nanotubes) and nanostructures, biomacromolecules. A detailed understanding of the structure and dynamics of these systems is a difficult and fundamental task, the solution of which is needed in numerous applications in nano- and biotechnology, material science and medicine.

Independently of the nature of the molecular systems (biological or none), their size is typically on the nanometer scale. This creates rather close and fruitful interdisciplinary interconnection of nano- and biomolecular research with a strong mutual feedback. Apart from structural characterization, there are many interesting dynamical phenomena involving Meso-Bio-Nano molecular systems. In general, this interdisciplinary field of research studying structure-formation and dynamics of animate and inanimate macromolecular matter on the molecular level and all the related phenomena, called Meso-Bio-Nano science, bundles up several traditional disciplines under a common theme.

The range of concrete scientific foci in this field is rather broad. They may include: structure and dynamics of clusters, nanoparticles and biomolecules; clustering, self-organization, growth and structure-formation processes, their multiscale nature and the scaling laws; cluster and biomolecular ensembles, hybrid bio-nano systems, nanostructured materials; surface phenomena; nanoscale phase transitions; protein folding; thermal, optical and magnetic properties; collective phenomena; electron/spin transport and molecular electronics; nuclear magnetic resonance; collision, fusion, fission and fragmentation processes; radiation phenomena and radiobiological effects; important applications, e.g. ion-beam cancer therapy, radiosensitization by metal nanoparticles; novel light sources, like crystalline undulators and crystalline undulator based lasers.

In this introductory talk I would like to highlight several important theoretical and experimental challenges and recent achievements of this highly interdisciplinary field of research. Their choice is linked tightly to the topics that will be presented and discussed at the DySoN 2012 Conference..

Mo-I-1

NOVEL ANALYSIS OF DYNAMICS AT THE NANOSCALE

Julius Jellinek and Darya Aleinikava

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An analysis of the relationship between dynamics and statistical mechanics of finite systems based on densities of states will be presented. A new, general and robust methodology for computation of anharmonic densities of states applicable to any degree of anharmonicity will be formulated. This density of states is computed from data accumulated in the course of molecular dynamics simulations. The utility of the new methodology will be illustrated in applications to atomic clusters.

NEW INVESTIGATIONS OF CORONENE CLUSTERS

Ph. Bréchnignac¹, C. Falvo¹, P. Parneix¹, T. Pino¹, O. Pirali¹, C. Joblin², D. Kokkin², A. Bonnamy²
M. Rapacioli³, F. Spiegelman³, L. Dontot³, A. Gamboa³, G. Garcia⁴, L. Nahon⁴

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The presence of polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM) was suggested in the mid-80s. Since then, their ubiquity and their important role in the physico-chemical evolution of the ISM have been confirmed through many observational studies of the "Aromatic Infrared Bands" (AIB). Interstellar PAHs have also been proposed as possible carriers of some Diffuse Interstellar Bands (DIBs). These absorption bands, seen in the spectra of reddened stars from the visible to the near infrared, constitute a major astrophysical issue.

In recent years, high spatial resolution observations in the AIBs range have been conducted in specific regions like reflection nebulae. Some of them suggest the possible presence of PAH clusters in the transition region of the PhotoDissociation Regions [1]. Since very little information is presently available on the physical and chemical properties of these clusters [2,3], it is calling for new systematic experimental and theoretical studies directed towards validation of their presence in interstellar environments and to constrain their survival therein. It is one of the goals of the collaborative project GASPARIM [4].

We will report about new experiments conducted at the SOLEIL synchrotron facility, using the molecular beam chamber SAPHIRS and the photoelectron-photoion coincidence (PEPICO) spectrometer DELICIOUS II [5] on the VUV beam line DESIRS. Neutral cold coronene clusters were generated by supersonic co-expansion in He/Ar out of an oven which can be heated up to 500°C. The skimmed resulting molecular beam crossed the monochromatized VUV light beam within the plates of a double Time-Of-Flight arrangement with imaging capabilities for photoelectrons. By tuning the VUV wavelength and by using the imaging capabilities of the DELICIOUS II spectrometer, this set-up provides a unique way to explore the properties of the clusters as a function of their size. Total (or with partial electron energy selection) photoion yield curves have been measured. They exhibit a series of autoionizing states in the case of the monomer and the dimer, for which the total final states of the cations can be retrieved. Ionization thresholds, vibrational and electronic structures of both the neutral and the cationic clusters can be derived from TPEPICO data analysis. These experimental data will be discussed in relation to theoretical predictions [6].

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ON ELECTRONIC EMISSION FROM IRRADIATED CLUSTERS AND NANO STRUCTURES

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We discuss the non adiabatic dynamical response to laser irradiation of clusters [1] and small organic molecules, possibly in contact with an environment (insulating substrate or matrix). The electronic degrees of freedom are treated at a microscopic quantum level through Density Functional Theory (DFT) in the time domain [2]. A proper account of electronic emission requires some dedicated treatment, especially when ionization is to be explicitly followed in time. We have thus included elaborate theoretical methods to treat the well known hindrance constituted by the Self Interaction Problem in the simple and robust Local Density Approximation of DFT [3,4]. The description of electrons is complemented by a classical Molecular Dynamics treatment of ions. Environment is, when necessary, included via a dynamical hierarchical modelling in the spirit of Quantum Mechanical/Molecular Mechanical approaches of quantum chemistry [5,6,7,8].

A major focus of these studies concerns the properties of ionized electrons. We discuss in particular photoelectron spectra (PES) and photoelectron angular distributions (PAD) in relation to recent experimental results. Experimental results provide here a challenging environment for theoretical modelling. But such observables are easily attainable within the formalism we have developed and calculations lead to encouraging results.

We also consider the impact of variations of laser frequencies, especially when exploring the newly and widely opening domain of FEL frequencies. We show that the use of such frequencies at moderate laser intensities might also constitute a key tool of analysis of cluster properties, in complement to studies performed in the visible. The complementing case of organic molecules is also considered in this respect.

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Mo-II-1

SPIN ACCOMMODATION AND GEOMETRIC EFFECTS IN CATALYSIS: BREAKING POLAR COVALENT BONDS VIA COMPLEMENTARY ACTIVE SITES

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Due to quantum confinement, the electronic states in metal clusters can be grouped into electronic shells, similar to the electronic shells in atoms. This shell structure leads to variable reactivity of clusters with reagents like O₂. For example, silver cluster anions [Ag_n]⁻ have recently been found to exhibit variable reactivity with oxygen in even electron systems but rapid etching in odd electron systems. The experimental studies also find an unusual magic cluster, namely, [Ag₁₃]⁻ that exhibits unique stability against reactivity with oxygen. Similar behavior has also been observed in the reactivity of Al_n⁻ clusters. Here, while bulk aluminum readily oxidizes in the presence of oxygen, an Al₁₃⁻ cluster is found to be relatively inert. I will demonstrate that these reactivity patterns are related to the spin accommodation. This behavior is rooted in the fact that the ground state of O₂ is a spin triplet, the breaking of the O-O bond requires the filling of the minority lowest unoccupied molecular orbital's (LUMO's) in ³O₂ and the process can be thought of as a spin multiplicity 3 → 1 excitation of the oxygen half of the complex. I will show that the reactivity of clusters is then correlated with the spin excitation energy of the clusters to accommodate the spin excitation. Clusters with filled electronic shells and the large separation between filled and unoccupied shells require large energy for undergoing a spin excitation and exhibit reduced reactivity. I will further show how clusters like [Ag₁₃]⁻ acquire large spin excitation energy via a shell closure at 14 electrons that arises due to a crystal-field like splitting of the 1D-orbitals due to deformation of the cluster atomic structure.

While the electronic shells control the reactivity with O₂, reactivity with molecules having polar covalent bonds exhibits different patterns involving the geometry. For example, experiments on the reactivity of aluminum cluster anions with water show (1) that some clusters with open electronic shells such as Al₂₀⁻ do not reveal any significant reactivity with water while (2) selected clusters including even some with closed electronic sub-shells can exhibit strong reactivity towards water. Similar patterns are also observed for the reactivity of aluminum cluster anions with methanol and formaldehyde. Our theoretical studies show that these behaviors are rooted in the non-uniform distribution of charge densities on cluster surfaces and hence have a geometric rather than an electronic origin. I will show that clusters with non-uniform charge distributions are often marked by Lewis-acid and Lewis-base complementary sites that may stimulate the breaking of polar bonds enabling an atomic level control of reactivity. Such pairs can break hydroxyl and even stronger C=O carbonyl bond of formaldehyde. These paired active sites establish the potential use of these geometrically driven centers in devising precursors for synthesizing chemicals or radicals that might find use in production of fine chemicals.

STRUCTURAL TRANSFORMATIONS IN FERROELECTRIC POLYMERS AND METAL-PROTEIN COMPLEXES

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Recent advances in multiscale methods and high performance computing allow for reliable first-principles predictions of complex nanostructured materials and even chemical and biological processes. This talk will discuss two topics: (i) novel nanoscale energy storage mechanisms in ferroelectric polymers that enable ultrafast capacitors with very high power densities, (ii) simulations of solvated biomolecules and of the role of transition metal atoms in biological processes and diseases.

Polyvinylidene fluoride (PVDF) with a small concentration of chlorotrifluoroethylene (CTFE) stores much more energy than current capacitor materials. In a recent work, we suggested that the ultra-high energy storage in P(VDF-CTFE) is due to formation of nanostructured domains that undergo an electric-field-induced phase transition from the non-polar alpha to the polar beta phase [1]. We have now mapped out the phase transformation pathway as a function of the electric field for both pure PVDF and P(VDF-CTFE). We show that the admixture of CTFE has a dramatic effect on the transformation barriers, both in a thermally induced transformation and in high electric field [2]. The admixture of suitable copolymers can thus be used to tune the high-field behavior of PVDF for high-power density energy storage applications.

One of the most important challenges in quantum simulations of biomolecules is efficient and accurate inclusion of the solvent, because the solvent atoms usually far outnumber those in the biomolecule of interest. We have developed a hybrid method that allows for explicit quantum-mechanical treatment of the solvent at low computational cost. In this method, the biomolecule and its first solvation shells are described by Kohn-Sham density functional theory (DFT), while more distant solvent molecules are treated by orbital-free DFT. We have used this method to investigate the binding of copper ions to proteins involved in prion (PrP) and Parkinson's diseases. Our results for PrP [2] show how this protein can bind multiple copper ions while undergoing complex structural rearrangements and becoming more resistant to misfolding. It can thus act as a copper buffer and has a positive effect in prion diseases. For alpha-synuclein, the Parkinson's disease (PD) protein, we show that Cu binding modifies the protein structurally, making it more susceptible to misfolding -- an initial step in the onset of PD [3].

In collaboration with V. Ranjan, M. Hodak, F. Rose, M. Buongiorno Nardelli and W. Lu.

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ROLE OF THE ACTIVE AND INERT SUPPORTS IN ENHANCED CATALYTIC ACTIVITY OF GOLD CLUSTERS

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The specific role played by the support in catalytic activity of small gold clusters will be discussed. Two types of support are considered—the “inert” support of the hexagonal boron nitride (h-BN) and the “active” support of rutile TiO₂(110). Since the pioneering work of Haruta on the oxidation of CO by molecular oxygen on small gold nanoparticles [1] an extensive interest has been devoted to understanding the catalytic properties of gold; see, e.g. [2-4] and references therein. Gold clusters possess unique catalytic activity in various oxidation and hydrogenation reactions. The high selectivity of gold clusters at mild temperatures makes them very attractive for many industrial applications. However, in spite of intensive experimental and theoretical studies the origin of catalytic activity of gold nanoparticles remains highly debated.

In the present work we demonstrate that adsorption, catalytic activation and dissociation of O₂ on the h-BN supported small gold clusters can be affected by the interaction with the support via electron pushing and donor/acceptor mechanisms [5-7]. It is shown that even weak interaction of gold clusters with the defect-free “inert” h-BN surface can have an unusually strong influence on the binding and catalytic activation of the molecular oxygen. Although the defect-free h-BN surface does not act as a good electron donor for the supported O₂-Au, it promotes an electron transfer from the Au to O₂, pushing electrons from the gold to the adsorbed oxygen. In the case of defected h-BN surface gold clusters can be trapped effectively by N or B vacancy and impurity point defects. Strong adsorption on the surface defects is accompanied by the large charge transfer to/from the adsorbate. The excess of the positive or negative charge on the supported gold clusters can considerably promote their catalytic activity. Therefore, the h-BN surface (pristine or defected) cannot be considered as an “inert” support.

We also demonstrate that the rutile TiO₂(110) support energetically promotes H₂ dissociation on gold clusters [8]. We show that the formation of the OH group near the supported gold cluster is an important condition for H₂ dissociation. We demonstrate that the active sites towards H₂ dissociation on the supported gold clusters are located at corners and edges of the gold cluster in the vicinity of the low coordinated oxygen atoms on TiO₂(110). Thus catalytic activity of a gold nanoparticle supported on the rutile TiO₂(110) surface is proportional to the length of the perimeter interface between the nanoparticle and the support.

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ELECTRON ATTACHMENT TO MOLECULES IN A CLUSTER ENVIRONMENT

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Dissociative electron attachment (DEA) is one of the most important processes through which low-energy electrons deposit energy and induce chemical transformations. In biological systems, it is important to know how these fundamental mechanisms are affected and modified in the presence of vital cellular components, in particular water [1]. The effects of a cluster environment in DEA are also important in beam- and photon-induced surface chemistry and atmospheric science. In particular, the DEA of electron trapped in ice to chlorofluorocarbons plays an important role in the ozone-depletion chemistry in polar stratospheric clouds. In the experiments of Lu and Sanche, it was shown that due to its strong trapping properties, ice water strongly enhances DEA processes in halocarbons [2] and hydrogen halides [3].

In the present work low-energy DEA to the CF_2Cl_2 and CF_3Cl molecules in a water cluster environment is investigated theoretically using the multiple-scattering approach [4]. Calculations are performed for the water trimer and water hexamer. It is shown that the DEA cross section is strongly enhanced when the attaching molecule is embedded in a water cluster, and that this cross section grows as the number of water molecules in the cluster increases. This growth is explained by a trapping effect that is due to multiple scattering by water molecules while the electron is trapped in the cluster environment. The trapping increases the resonance lifetime and the negative ion survival probability. This confirms qualitatively existing experiments on electron attachment to the CF_2Cl_2 molecule placed on the surface of H_2O ice. The DEA cross sections are shown to be very sensitive to the position of the attaching molecule within the cluster and the orientation of the electron beam relative to the cluster.

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IONIZATION OF BIOMOLECULAR TARGETS BY ION-IMPACT: INPUT DATA FOR RADIOBIOLOGICAL APPLICATIONS

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The emission of secondary electrons is an important step in the multiscale description of ion beam cancer therapy [1]. Nowadays, theoretical efforts have concentrated mainly in the study of electron ejection from liquid water, the main constituent of tissue [2, 3]. Nonetheless, the final damage of the cell depends on ionization of cellular structures in the nano- or mesoscale, such as chromatin, DNA components or proteins, and cross sections for these targets are still scarce [4, 5]. In this contribution, a semiempirical method will be introduced, based on the dielectric formalism and on a parameterization of the experimental optical energy-loss function of organic compounds [6]. This model allows estimating single differential (in ejection energy) cross sections for the ion-impact ionization of a wide number of biological targets, such as DNA and its molecular components (i.e., bases and backbone), proteins and its components (i.e., amino acids), or lipids, among others. The knowledge of these basic data permits to obtain other important magnitudes, such as total ionization cross sections, number of electrons emitted per unit path length or average kinetic energy of the ejected electrons. In this way, we are able of obtaining, with a simple approach, useful information for the comparative study of radiation damage in different cellular substructures, as well as input data for detailed simulations of radiation transport in a realistic biological environment.

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Mo-IV-1

(PbS)₃₂: A BABY CRYSTAL

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Theoretical calculations based on density functional theory have found (PbS)₃₂ to be the smallest cubic cluster for which its inner (PbS)₄ core enjoys bulk-like coordination. Cubic (PbS)₃₂ is thus a “*baby crystal*”, i.e., the smallest cluster, exhibiting six-fold coordination, that can be replicated to obtain the bulk crystal. The calculated dimensions of the (PbS)₃₂ cluster further provide a rubric for understanding the pattern of aggregation when (PbS)₃₂ clusters are deposited on a suitable surface, i.e., the formation of square and rectangular, crystalline nano-blocks with predictable dimensions. Experiments in which mass-selected (PbS)₃₂ clusters were soft-landed onto a HOPG surface and the resulting aggregates imaged by STM provide evidence in direct support of the computational results.

Mo-IV-2

OSTWALD RIPENING AND A TEST-TUBE MODEL FOR RAINFALL

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Ostwald ripening is an intriguing phenomenon, which can play an important role in the evolution of nanoscale structures. After illustrating the effect with the aid of some simulations of the dynamics of atoms on surfaces, I shall describe a novel application of the Lifshitz-Slezov theory [1] of Ostwald ripening.

The initiation of rainfall is a complex and imperfectly understood physical process, which is fundamentally important to explaining the life cycle of clouds (and therefore our climate), see, e.g. [2]. I will discuss some simple but very elegant experiments by Jürgen Vollmer and co-workers, who have produced a test-tube model for rainfall in a convectively stable atmosphere. The experiment involves slowly changing the temperature of two partially miscible liquids. As they become less miscible, microscopic droplets are nucleated and move towards the interface. This produces a cyclic variation of the turbidity of the liquid, with period Δt . I model droplet growth by a period of Ostwald ripening, which is treated using the approach of Lifshitz and Slezov, followed by a finite-time runaway growth of droplet sizes due to larger droplets sweeping up smaller ones. The theory predicts that the period Δt to arrive at precipitation is related to the temperature sweep rate ζ by $\Delta t \sim \zeta^{-3/7}$, in excellent agreement with the experiment.

Finally I shall discuss the extent to which this weather cycle in a test-tube is relevant to real clouds.

The talk will draw upon the results of collaborations with Jürgen Vollmer and his students Tobias Lapp and Martin Rohloff at the Max-Planck-Institute for Dynamics and Self-Organization, Göttingen.

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DYNAMIC ORDERING OF IONS AROUND DNA HELIX

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In water solution with enough concentrations of alkali metal ions the DNA macromolecule takes the form of double helix. The positively charged ions neutralize the negatively charged phosphate groups of DNA backbone that is one of the most important factors in the stability of the double helix. Under sufficient counterions concentration a regular structure of ions and DNA phosphate groups must be formed in solution. Such ordered structure of ions around DNA we consider as an ionic lattice, the formation of which may be observed in vibrational spectra. The increasing of counterion concentration with the simultaneous decreasing of solution volume leads to formation of DNA-salt complex. Such complexes are observed as microscopic textures on a surface after solution evaporation. The formation of textures and their shape are sensitive to concentration and type of metals ions in initial solution of DNA. The report presents a theoretical approach that describes the ordering of ions around DNA under various conditions of ion-hydrate environment of macromolecule.

Considering DNA with counterions as ionic lattice a spatial phenomenological model of dynamics of ions and phosphate groups was developed [1-3]. The modes of ion vibrations are found for DNA with Na^+ , K^+ , Rb^+ , Cs^+ , and Mg^{2+} ions, and frequencies, amplitudes, and Raman intensities are calculated. The results show that the frequencies of ion vibrations depend on counterion type and decrease from 180 to 100 cm^{-1} as ion mass increases. The vibrations of heavy ions are more intensive in the Raman spectra of DNA in contrast to the vibrations of light ions, which have very low intensity. The counterions of different masses influence the dynamics of the structural elements of the double helix in different way. Heavy ions (Rb^+ , Cs^+) disturb the internal dynamics of the double helix, while light ions (K^+ , Na^+) do not influence the internal dynamics of DNA.

The ordering of ions around DNA in concentrated salt solution is studied by the developed approach based on the Debye-Hückel theory of electrolyte solutions and theory of ionic crystals [4]. The electrostatic energy is calculated for the ions around DNA in solution with the excess salt. The results show that the process of ions ordering around DNA begins at a lower concentration of excess salt, compared with pure salt solution. More earlier ions ordering determines the formation of DNA-salt complexes. The ability of salts to induce the formation of DNA aggregates is found to be in the following order $\text{KCl} > \text{NaCl} > \text{RbCl} > \text{CsCl} > \text{LiCl}$. The obtained data qualitatively describe the formation of experimentally observed textures in DNA films with the chlorides of alkali metal ions.

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ION-INDUCED CHEMISTRY IN MOLECULES AND CLUSTERS

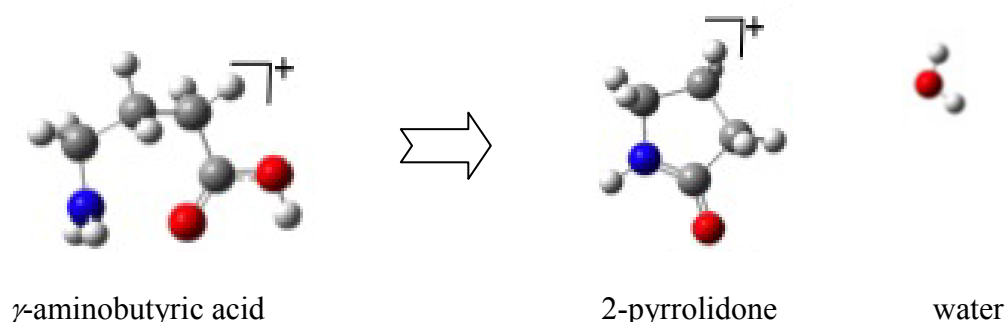
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When low energy ions (in the keV region) interact with complex systems like clusters of complex molecules, energy and charge will be transferred and the subsequent interaction between individual sub-systems can lead to the initiation of chemical reactions. In many cases it has been shown [1], that the transferred energy and the excess charge is rapidly redistributed among the large number of degrees of freedom all over the cluster volume, and a diminution of the fragmentation yield of the cluster components is observed with respect to the case where an individual molecule collides in the gas phase. However, in particular, when the cluster consists of large molecules like fullerenes, amino acids or polycyclic aromatic hydrocarbons, there is the possibility that one of the components is transformed by the collision into a highly reactive species which likes to react immediately with one of its neighbors before the system fragments. In this way, weakly bound systems (van der Waals or hydrogen-bonded) can be transferred into rather stable covalently-bound molecules.

These phenomena have been observed in many different systems and we will present some of the following examples:

- Xe²⁵⁺ ion-induced coalescence of large fullerenes in clusters of C₆₀ fullerenes [2];
- formation of C₁₁₉/C₁₁₈ after collisions of He²⁺ ions with clusters of C₆₀ fullerenes;
- production of polypeptides in collisions of He²⁺ ions with clusters of β -alanine;
- protonation processes after clusters ionization;
- carbon addition reactions in clusters of pyrene;
- reactive fragmentation processes in complex molecules like GABA [3] (see figure below).



These studies have been performed in collaboration between several teams: CIMAP (Caen), Stockholm University (H. Cederquist et al.), KVI (T. Schlathölter et al.), Aarhus University (P. Hvelplund et al.) and Universidad Autonoma de Madrid (F. Martin et al).

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**IRRADIATION OF MULTI-WALLED CARBON NANOTUBES
BY PROTON BEAMS AT NORMAL INCIDENCE**

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We study, both experimentally and theoretically, the irradiation with 2 – 10 keV proton beams impinging normally to the axis of a multi-walled carbon nanotube (MWCNT). In the experimental setup the MWCNTs are dispersed on top of a holey amorphous carbon (a-C) thin foil and the proton energy loss distribution is measured by the transmission technique. The resulting energy loss spectra in the forward direction show two well differentiated peaks (see Fig. 1), whose origin is elucidated by using a semi-classical simulation of the proton trajectory through the nanotube. We conclude that the experimental low energy-loss peak corresponds to quasi-planar channelling of protons moving between the outer walls of the MWCNT, whereas the experimental high energy-loss peak is mainly due to protons traversing the supporting a-C substrate after moving through the MWCNTs in quasi-planar channelling.

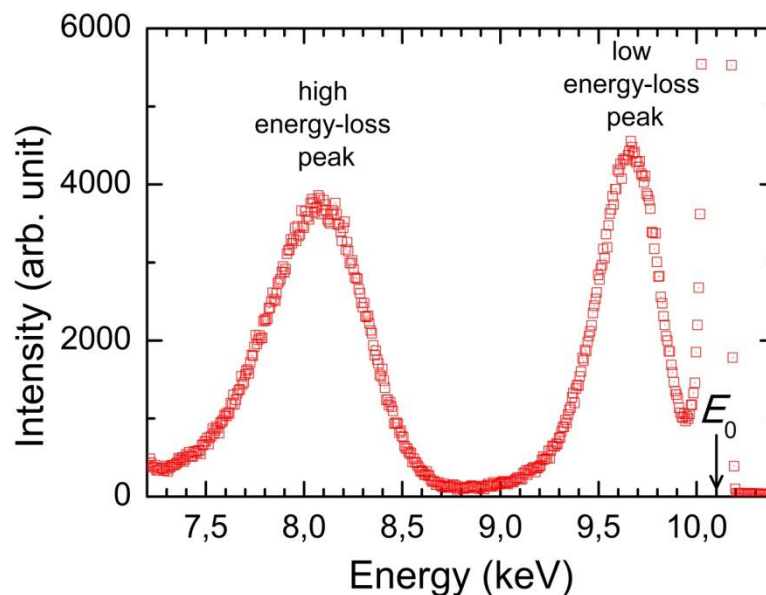


Figure 1: Energy spectrum of a proton beam incident with $E_0=10.1$ keV perpendicularly on MWCNTs whose average inner and outer diameters are 5 nm and 27 nm, respectively.

Tu-I-3

NON-ADIABATIC DYNAMICS IN POLYATOMIC MOLECULES BY FEMTOSECOND PHOTOELECTRON IMAGING

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

The laser induced predissociation dynamics of the *B* Rydberg state of CH₃I following two-photon absorption of a pump pulse was studied. The predissociation lifetime was measured to be 1.55 ps induced by the crossing between the *B* state and the repulsive *A*-band. Two possible predissociation channels were observed originating from (a) direct coupling between the *B* state and the repulsive ³Q₀ state and (b) a second crossing between the ³Q₀ and ¹Q₁ states after the coupling between the *B* and ³Q₀ states, respectively.

The electron dephasing mechanism of S₁ (B₂) state of *p*-bromofluorobenzene is determined to be the intersystem crossing (ISC) from the S₁ (B₂) to the T₁ (B₂) state and predissociation S₁ (B₂) via T₁ (B₁) state. The lifetime of S₁ (B₂) and T₁ (B₂) is determined to be 40ps and 33ps from the decay of the photoelectron signal.

The intramolecular vibrational energy redistribution (IVR) induced by a Fermi resonance in the S₁ low energy regime of *p*-difluorobenzene has been experimentally observed for the first time. The corresponding photoelectron angular distributions (PADs) clearly reflect each Fermi component character of the resonance 5¹... 6². The oscillation period for the IVR is estimated to be less than 20 ps.

Non-adiabatic alignment of the asymmetric molecule on excited state by femtosecond laser pulse was observed on real time via time-resolved photoelectron angular distributions (TRPAD). Surprisingly, the molecular-axis alignment revival at as long as 296 ps of S₁ *o*-dichlorobenzene was observed.

Tu-II-1

ASSESSING QUANTUM THERMAL BATHS FOR FINITE SYSTEMS

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Nuclear quantum effects are important for weakly bound or light atoms and at low temperatures. They are manifested by residual energy stored as zero-point vibrations, tunneling, and possible exchange effects in bosonic systems. Unfortunately, the vibrational Schrodinger equation is difficult to solve except for very small systems. Quantum thermal baths (QTBs) have been proposed in the recent years as an alternative to the convenient, but still computationally expensive schemes based on path integrals. The QTB method relies on propagating a stochastic Langevin equation with a correlated (colored) noise designed to produce a power spectrum which satisfies the quantum fluctuation-dissipation theorem. As such, its numerical cost is close to that of a standard classical Langevin equation, making it a very promising technique for large-scale atomic and molecular systems.

In the present contribution, we discuss the application of the QTB approach for gas-phase systems, their equilibrium properties and vibrational spectroscopy. The implementation of the method is described, with an emphasis on specific computational aspects involved in the generation of the colored noise. The performance of the method is assessed by comparison with dedicated path integral molecular dynamics simulations for simple ionic clusters, as well as polycyclic aromatic hydrocarbons.

In another application, we show that cationic neon clusters containing up to 57 atoms exhibit some surprisingly strong vibrational delocalization, which is sufficient to blur the picture of well-defined isomers. The extent of delocalization, measured by the dispersion of the inherent structures within the ground state wavefunction, correlates with enhanced stabilities in mass spectra.

DIFFUSION AND NANOINDENTATION PROCESSES IN TITANIUM AND NICKEL MATERIALS

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We report on the results of classical molecular dynamics simulation of the diffusion processes occurring at the nickel and titanium interface. The interactions between metal atoms are treated using Finnis-Sinclair [1] potential. From the simulations we derive the diffusion coefficient for Ni and Ti atoms. The dynamics of Ni₅₅ cluster on the titanium surface in the presence of water environment is investigated. Investigation of surface diffusion is of a current interest since it is involved in many important processes, such as crystal and film growing, evaporation, chemical surface reactions, catalysis and condensation [2]. We analyze the dynamics of nickel atoms in the cluster; describe clusters' structural rearrangements due to the interaction with titanium surface and derive its surface diffusion coefficient.

We also present the results of the molecular dynamics simulations of nanoindentation [3] of titanium crystal. The dependence of the total energy of the system and the force acting on the indenter as a function of the indenter penetration depth is studied. We show that at the initial part of the total energy of the system decreases due to the interaction between the indenter and titanium surface, while further displacement of the indenter leads to the damage of the crystalline structure of the material and to the consequent increase of the total energy of the system.

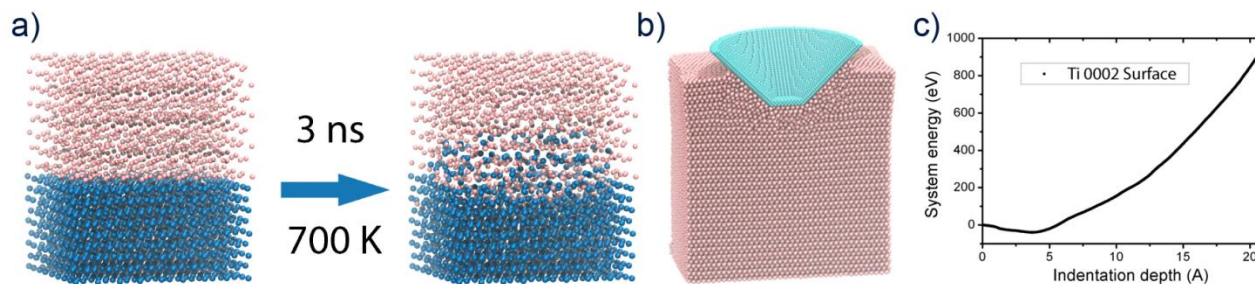


Figure 1: a) Interpenetration of the nickel and titanium atoms due to the diffusion across crystal interface. b) Indentation of titanium crystal by infinitely stiff indenter. c) The dependence of the total energy of the titanium/indenter system on the indentation depth.

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Tu-II-3

DYNAMICS OF MARTENSITIC STRUCTURE AT TiNb-BASED QUENCHED ALLOYS UNDER HEATING AND LOADING

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It is well known that there are only two stable phases in pure Ti and solid solutions on its base: high temperature cubic (bcc or “beta”) phase and lower temperature hexagonal (“alpha”) phase. Alloying of Ti by bcc elements (Nb, Ta, Mo etc.) changes structure type of quenched solid solution on the way of rearrangement from hexagonal (alfa) phase till (cubic) beta phase. So, some other metastable phases could be formed dependent on alloying, heat treatment and pressure processing. The tailoring of metastable structures at reasonable processing leads to such inelastic phenomena as shape memory, pseudo-elasticity, high damping capacity, negative temperature dependence of electric resistivity etc. The alloys are attractive for medical applications as metallic implant materials combining superelasticity with biocompatibility comparable to that of pure Ti.

Ternary and quaternary Ti–Nb-based alloys have been extensively investigated during the last several years and the results confirm the possibility of producing Ni-free, Ti-based solid solution alloys with shape memory effects connected with reversible β to α'' martensitic transformation [1,2]. In this work, products of martensitic transformation of biocompatible quenched Ti-(Nb, Ta) alloys, especially metastable orthorhombic α'' and cubic β phases have been studied by elastic E and G moduli determination, thermal analysis (DTA), tensile tests and nanoindentation.

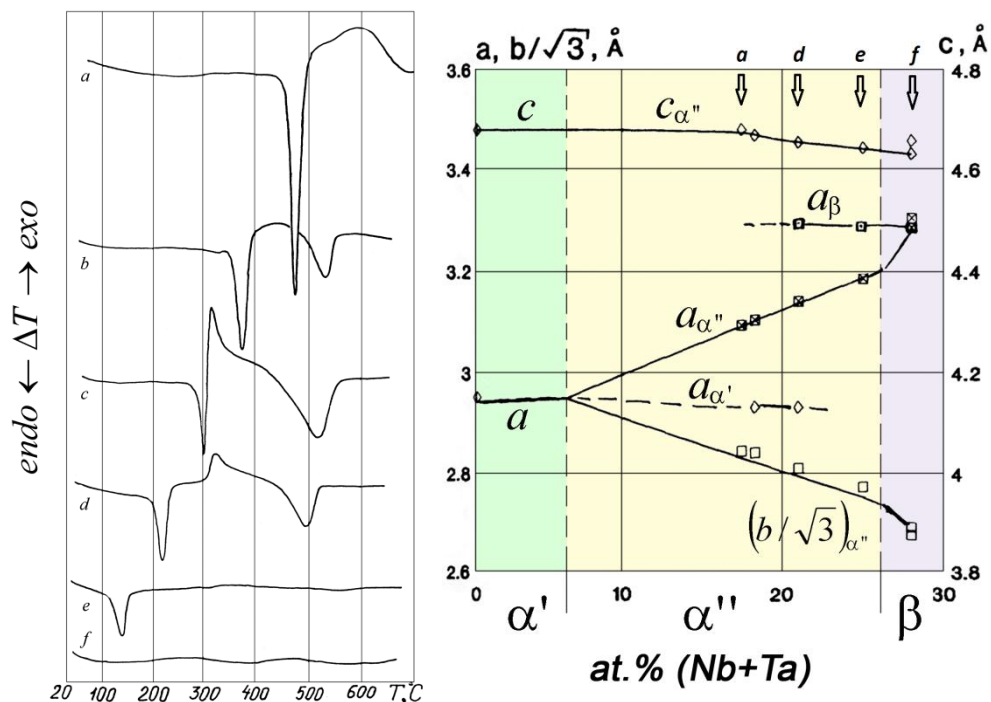


Fig.1 The effect of alloying on temperature range of martensitic transformation (a) and distortion of orthorhombic lattice cell (b)

Tu-II-3

The experimental results were analyzed taking into account XRD data on phase composition, as well as on degree of distortion $R=\sqrt{3a/b}$ of orthorhombic α'' -martensite (Cmcm space group) according to Yu.A. Bagariatskii's diagram of transition [2,3]. It was found that experimental realization of superelasticity (up to 2,5 % of returnable deformation) on tensile mechanical tests was closed to its theoretical limit [3] and it was observed at alloys having extremely low Young's modulus (about 60 GPa and less) and the largest rhombic distortion (about $R=1.13-1.16$) of unit cell. Also it was noted a high thermal stability of the martensitic structure against thermal cycling [4].

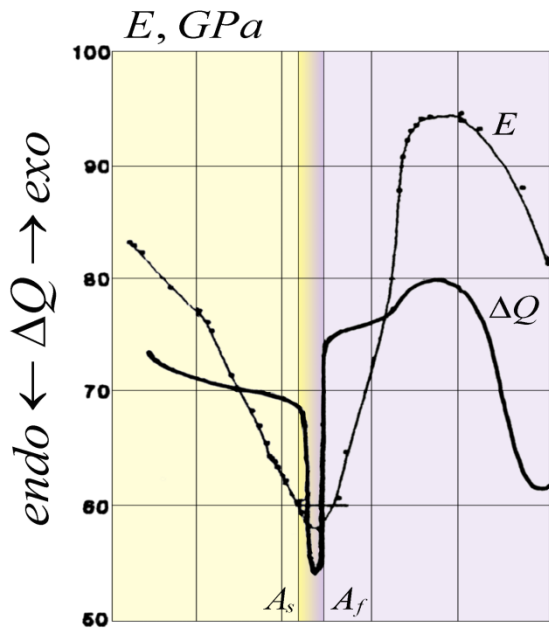


Fig.2 Softening of Young's (E) modulus at heating through A_s - A_f range

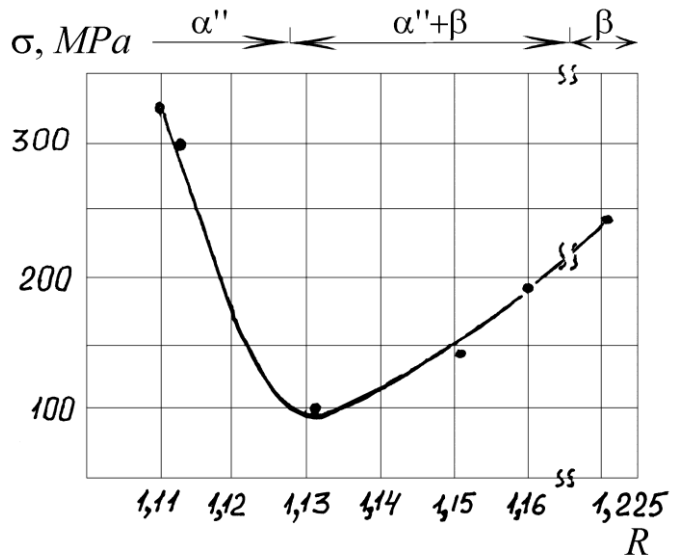


Fig.3 Pseudo yield stress vs. distortion of orthorhombic unit cell

So, shape memory and pseudo elasticity observed in TiNb based alloys are due two sequential mechanisms: orthorhombic distortion and martensitic transformation.

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ATMOSPHERIC DEGRADATION OF SILVER NANOFRACTAL BY TRACE AMOUNT OF CHLORINE

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The fragmentation mechanisms induced by atmospheric corrosion are studied on silver nanofractal islands obtained from physical method. Those nano-fractals formed by deposition and diffusion of silver clusters on cleaved graphite surfaces exhibit dendritic morphologies that highly sensitive to any perturbation. After ageing by exposure to the ambient air, these structures reveal two competitive fragmentation mechanisms due to chlorine and sulphur pollution as the main agents for fractal degradation. To understand the role of the chlorine in the stability and the observed fragmentation of Ag dendritic nanostructures, we have studied computationally a model system using density functional theory. It relates to the diffusion of Ag_n and Ag_nCl_m ($n=1$ to 4) clusters on Ag(111) surface. Based on our calculated energy barriers, Ag_nCl_m clusters are more mobile than Ag_n clusters. It has to be noted that, the chemically induced fragmentation differs from the morphological transition of the fractal shape induced by temperature effects.

SUPPORTED MASS-SELECTED CARBON CLUSTERS: THERMALLY AND CHEMICALLY DRIVEN SURFACE MODIFICATIONS

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We have applied low-energy cluster ion beam deposition [1] of mass selected non-IPR fullerenes towards designing new materials on the macro- and mesoscopic length scales. The talk will show to which extent the dynamics of the cluster-surface interaction can be exploited to create carbon nanomaterials with different topographies [2]. The mesoscopic-scale structures initially formed on the surface appear to be metastable due to the unique molecular properties of the deposited fullerene cages. They can be converted into more stable topographies simply by extended thermal treatment or by chemical doping (e.g. with electron donors). Such treatment results in maximization of the coordination number of the component carbon cages – thus leading to significant changes in topography. This observation has been exploited in order to decorate defect-patterned substrates with periodically aligned fullerene islands. Thermally induced rearrangement of 2D islands on the mesoscopic scale led us to also study related transformations of corresponding macroscopic 3D fullerene films. It turns out that apart from the thermal desorption of less coordinated cages, thermal treatment of 3D fullerene films considerably modifies their vibrational, electronic and mechanical properties - as probed by macroscopically averaging spectroscopic methods. For instance C_{58} solids [3] become converted from wide-gap into narrow-band semiconductors, whereas the $-C_{58}-C_{58}-C_{58}-$ oligomers as main constituents become additionally stabilized due to further $-C-C-$ bonding interactions. Such thermally activated 3D rearrangement on the molecular level is responsible for a pronounced strengthening of the macroscopic materials properties (e.g. hardness and the Young's modulus). The same thermal treatment when applied to alkali-metal-doped fullerenes, $C_{58}Cs_x$, leads to qualitative modifications of the electronic and vibrational properties as well as a dramatic transformation of the surface topography. The resulting surface consists of dendritic island structures (mean size $<1\mu\text{m}$) thus indicating a thermally driven spinodal decomposition process (in analogy to binary metal alloys [4]).

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DYNAMICS OF NANOFRACTAL FORMATION AND FRAGMENTATION

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The self-organization of nanoparticles plays an important role in the process of nanostructure formation on a surface [1]. The understanding of the mechanisms of self-organization on the nanoscale may provide essential tool for the control and manipulation of nanoparticle's dynamics on a surface which will allow efficient obtaining of the desirable patterns of deposited materials [1-3].

We investigate the process of fractal formation on a surface and their post-growth relaxation. For this study we have developed a method that accounts for the internal dynamics of particles in a fractal [2,4]. We demonstrate that the detachment of particles from the fractal and their diffusion within the fractal and over the surface determines the shape of the islands remaining on a surface after the fractal fragmentation, see Fig.1. We consider different scenarios of fractal post-growth relaxation and analyze the time evolution of the island's morphology. The results of our calculations are compared with available experimental observations, and experiments in which the post-growth relaxation of deposited nanostructures can be tested are suggested [2,3].

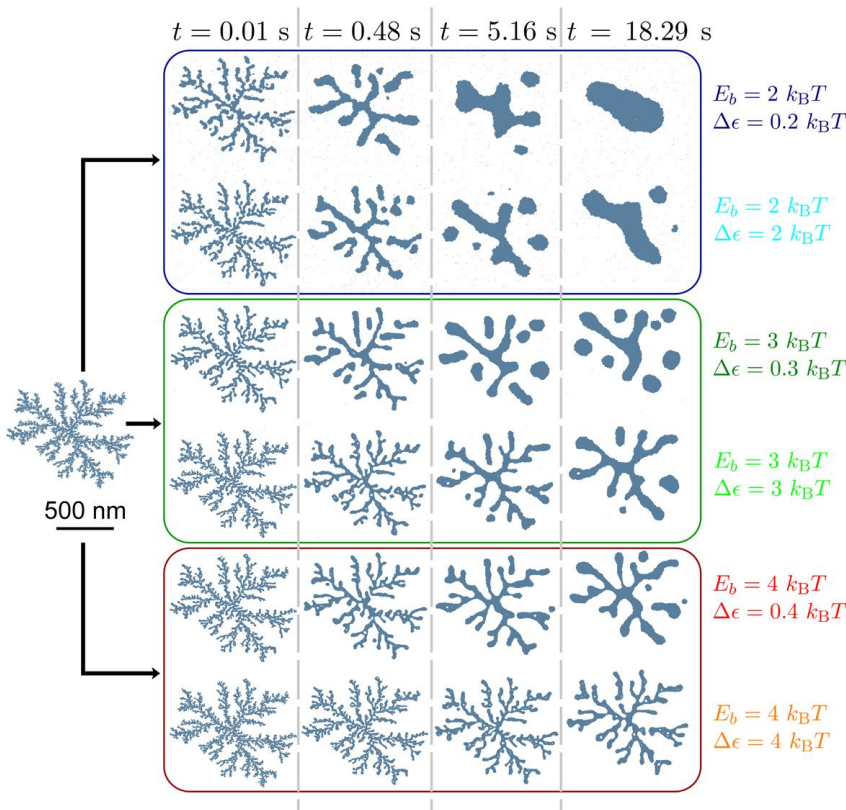


Figure 1: Evolution of a fractal structure on a $4.3 \times 5.0 \mu\text{m}^2$ substrate with periodic boundary conditions. The initial fractal structure, consisting of 38,012 particles (shown left) undergoes fragmentation in different final states depending on the interparticle interactions in the system (shown right). Numbers above the images indicate the simulation time t at which the corresponding snapshots were rendered.

Tu-III-3

The presentation will advertise a new software package MBN Explorer (www.mbnexplorer.com) [4] that was successfully used to study of nanofractal formation and fragmentation. The talk will give an overview of the capabilities of the program and its computational efficiency with particular emphasis of stochastic Monte-Carlo based dynamics used for studying selforganization processes on a surface, but other features of the program will also be discussed.

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MULTISCALE PHYSICS OF ION INDUCED RADIATION DAMAGE

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The scientific interest in obtaining a deeper understanding of radiation damage is motivated by the development of ion-beam cancer therapy and other applications of ions interacting with biological targets [1,2]. This field has attracted much attention from the scientific community, atomic and molecular physics in particular. Among these studies is the multiscale approach to the assessment of radiation damage induced by irradiation with ions [3, 4]. This method combines effects happening on a number of spatial, temporal, and energy scales. The goal of the multiscale approach is to quantitatively relate these effects to the cell damage and calculate the relative biological effectiveness (RBE) and other macroscopic quantities. The main issues addressed by the multiscale approach are ion stopping in the medium, the production and transport of secondary electrons produced as a result of ionization and excitation of the medium, the interaction of secondary particles with biological molecules, the most important being DNA, the analysis of induced damage, and the evaluation of the probabilities of subsequent cell survival or death.

The milestones in the development of the multiscale approach were the calculations of the Bragg peak, the estimation of DNA strand breaks yields by secondary electrons, calculation of the radial dose, and assessment of the complex DNA damage [4]. A special investigation is devoted to DNA damage as a result of thermomechanical effects caused by ions [4-7]. These effects follow a dynamical change in temperature and pressure within a small cylinder surrounding the ion's path leading to a cylindrical shock wave, which may rupture bonds in DNA molecules and also provides an effective mechanism of transport of reacting species, which may damage a DNA molecule several decades of nm away from the path. The understanding of such a possibility evolved from the estimates of the temperature increase in the medium as a result of ion propagation [5] to the analysis of thermal and pressure spikes in liquid water and further to the analysis of the shock wave in the medium [6] and modeling of its action on biological molecules [7].

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LANTHANIDE NANOPARTICLES: TOWARD THERANOSTIC IN HADRONTHERAPY

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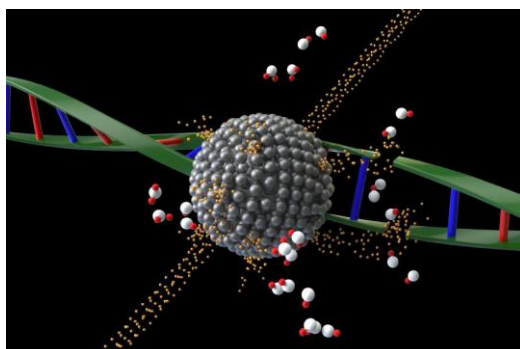
The main techniques used to treat cancer (surgery, chemotherapy, and radiotherapy) cause severe side effects to the patients due to strong damage and poisoning in the healthy tissues. The improvement of targeting and efficiency of the treatments is a challenge for future developments.

In this respect, protontherapy and hadrontherapy, which use fast protons and carbon ions as ionizing particles, have specific advantages. The ballistic effect of the fast ions interacting with the biological matter (the Bragg peak) enhances the dose deposition into the tumor. It thus improves the preservation of the tissue sited behind. However the dose deposited at the entrance of the track is not negligible.

To improve the performances of proton/hadrontherapy, the group of S. Lacombe is developing a **new strategy where metallic nanoparticles (<3nm) are combined with fast ion irradiation** [1]. A multiple-scale approach, from DNA molecule to living cells, is adopted by the group to quantify and to characterize the efficiency of potentially active nanodrugs. The group has shown for the first time that platinum and gadolinium nanoparticles amplify efficiently the radiation effects of fast ions. They have shown that the addition of nanoparticles enhances the induction of **nanometric damages** (>2-3 nm).

In order to predict and control the effect of nanodrugs, it is urgent to better understand the **elementary mechanisms involved in the activation of the nanoparticles**. As a first attempt, the group ascribes the effects of nanoparticles to fast electronic cascades activated by electrons emitted along the ion tracks. But simulations and physics experiment are needed to confirm this hypothesis.

As an end point, the use of nanodrugs in hadrontherapy is a very promising strategy to improve the therapeutic index of cancer treatments, but a deep understanding of the mechanisms is needed to quantify and control the dose deposition in bodies and to evaluate the feasibility of this protocol.



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ELECTRON AND POSITRON SCATTERING WITH NANOSTRUCTURES (ATOMIC CLUSTERS AND MACROMOLECULES)

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Electron and positron scattering cross sections are relevant for many applications in material and biomedical sciences. Media of interest for these applications are mainly in the condensed phase while most of calculations and experiments devoted to obtain cross section data are carried out for isolated atoms and molecules. In this contribution we present a method to derive accurate scattering parameters for electrons and positrons interacting with atomic cluster (dimer, trimer, tetramer, etc..) and macromolecules (DNA nucleotides) as a transitional procedure to accomplish model particle interactions in the condensed phase.

Scattering calculations will initially focus on atoms constituting the target of interest, namely H, C, N, O, Ar, by using an optical potential method [1-2] and then we will apply the Screened Corrected Additivity Rule (SCAR) procedure [3] to model the geometrical properties of the nanostructures. Through a coherent addition of the scattering amplitudes we will present results of differential and integral elastic cross as well as inelastic integral cross sections over a broad energy range, from 1 to 1000 eV for representative argon clusters and DNA components. Details on the experimental validation of the present data will be finally provided.

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PHOTOIONIZATION OF CLUSTERS AND FULLERENES

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The main goal of the present study is to determine a role of many-electron effects in the description of photoionization of metal clusters, fullerenes and endohedral fullerenes. In this contribution the results of recent calculations of electronic structure and photoionization cross sections of these systems are discussed.

The calculations of photoprocesses are performed within the consistent many-body theory based on the spherical jellium model. The single-electron energies and wave functions of valence-electron system are determined both within the Hartree-Fock (HF) and local density (LDA) approximations. Then, using the HF or LDA wave functions of excited states the photoionization amplitudes and cross sections are calculated within both the single-electron approach and the random phase approximation with exchange (RPAE).

Within the spherical jellium model the detailed ionic structure of the system is smeared out and substituted by the uniform, spherically symmetric distribution of the positive charge. For metal clusters the ionic core is represented by the uniformly charged full sphere [1] and this model produces rather good description of photoionization process. The simplest model for C₆₀ ionic core is the uniform distribution of positive charge ($Z=240$) over spherical layer of the finite thickness [2]. However, the calculations show that the ground state properties of fullerenes cannot be described properly by the standard jellium model which produces, in particular, incorrect electron density distribution [3]. On the other hand, the photoionization process in the vicinity of the collective plasmon excitation depends strongly on the electron density. Therefore, one needs to improve the description of the ground state in order to get a correct behavior of the photoionization cross section. For this purpose we introduce a new pseudopotential [3] which originates from the comparison of results obtained within the accurate *ab initio* and the jellium model frameworks. Including this pseudopotential as a correction to the standard jellium model we improve the fullerene's ground state, in particular, introducing effects of the sp²-hybridization of carbon atomic orbitals. The modified ground state is used for the RPAE photoionization cross section calculations. Preliminary results show better description of resonance shape and correlation between two surface plasmons. Meanwhile, there are some limitations of the approach which will be discussed in the presentation.

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STUDY OF COLLECTIVE ELECTRON EXCITATIONS IN FULLERENES

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We present the results of investigation of the collective excitations in C_{60} in the process of inelastic scattering of electrons. By means of the theoretical model [1] developed recently we demonstrate that the cross section of inelastic scattering of fast electrons on fullerenes is determined, to a great extent, by the three contributions. They arise from the three plasmons (the symmetric and antisymmetric modes of the surface plasmon, and the volume plasmon) which are excited in the fullerene under the action of a non-uniform external field of the charged projectile (Fig. 1). The formation of the three plasmons is the main feature of the electron impact ionization of fullerenes. This is in contrast to the process of photoionization where only two modes of the surface plasmon can be excited by the uniform field of an electromagnetic wave.

We show that the shape of the electron energy loss spectrum varies with the scattering angle. This variation is due to the electron diffraction at the fullerene shell. At small angles, the inelastic scattering cross section is determined mostly by the symmetric mode of the surface plasmon, while at larger angles, the antisymmetric surface and the volume plasmons become prominent [2, 3].

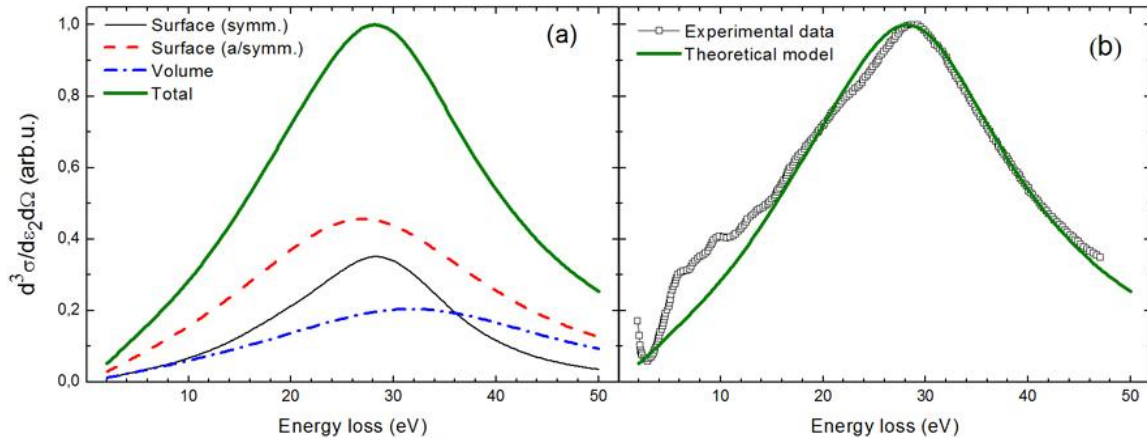


Figure 1: Comparison of the theoretical results with the experimental electron energy loss spectrum [2 – 4] measured at the scattering angle $\theta = 5^\circ$.

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COHERENT MULTIPHOTON PHOTOELECTRON EMISSION FROM INDIVIDUAL, SUPPORTED METALLIC NANOPARTICLES

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Metallic nanoparticles are finding use as highly efficient light absorbers in solar cells, subdiffraction-limited light guides in optical communications, photothermal anti-cancer agents in medicine and SERS substrates in single-molecule detection applications. The underlying reason for this plethora of potential applications is a plasmon – a collective oscillation of the conduction electrons within a metallic nanoparticle in response to an incident electromagnetic field. The plasmon is highly sensitive to the particle composition, its environment and detailed shape. While modern synthetic methods control these factors to a high degree, sample inhomogeneity remains an issue. Single-particle techniques are thus essential for understanding the complex relationship between particle structure and its properties.

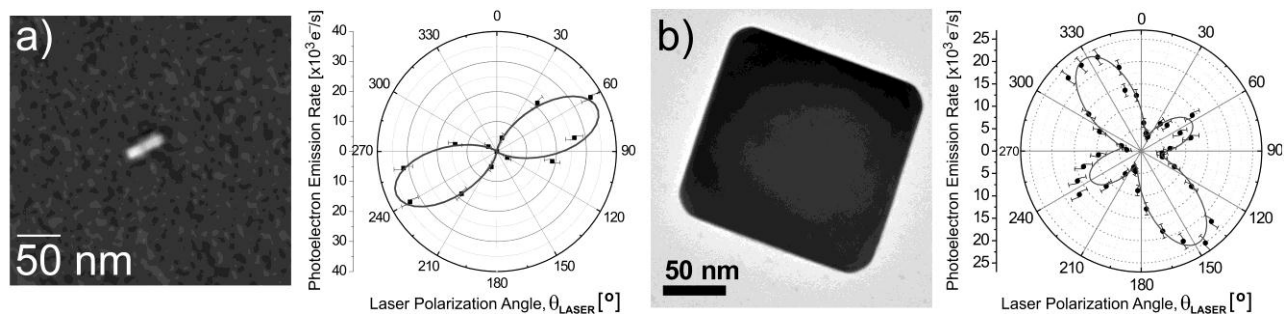


Figure 1: SEM/TEM images of a (a) Au nanorod and (b) Ag nanocube accompanied by polar plots of multiphoton photoemission vs laser polarization angle in the same reference frame (θ_{LASER}).

We have recently introduced scanning photoionization microscopy (SPIM) as a powerful, highly sensitive, single-particle technique for studying individual, supported nanoparticles [1,2]. In this technique, photoelectron emission from single nanoparticles following multiphoton absorption is measured. We show that in metallic nanoparticles coupling of incident radiation to localized surface plasmon (LSP) modes is essential for efficient photoelectron emission. For example, strongest photoelectron emission is observed when a plasmon is resonantly excited as well as when the incident laser polarization is aligned with the direction of the resonant plasmon mode (Fig. 1). It is shown that the observations are well described in terms of a coherent multiphoton photoelectric effect. The mechanism thought to occur on metallic surfaces upon femtosecond excitation is enhanced by several orders of magnitude in case of nanoparticles due to the local near-field enhancement that arises upon resonant excitation of a LSP. The finding not only opens a pathway for studying plasmons in nanoparticles that are much smaller than typically studied in conventional

We-II-3

optical microscopies, but also highlights the SPIM technique as a potential route to map local electric field enhancements in nanoparticles and nanostructures.

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We-III-1

OBSERVATION OF UNDULATOR RADIATION AT CHANNELING OF ELECTRONS AT MAMI

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At channeling the directions of charged particles are closely aligned with atomic rows (strings) or crystal planes, and their motion is governed by many correlated collisions with the crystal atoms. As a result, the particles are steered along strings or planes and all cross-sections associated with the interaction of charged particles with matter are substantially changed in comparison to amorphous matter. Although the potential depths are in the laboratory frame only in the order of some tens of eV, transitions between quantum states or the transverse oscillatory motion may result in photons with energies in the range between keV to multi MeV if the relativistic particle energies are in the range between a few MeV to some GeV, respectively. This so called channeling radiation is well known and was investigated in many papers. Experiments performed with electrons in the energy region between 180 and 1500 MeV at the Mainz Microtron MAMI are described in Ref. [1].

If the crystal planes are periodically bent at the direction the particle moves, undulator-like radiation in the hundreds of keV up to the MeV region may be emitted in addition to channeling radiation. The possibility to produce such radiation by means of positron channeling was discussed in a number of papers, see e.g. Ref. [2]. However, the demonstration and utilization of such devices hampers from the fact that high quality positron beams in the GeV range are not easily available, see e.g. Ref. [3], in contrast to electron beams. It was suggested in Ref. [4] that by means of planar channeling of ultrarelativistic electrons in a periodically bent single crystal the production of undulator-like radiation should also be possible.

There are several possibilities to realize crystalline undulator targets. Our approach is based on the production of graded composition strained layers in an epitaxially grown $\text{Si}_{1-x}\text{Ge}_x$ superlattice [5]. Because of the slight difference in the lattice constants between Si and Ge, adding a small content x of Ge to Si in a molecular beam epitaxy (MBE) growing process results in strain in the crystal and a bending of the crystal lattice. By varying the concentration x in the $\text{Si}_{1-x}\text{Ge}_x$ superlattice linearly and periodically [6], undulating (110) planes can be obtained.

Undulator crystals produced at the Aarhus University (UAAR) have been tested with the high quality electron beam of the Mainz Microtron MAMI. Experiments have been performed with 4-period epitaxially grown strained layer $\text{Si}_{1-x}\text{Ge}_x$ undulators with a period length $\lambda_U = 9.9 \mu\text{m}$. The experimental setup is described in Ref. [7]. The aim of these experiments was to characterize the bending features of the undulator crystals, and to explore its radiation emission characteristics.

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At goniometer scan signals, generated with electrons which had emitted a high energy bremsstrahlung photon, a characteristic broadening of the base width has been observed which amounted to about a factor of two for the (110) plane of the undulator crystal in comparison to a flat reference crystal. This broadening has been interpreted as a shift which originates from the maximum slope of an assumed sinusoidal function of the undulator crystal. Under this assumption amplitude of 4.0 Å has been deduced.

A broad excess yield around the theoretically expected photon energies of 0.069 and 0.637 MeV has been observed at (110) planar channeling for electron beam energies of 270 and 855 MeV, respectively. However, the peaks seem to be shifted to lower energies. This effect is not yet fully understood and is subject to further investigations. Possible reasons may be found in a non-sinusoidal undulator structure, and/or interference phenomena with bremsstrahlung or channeling radiation.

A simple analytic model is presented which explains both experimental observations, and may show into the direction for producing undulators with the wanted sinusoidal structure.

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We-III-2

CRYSTALLINE UNDULATOR AS A SOURCE OF COHERENT RADIATION

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Development of coherent radiation sources for a wavelength λ below 1 Å is a challenging goal of modern physics. Sub-angstrom wavelength powerful spontaneous and, especially, coherent radiation will have many applications in basic science, technology and medicine. In particular, they may have a revolutionary impact on nuclear and solid state physics as well as on life sciences.

The present state-of-the-art lasers are capable for emitting electromagnetic radiation from the infrared to ultraviolet range of the spectrum. Currently, there is one Free-Electron Laser (FEL) operating in the X-ray range ($\lambda \approx 1$ Å) [1]. Several other FEL X-ray facilities are either under construction or undergo advanced technical design work. Moving further, i.e. into the hard X or gamma ray band, is not possible without new approaches and technologies.

In the talk we discuss one of such novel approaches. The main phenomenon addressed is the radiation formed in a Crystalline Undulator (CU) [2]. In this device (see the figure) electromagnetic radiation which is generated by a bunch of ultra-relativistic particles channeling through a periodically bent crystalline structure. Such a system becomes a source of intensive spontaneous monochromatic radiation and, under certain conditions, also a source of the laser light [3]. A laser based on the CU could produce photons with $\lambda=0.01-0.1$ Å (the corresponding photon energy range is from tens-hundreds keV up to MeV region). Thus, its photon energy range starts where conventional FEL devices tail-off.

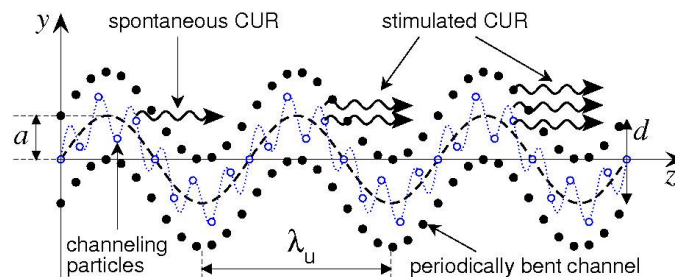


Figure 1: Schematic representation of CU [2,3]. The closed circles mark the atoms belonging to two neighbouring crystallographic planes (separated by the interplanar distance d) which are periodically bent. The period λ_u and amplitude a of bending satisfy the condition $\lambda_u \gg a \gg d$ (the y - and z -scales are incompatible in the figure!) Thin dotted line illustrates the trajectory of the particle (open circles), which propagates along the centerline (the undulator motion) and, simultaneously, undergoes channeling oscillations.

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NEW TRENDS FOR MANIPULATION OF CHARGED PARTICLE BEAM VIA COHERENT INTERACTIONS IN CRYSTALS

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Coherent interactions have proven to be an interesting technique to steer high-energy particle beams with the aim to aid or replace the traditional components of an accelerator for extraction, focusing, collimation, emission of coherent electromagnetic radiation and more. Nowadays, owing to the availability of crystals fabricated through most modern techniques of silicon micro-machining, specially designed crystal geometries can be tailored to investigate coherent interactions within a crystal. This availability has boosted research further and led to the discovery of new effects.

Planar channeling in a bent crystal has been the first effect to be studied. With the advent of a new generation of crystals, single-pass deflection efficiency exceeded 80% for protons at 400 GeV, i.e., a performance very close to the maximum theoretical limit. To date, planar channeling offers the best credentials for particle beam manipulation. In this sense, an experiment is under way by the UA9 collaboration with a study on beam halo collimation aimed at its application to the Large Hadron Collider. Planar channeling for negatively charged particles was also demonstrated to work with surprisingly high efficiency, too.

Aside from channeling, a new coherent effect in bent crystals, which could be used for beam manipulation, is volume reflection. Since its discovery in 2006, this effect offers extraordinary high efficiency and wide angular acceptance. The extent of deflection is somewhat limited especially at highest energies though some schemes to excite repeated volume reflections in an array of quasi-parallel crystals demonstrated that this scheme is a viable way for manipulation of either positively or negatively charged particles.

Very interesting effects from the physical point of view are axial and quasi-axial effects. With proper choice of the crystal geometry, axial channeling proved to be highly efficient with both signs of the particles. Among quasi-axial effects, special attention owes to multi-volume reflection within one crystal, a situation where planar-like and axial-like dynamics merge together. Each of the above coherent effects is accompanied by emission of x-ray radiation, a topic that deserves special attention as itself.

A very recent innovation in beam steering via interaction with an unbent crystal is the use of half wavelength crystals and the consequent effect of mirroring suffered by the particles traversing the crystal. Particles undergo half an oscillation and exit the crystal with reversal of the transverse momentum, resulting in beam deflection. This effect has been studied at relatively low energy (at some MeV) though it is considered for investigation beyond this range.

In summary, coherent interaction with bent and unbent crystals is a hot topic in particle accelerators, a research branch that is way far from exhaustion with blooming of experimental results and theoretical understanding. We review current state of the art for research in coherent interactions for steering charged particles and in its pertaining technology with a special attention to the practical applications to the physics of accelerators.

MESOSCOPIC SUPERSOLID OF DIPOLE CLUSTERS

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A mesoscopic system of dipolar bosons trapped by a harmonic potential is considered. The system has a number of physical realizations including dipole excitons, atoms with large dipolar moment, polar molecules, Rydberg atoms in inhomogeneous electric field.

We carry out a diffusion Monte Carlo simulation to define the quantum properties of a two-dimensional system of trapped dipoles at zero temperature. Temperature effects are also studied by path integral Monte Carlo method.

In dimensionless units the system is described by two control parameters, namely the number of particles and the strength of the interparticle interaction. We have shown that when the interparticle interaction is strong enough a mesoscopic crystal cluster is formed. As the strength of interactions is decreased a multi-stage melting takes place. Off-diagonal order in the system is tested using natural orbitals analysis. We have found that the system might be Bose condensed even in the case of strong interparticle interactions. There is a set of parameters for which a spatially ordered structure is formed while simultaneously the fraction of Bose condensed particles is non zero. This might be considered as a realization of a mesoscopic supersolid.

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We-IV-2

FROM PAULI'S BIRTHDAY TO CONFINEMENT RESONANCES: A POTTED HISTORY OF QUANTUM CONFINEMENT

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Quantum Confinement is in some sense a new subject. International meetings dedicated to Quantum Confinement took place only recently in Mexico City (the second was in September 2011 and the first, a year before). However, at least in principle, the subject has existed since a very long time. Surprisingly perhaps, it lay dormant for many years, for want of suitable experimental examples. However, when one looks carefully at its origin, it turns out to have a long and distinguished history. In fact, the problem of quantum confinement raises a number of very interesting issues concerning boundary conditions in elementary quantum mechanics and how they should be applied to real problems. Some of these issues were missed in the earliest papers, but are implicit in the structure of quantum mechanics, and lead to the notion of Confinement Resonances, the existence of which was predicted theoretically more than ten years ago. Although, for several reasons, these resonances remained elusive for a very long time, they have now been observed experimentally, which puts the whole subject in much better shape and, together with the advent of metallofullerenes, has contributed to its revival.

Posters

ION SYNTHESIS OF METAL NANOPARTICLES

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Composite materials containing metal nanoparticles (MNP) are now considered as a basis for designing new photonic media for optoelectronics and nonlinear optics. Simultaneously with the search for and development of modern technologies intended for nanoparticle synthesis, substantial practical attention has been devoted to designing techniques for controlling the MNP size. This is caused by the fact that the properties of MNPs that are required for various applications, take place up to a certain MNP size. One of the most promising enhanced fabrication methods to synthesize MNPs is ion implantation because it allows reaching a high metal filling factor and a control of MNP sizes [1]. A most critical parameter of ion implantation is ion dose, which determines the implant amount. When the concentration of implanted metal ions exceeds the solubility limit of metal in dielectric matrices, the system relaxes by nucleation and growth of MNPs. Recent results on ion-synthesis and nonlinear optical properties of silver, copper and gold nanoparticles in surface area of various silicate glasses are presented. Composites prepared by the low energy ion implantation are characterized with the growth of MNPs with a size distribution in the depth of thin area of irradiated substrate surface. Fabricated structures lead to specific optical nonlinear properties in wide spectral area from UV to IR such as nonlinear refraction, saturation and two-photon absorption, optical limiting. Their nonlinear optical characteristics strongly depend on variations of nanoparticles size. The practical recommendations for fabrication of composites with implanted metal nanoparticles for optical components are suggested.

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ENERGY LOSS DISTRIBUTION OF ENERGETIC CARBON BEAMS IN LIQUID WATER

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Cancer treatment with swift heavy ion beams is much more efficient than conventional photon or electron beam radiotherapy, which deposit a substantial fraction of their initial energy near the entrance surface of the irradiated tissue, causing undesirable damage, especially for deep-seated tumors. However, energetic ion (like proton or carbon) beams have a well defined penetration range, do not suffer significant angular scattering, and lose most of their energy in a well localized region near the end of their trajectories, the so-called Bragg peak. This characteristic behavior allows high doses delivering in the tumor target with low effect in the surrounding normal tissue.

Liquid water is a major component of living tissue, so the energy deposited by energetic carbon beams in this target is important for dose distribution studies in carbon beam cancer therapy.

In this communication, we present the energy loss distribution of carbon beams in liquid water calculated with the dielectric formalism together with an accurate description of the electronic excitation spectrum of the target, which is obtained from available experimental optical data properly extended to non vanishing momentum transfers. We also discuss the effects of different descriptions of the electronic charged density of the carbon projectiles.

**MODELING OF WATER CLUSTERS FORMATION PROCESSES IN THE
INNER ATMOSPHERE OF COMETS**

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The kinetics of molecular clusters formation is of great interest for large number of applications in science and technology. In particular, preliminary estimations of near-nucleus comets' atmosphere parameters affected strongly by water clusters formation processes [1] are required for correct interpretation of experimental results and theoretical predictions.

The powerful tool for numerical investigation of rarefied comet atmospheres is the direct simulation Monte Carlo (DSMC) method [2]. The model of water clusters formation for the DSMC technique was developed on the base of the kinetic approach [3, 4]. The model takes into account hierarchy of kinetic processes from water dimer formation by binary and triple collisions up to molecule-cluster and cluster-cluster associations. The probabilities of association acts under particles collisions, the influence of intra-molecular vibrations of water molecules in clusters on cluster decay rate were analyzed.

The influence of nucleus gas productivity on intensity of cluster formation process in comet water jets was investigated using the developed clusterization model and the DSMC technique. The data on resulting condensation mass, size distributions of observed water clusters, velocities, internal energies of clusters were obtained. The effect of condensation on flow structure was discussed.

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**CATALYSIS DRIVEN BY SUBNANO-SPACE POLARIZED CHARGES
CREATED BY SUPPORTED BI-ELEMENT CLUSTERS**

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Since the discovery of clusters in an atomic beam 40 years ago, a number of fundamental properties originating from their many-body and tiny natures have been unveiled. For instance, electrons in a metal cluster are confined but delocalized in it. One can obtain high performance functions by amplifying these cluster-specific properties controllably in a wide dynamic range on/in an appropriate surface and interior of a solid material, a solution and a gas atmosphere. They are further tuned precisely in electric, magnetic and chemical fields with internal species such as dopants and ligands as well as the corresponding external fields.

We have created successfully two-dimensional charge polarization in a subnano-space due to electron accumulation at an interface between a monatomic-layered Pt cluster disk and a substrate Si surface [1-4]; the electrons are transferred from the cluster disk to the subnano-space interface in a similar manner as the Schottky barrier junction, while the counter positive charge is delocalized in the cluster disk. This can be controlled precisely through one-by-one doping of an electron-donor or acceptor atom into the cluster [5].

It is straightforward that the polarized charges promote catalytic activity significantly, because rich charges are favorable for the reduction and oxidation of molecules, which are defined as capture and release of electrons, respectively. Focusing on the catalysis as a global key issue of energy and materials we are confronted with, we present a high-performance catalytic activity of the Pt cluster disk on the Si substrate in thermal oxidation of CO, which is promoted further by doping only a single Ag atom as the electron donor.

The controlled atom doping to the cluster was carried out by deposition of uni-atomic-composition bi-element clusters, Pt_NAg_M [5,6]. The cluster ions were generated in a dual-magnetron cluster-ion source, their atomic composition was definitely selected by passing through a quadrupole mass filter, and the deposition was made by cluster impact [7] onto the Si(111)- 7×7 reconstructed surface. The cluster density was maintained at less than 0.05 nm^{-2} to avoid any undesirable cluster-cluster interactions on the substrate. Then, the substrate surface was terminated with hydrogen for their protection against the reactants. Temperature-programmed desorption (TPD) mass spectroscopy [6] and flow-reaction (FR) mass spectroscopy were employed to obtain the mechanism and the kinetics for the catalytic reaction; the intensity of the reaction product, CO_2 , was measured as a function of the cluster temperature at limited amounts of the reactants adsorbed and with continuous supply of the reactants in TPD and FR, respectively. Sensitive detection was achieved using isotope-labeled $^{18}O_2$ and $^{13}C^{16}O$ as the reactants.

Figure 1 shows the TPD results of the Pt₃₀ disks at various amounts of the reactants. Discernible are two sharp peaks below 200 K and four broad ones at the higher temperatures. The peak temperatures do not change with the dose amount or the Pt-Ag replacement, but the peak ratios do.

In comparison with the same reaction on the Pt(111) surface [8], the peak at 130 K is assigned to the CO oxidation by the molecularly adsorbed O₂^{δ-} (α site) in the Langmuir-Hinshelwood (LH) mechanism. The interatomic distance of O₂^{δ-} is elongated by electron capture into its anti-bonding molecular orbitals from the cluster disk. This is lower by ~15 K than that of the Pt(111) surface. The peak at 185 K is inherent to the clusters, and assignable to another molecular O₂^{δ-} site (α') in the LH mechanism. Those observed between 270 and 450 K are assigned to the dissociatively adsorbed O (β_i sites). The β sites of the Pt cluster disk have larger branching fractions than those of the Pt(111) surface, and are promoted further by the substitution of Pt with only the single-atom Ag as the electron donor. These results indicate that the catalytic activity is enhanced by the more negative charge in the subnano space through the more efficient activation of O₂.

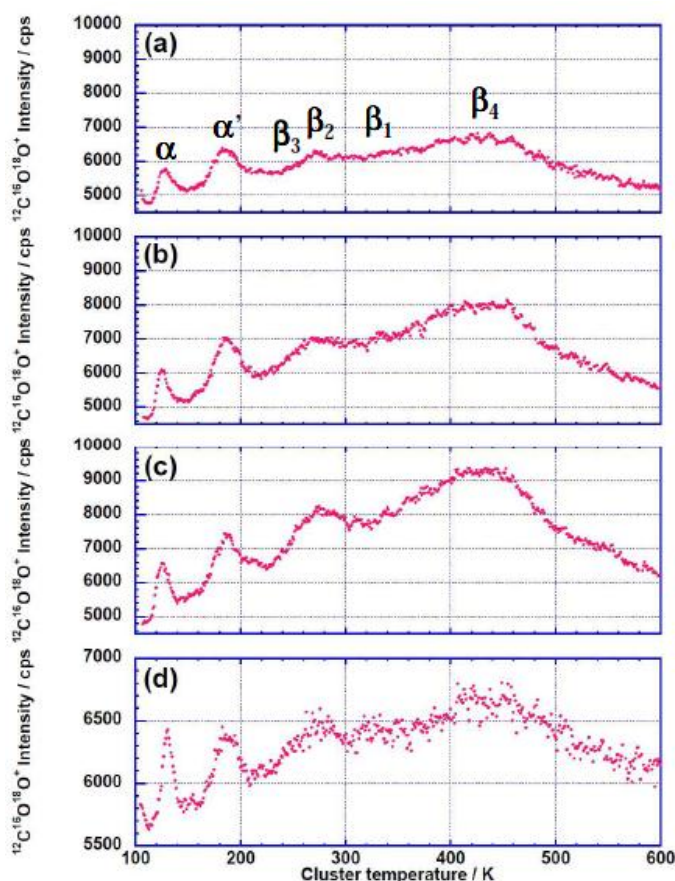


Figure 1: TPD results of CO oxidation on Pt₂₉Ag₁ supported on Si surface with dose amounts of ¹⁸O₂ and ¹²C¹⁶O at (a) 0.2 L, (b) 0.5 L, (c) 1 L and (d) Pt₃₀ at 1 L. Peak assignment is shown in panel (a).

The reaction probabilities per Pt atom of both the α and β sites decrease with the dose amount of the reactants. This is recognized as spillover of the reactants, i.e. they escape from the clusters before the completion of the reaction. Indeed, the relative branching ratio of the α sites to the β ones becomes smaller with the dose amount due to the faster spillover rate for O₂ than CO and O. This shows an important role of the substrate as a reactant reservoir for the cluster catalysts.

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PS-05

MASS-SELECTED PHOTODISSOCIATION STUDY OF AlPb_N^+ CLUSTERS ($N = 7-16$): EVIDENCE FOR THE EXTRAORDINARY STABILITY OF AlPb_{10}^+ AND AlPb_{12}^+

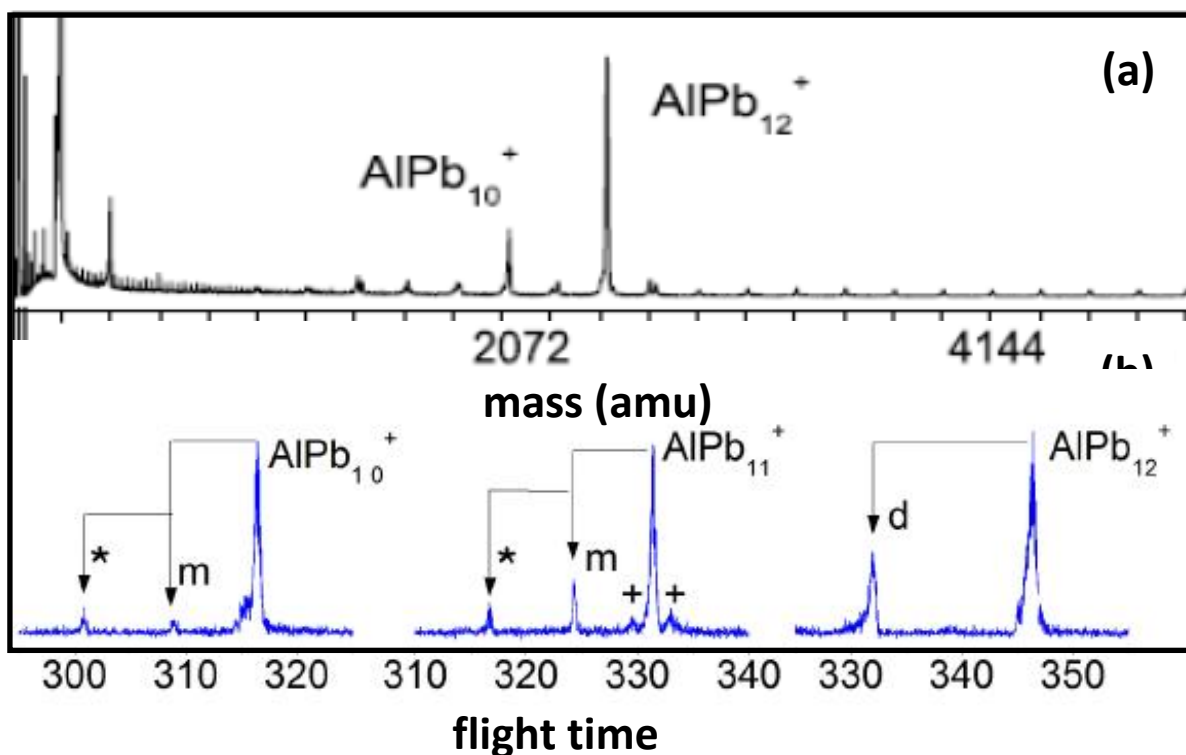
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We report on the fragmentation pathways and dissociation energies of AlPb_n^+ ($n = 7-16$) clusters. The clusters are produced with pulsed laser vaporization and studied in a supersonic molecular beam. They are mass-selected and photodissociated with 532 and 355 nm laser light. Photofragments are thereafter mass-separated in a tandem reflectron time-of-flight mass spectrometer. Bare Pb_n^+ ($n = 8-16$) clusters prefer atomic Pb evaporation, with the exception of Pb_{15}^+ that fragments by loss of a Pb_2 dimer to form the stable Pb_{13}^+ cluster, in line with computational predictions [1]. The smallest AlPb_n^+ ($n = 7-11$) also show mainly atomic Pb evaporation, while the favored fragmentation pathway of larger aluminum doped lead clusters ($n = 12-16$) involves Pb_2 and Pb_3 fragments. AlPb_{10}^+ and AlPb_{12}^+ are the most intense fragments of several larger cluster sizes, confirming the superatom character of these two clusters [2]. Dissociation energies for the most facile fragmentation channel are bracketed from the measured laser fluence dependencies of daughter intensities using a detailed balance model [3,4].



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PSEUDOPOTENTIAL CORRECTION TO THE JELLIUM MODEL FOR FULLERENES

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A new type of a correction for a more accurate description of fullerenes within the spherical jellium model is considered. The correction represents a pseudopotential which originates from the comparison between the results of an accurate *ab initio* and the jellium model calculations.

Contemporary software for quantum-chemical calculations (e.g., Gaussian 09 [1]) provides an accurate quantitative description of the ground state of many-particle systems and allows one to obtain information on geometrical and chemical properties of the system. However, the description of dynamic properties, which play an important role in the process of photoionization, by means of such programs faces significant difficulties. Thus, collective electron excitations in fullerenes, which lie in the continuous spectrum, have not been described so far by means of quantum-chemical programs. However, this can be achieved within simplified model approximations, e.g. the jellium model.

Within the jellium model a detailed ionic structure of the system is smeared out and substituted by the uniform distribution of the positive charge. The simplest approach for the ionic core of a fullerene is the uniform distribution of the positive charge over a spherical layer of the finite thickness [2]. However, the calculations show that the ground state properties of fullerenes cannot be described properly by the standard jellium model which produces, in particular, unreliable values for the total energy of the system [3].

In this contribution we introduce a structured pseudopotential for calculations of the ground state of the C₆₀ and C₂₀ fullerenes which originates from the comparison of an accurate *ab initio* calculation with the jellium-based one [4]. It is shown that such a correction to the standard jellium model allows one to introduce effects of the sp²-hybridization of carbon atomic orbitals into the model. Therefore, it may be considered as a more physically meaningful correction as compared to the structureless square well pseudopotential which has been widely used earlier (see, e.g., [3]). The results of calculations of the ground state of C₆₀ and C₂₀ within the “modified” jellium model, and the Hartree-Fock and local density approximations are discussed.

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CARBON CLUSTERS AS AN EXAMPLE FOR SELF-ORGANIZATION

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According to the main principles of self-organized criticality (SOC) concept [1], there is a number of giant dissipative dynamical systems which are able to accumulate small external perturbations. Mathematical criterion of self-organization is a power-law behavior of avalanche size probability density. Several systems have been shown to exhibit SOC in terms of finite-size scaling as well as power law avalanches, such as pile of rice, magnetic vortices in superconductors [2] etc. The aim of this work is to show that carbon clusters such as nanotubes and graphite powder can serve as convenient objects for experimental investigations of SOC. Self-organized criticality can be experimentally observed as a power-law behavior of the resistance, which is controlled by the applied voltage. The initial samples, used in this study, were in the form of multiwalled carbon nanotubes (CNTs) with 20–70 nm diameter and up to 150 nm length [3]. We investigated the static CVC of the samples in the current generator regime. The samples were formed on the surface containing current contacts (the distance between the contacts is 0,7 mm), with the help of well-known technique of creating "sand pile" [4]. Fig. 1 shows the geometry of the experiment.

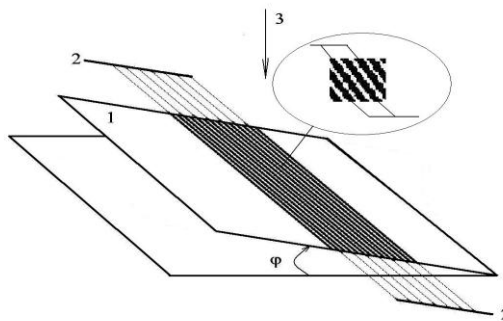


Figure 1: The geometry of the experiment: 1 – the plane forming a heap, φ – the angle of the plane, 2 – current contacts, 3 – line submission of portions of the powder.

At the beginning we carried out experiments to determine the critical angle of SOC for the samples. Critical angle corresponds to the avalanche, and hence a sharp increase in resistance, because dramatically reduced the amount of matter in the field measurements. We need to measure the slope of the heap (φ_c) for «avalanches» of CNTs. We present here the experimental study results of the evolving sand pile resistance dynamics. The φ_c value corresponds to the sharp increase in resistance is 30° and 70° for CNTs. We present a study of the static voltage-current characteristics which vary from ohmic ($U_{\min}=2V$) to breakdown ($U_{\max} \sim 20V$) on

above mentioned samples. The typical CVC for CNTs samples with a region of sharp current increase with U_{\max} and developing instability are obtained. Close to the critical voltage U_{\max} , the $I-V$ curves are typical of the thermally induced destruction for CNTs samples; at voltages $U < U_{\max}$, the ohmic $I-V$ behavior is observed. At voltages close to the critical one, the detailed shape of the $I-V$ curve is typical of multi-walled CNTs [5]. Typical dependencies of CNTs resistance R by the number of material portions n are shown at the Fig. 2. The power-law behavior of $R(n)$ typical for SOC is observed. Dependency of line slope (B) by voltage (see Fig. 2) can be an evidence of inter-nanotube circuits influence to the critical state formation. Line slopes of CNTs powder are: $B = -1,52$ (U_{\min}), $B = -0,28$ (U_{\max}).

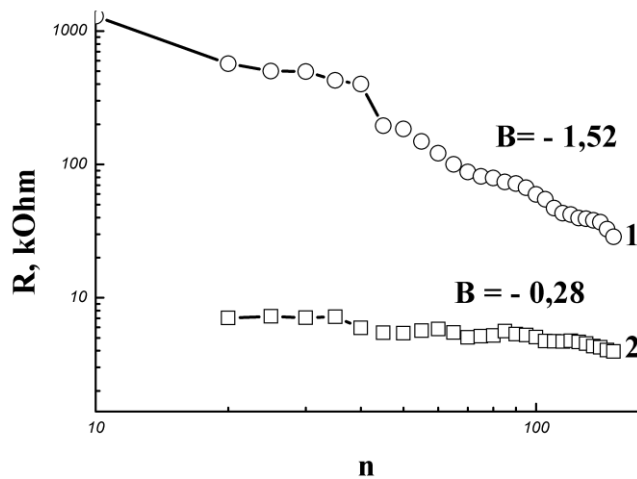


Figure 2: The resistance R of CNTs samples at U_{\min} (1) and U_{\max} (2) as a function of n . Best fit line slope- B .

We have presented that the experimental method of measuring the electrical resistance of the lateral layers at certain slopes of the surface, where the sample is formed on the basis of entangled bunches of multiwalled nanotubes can be used to study SOC in the sand heap technique. It was shown experimentally that the appeared self-maintained critical state can be controlled using an external electric action. We found that, in prebreakdown electric fields, likely, analogs of thermally controlled avalanches appear, but the avalanches, unlike hard Type-II superconductors, do not cause destruction of the critical state and only change (decrease) the exponent in the SOC law.

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NONCOLLINEAR MAGNETIC PHASES IN MANGANITES

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Depending on the chemical composition and doping level, the doped manganites $R_xA_{1-x}MnO_3$ ($R = La, Pr, Nd, Sm$; $A = Ca, Sr, Ba$) with a perovskite structure can either be in the ferromagnetic state or have different types of antiferromagnetic (AF) order. Apart from simple antiferromagnetic structures of the G, A, and C types, there can arise more complex structures consisting of ferromagnetic chains antiferromagnetically ordered with respect to each other. All the aforementioned magnetic phases are collinear. However, the experiment has demonstrated that manganites contain not only collinear but also spiral magnetic structures.

The effective Hamiltonian in this study is the standard model Hamiltonian [1–3] $H = H_{DE} + H_{AF}$, where the double exchange Hamiltonian has the form

$$H_{DE} = \sum_{i\alpha\sigma} \varepsilon_{0\sigma} d_{i\alpha\sigma}^\dagger d_{i\alpha\sigma} + \sum_{\langle i,j \rangle > \sigma\sigma'} t_{ij}^{\alpha\beta} \{d_{i\alpha\sigma}^\dagger [U(\theta_i, \varphi_i)U^\dagger(\theta_j, \varphi_j)]_{\sigma\sigma'} d_{j\beta\sigma'} + \text{H.c.}\} - \frac{J_H S}{2} \sum_{i\alpha} (d_{i\alpha\uparrow}^\dagger d_{i\alpha\uparrow} - d_{i\alpha\downarrow}^\dagger d_{i\alpha\downarrow}) \quad (\sigma, \sigma' = \uparrow, \downarrow)$$

The Heisenberg Hamiltonian $H_{AF} = J_s \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ describes the antiferromagnetic exchange between the local spins \mathbf{S}_i and \mathbf{S}_j of the neighboring ions (J_s is the exchange Heisenberg parameter). The transformation U of the spinor components appears as a result of the rotation of the local system of the coordinates at each manganese atom, which accompanies any translation by the direct lattice vector. For spirals the translation invariance of the lattice is retained (see review [4]), which makes it possible to use the Bloch theorem for constructing the wave function and calculating the spectrum of noncollinear magnetic structures. The matrix element of the Hamiltonian of a noncollinear magnetic structure between the nearest spinors $\alpha(\beta)$ at atoms with indices i and j has the form $H_{ij\sigma\sigma'}^{\alpha\beta}(k) = \sum_{ij} t_{ij}^{\alpha\beta} (U_j^\dagger U_i)_{\sigma\sigma'} e^{ikR_j} \quad (\sigma, \sigma' = \uparrow, \downarrow)$.

Thus, the main result of transformation U is the appearance of the off-diagonal (in spin indices) matrix elements of the Hamiltonian of the interaction between the nearest neighbors.

The last expression allows to obtain the matrix of the Hamiltonian $H(\mathbf{k})$ of the noncollinear magnetic structures with the wave vector \mathbf{q} . If the spiral structures are considered, the Hamiltonian matrix can be easily written using the formulas derived in [3]. In the general case, in order to determine the region of existence of the spiral structures, it is necessary to minimize the total energy of the system with Hamiltonian according to the technique described in [3] with the inclusion of different spiral structures. In the proposed approach, we can also consider small magnetic clusters with arbitrary magnetic structure.

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STABLE ANIONS OF SMALL Xe CLUSTERS: MANY-BODY AB INITIO STUDIES

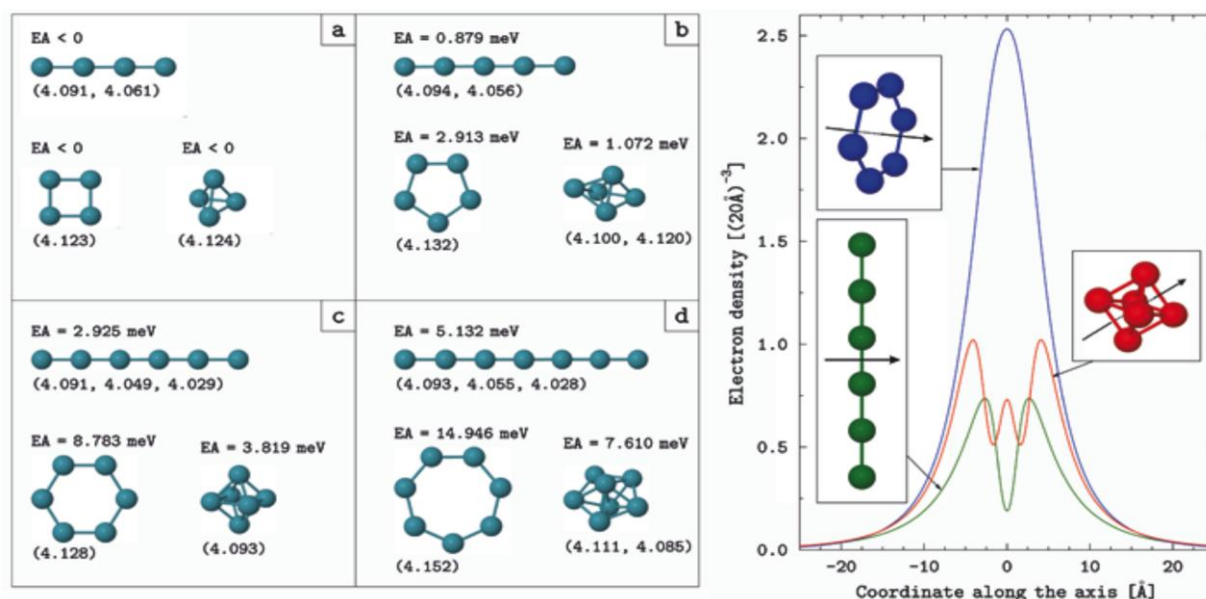
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It is known that the rare-gas atoms do not form stable anions. Can a cluster of these atoms support a bound anion? If the answer is positive, what are the minimum numbers of the atoms in a cluster which binds the extra electron? What are the electron binding energies for stable cluster anions? Till recently, these questions were addressed on the grounds of model approaches to the electron-cluster interaction. We report on extensive all-electron *ab initio* studies on anions of the Xe clusters [1]. There, major effort is required to include, in a rigorous quantum many-body formalism, the long-range electron correlation that plays a primary role in the binding. Cluster structures of different dimensionalities are investigated: conventional three dimensional, planar and linear structures of Xe clusters. Independently of the dimensionality of the cluster, the *minimal number* of Xe atoms required to form a stable cluster anion is found to be 5 atoms. Electron affinities are computed for clusters of 5, 6, and 7 atoms, and the planar clusters are found to form the most stable anions.



Left: Properties of the Xe clusters of different dimensionalities with 4 (a), 5 (b), 6 (c) and 7 (d) atoms. The clusters are shown by atomic spheres connected by bonds, with the radii of the spheres being 1.08 Å (half of the van der Waals radius of Xe). Indicated above each cluster are the electron affinities (EA) and the numbers given in brackets below each cluster are the internuclear separations in Å.

Right: Density of the attached electron for different dimensionalities of clusters made of 6 Xe atoms. The electron density is shown along the axes indicated by the arrows in insets, the centers of the axes coincide with the centers of the clusters.

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COMPUTER MODELLING OF CHANNELING EFFECT USING MBN EXPLORER SOFTWARE

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In the proposed talk we present and discuss implementation of relativistic equations of motion by means of the MBN Explorer [1] package and their application to modelling the channeling effect. The motion of individual electrons and positrons is simulated in the field created by crystal atoms. Each atom is treated as a screened point charge in the Moliere potential approximation. The crystalline structure is generated dynamically, and this allows one to efficiently simulate any desired number of crystal constituents. The effect of thermal vibration of crystal atoms is taken into account.

The projectile trajectory is calculated by solving the relativistic equation of motion using Runge–Kutta time step integration. This approach is compared to the previous work [2], based on a simplified treatment of the particle motion in a crystalline structure. Results are also compared to experimental data from work [3] which refers to the channeling process of 855MeV electron in a straight Si(110) crystal. It is shown that the current approach provides better consistency with the experimental results.

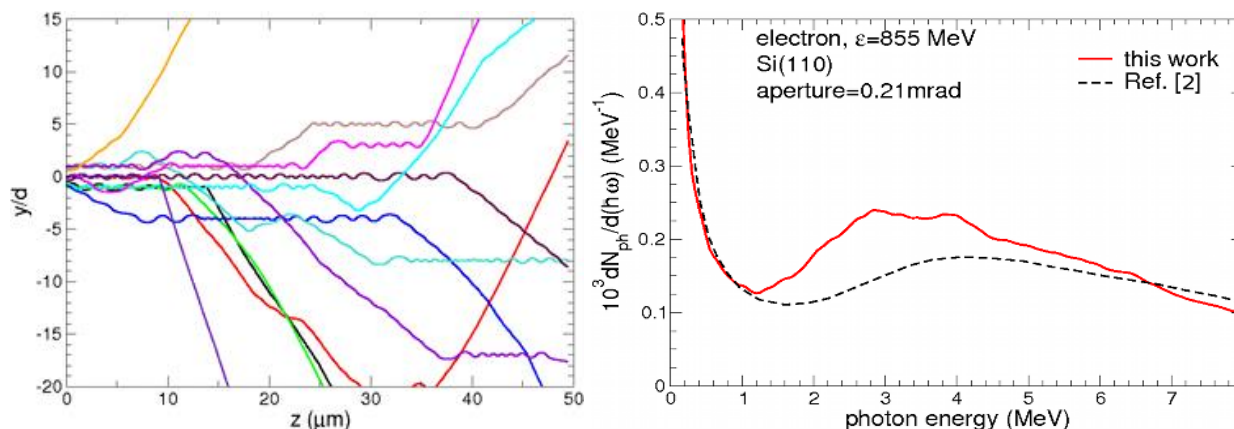


Figure 1: a) Example set of random trajectories of 855MeV electron channeling along Si (110). b) Comparison of radiation spectrum computed with MBN Explorer and code from Ref. [2]

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For notes

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Sunday, 30 September 2012

16 ⁰⁰ – 18 ⁰⁰	Participants registration
18 ⁰⁰ – 21 ⁰⁰	Conference reception

Monday, 1 October 2012

9 ⁰⁰ – 9 ³⁰	DySoN 2012 Opening Andrey V. Solov'yov
9 ³⁰ – 11 ⁰⁰	<i>Morning session I: Structure and dynamics of clusters, nanoparticles and biomolecules</i> <i>Chair: Jean-Patrick Connerade</i> Julius Jellinek Philippe Brechignac Eric Suraud
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<i>Morning session II: Nanoscale dynamical transitions and transformations</i> <i>Chair: Julius Jellinek</i> Shiv N. Khanna Jerry Bernholc Andrey Lyalin
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<i>Afternoon Session I: Nanoscale insights in biodamage</i> <i>Chair: Bernd Huber</i> Sandrine Lacombe Pablo de Vera Oral presentation of posters (Presentations 1-3)
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	<i>Afternoon Session II: Clustering and self-organization on the nanoscale</i> <i>Chair: Catherine Bréchnignac</i> Kit Bowen Michael Willkinson Sergiy Perepelytsya

Tuesday, 2 October 2012

9 ³⁰ – 11 ⁰⁰	<i>Morning session I: Collision processes involving nanosystems</i> <i>Chair: Eric Suraud</i> Bernd Huber Rafael Garcia Molina Bing Zhang
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<i>Morning session II: Thermo-mechanical, optical and magnetic properties of nanosystems</i> <i>Chair: Shiv N. Khanna</i> Florent Calvo Alexander Yakubovich Mikhail Petrzhek
13 ⁰⁰ – 13 ¹⁵	Conference photo

13 ¹⁵ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<i>Afternoon session I: Clustering and self-organization on the nanoscale</i> <i>Chair: Kit Bowen</i> Catherine Bréchnignac Artur Böttcher Iliia A. Solov'yov
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ¹⁰	Oral presentation of posters (Presentations 4-10) Open discussion

Wednesday, 3 October 2012

9 ³⁰ – 11 ⁰⁰	<i>Morning session I: Nanoscale insights into biodamage</i> <i>Chair: Rafael Garcia Molina</i> Eugene Surdutovich Gustavo Garcia Ilya I. Fabrikant
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<i>Morning session II: Collision processes involving nanosystems</i> <i>Chair: Andrei Korol</i> Vadim Ivanov Alexey Verkhovtsev Andrej Grubisic
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<i>Afternoon session I: Propagation of particles through medium</i> <i>Chair: Vadim Ivanov</i> Hartmut Backe Andrei Korol Vincenzo Guidi
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 17 ³⁰	<i>Afternoon session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i> <i>Chair: Andrey V. Solov'yov</i> Yurii Lozovik Jean-Patrick Connerade
17 ³⁰ - 18 ⁰⁰	Open discussion Conference Closing
19 ⁰⁰ – 22 ³⁰	Conference Dinner

Thursday, 4 October 2012

09 ⁰⁰ – 16 ⁰⁰	Conference tour
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