

**International Conference
"Dynamics of Systems on the Nanoscale"**

DySoN 2014 Conference

Crowne Plaza Edinburgh – The Roxburghe Hotel
Edinburgh, United Kingdom
May 19 - 23, 2014



Book of Abstracts

Editors: Nigel J. Mason and Andrey V. Solov'yov

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Preface

The Third International Conference "Dynamics of Systems on the Nanoscale" (DySoN 2014) will be held in Edinburgh, UK during May 19-23, 2014. The venue will be Crowne Plaza Edinburgh – The Roxburghe Hotel, 38 Charlotte Square, EH2 4HQ. The Conference will be preceded by the training course on Computational Methods for Complex Molecular Systems.

The DySoN conference has been built upon a series of International Symposia "Atomic Cluster Collisions" (ISACC 2003, 2007, 2008, 2009, 2011 and 2013). During these meetings it became clear that there is a need for an interdisciplinary conference, which will cover 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 Rome, Italy in 2010, and the second conference was held in St. Petersburg, Russia in 2012. Proceedings of DySoN 2012 were published in Journal of Physics: Conference Series (<http://iopscience.iop.org/1742-6596/438/1>). DySoN 2014 is the third conference in this series.

The DySoN 2014 Conference will promote the growth and exchange of interdisciplinary 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.

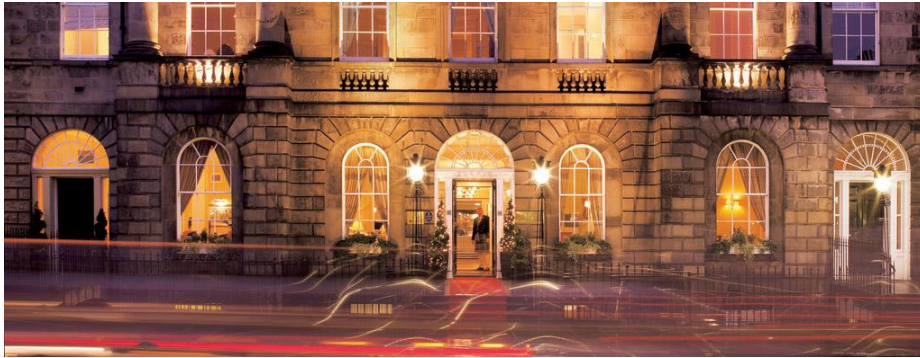
Although mesoscopic, nano- and biomolecular systems differ in their nature and origin, a number of fundamental problems are common to all of them: What are the underlying principles of self-organization and self-assembly of matter at the micro- and nano-scale? Are these principles classical or quantum? How does function emerge at the nano- and the meso-scale in systems with different origins? 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 entitled Meso-Bio-Nano (MBN) Science.

Experimental and theoretical aspects of these problems will be discussed at the DySoN 2014 Conference. Particular attention will be devoted to dynamical phenomena and many-body effects taking place in various MBN systems on the nanoscale that 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 Crowne Plaza Edinburgh - The Roxburghe Hotel, 38 Charlotte Square, Edinburgh, EH2 4HQ. The hotel is conveniently situated in a 15 minutes walking distance from Edinburgh's main railway station, The Waverley.

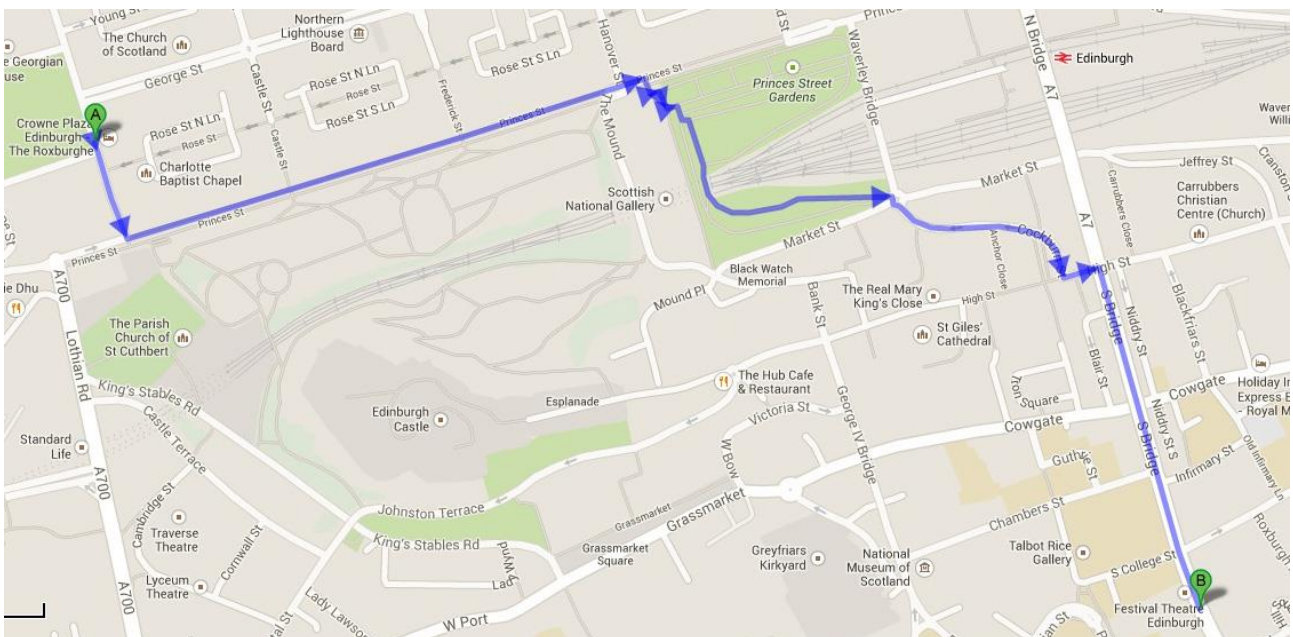


Conference Reception

The conference reception will be located in the hotel.

Conference Dinner

The conference dinner will take place at the Surgeons' Hall on Tuesday, May 22. Surgeons' Hall is situated at the Royal College of Surgeons of Edinburgh, approximately 2 km (25 minutes walk) from the conference venue. The map below shows the route from the Crowne Plaza Edinburgh – The Roxburghe Hotel (A) to the Surgeons' Hall (B).



Castle Visit

On Wednesday, May 21, there will be a visit to the Edinburgh Castle, Scotland's leading tourist attraction, and a key element of the Edinburgh World Heritage Site. More information about the Castle can be found via the following link: <http://www.edinburghcastle.gov.uk/>.

The tour will start at 14.30 from the conference hotel and end at 18.00.

Organizing Committee

| | |
|---------------------|--|
| Beverley Bishop | The Open University, UK |
| Andrei V. Korol | MBN Research Center and Goethe University, Germany |
| Nigel J. Mason | The Open University, UK |
| Andrey V. Solov'yov | MBN Research Center and Goethe University, Germany |

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- The Open University
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DySoN 2014 Conference Webpage

Updated information on the conference is available at the following webpages:
<http://www.open.ac.uk/science/physical-science-conferences/dyson-may-2014>

and

<http://www.mbnresearch.com/dyson-2014>

International Advisory Committee

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Germany

Dr. Surdutovich, Eugene

Oakland University
USA

Conference Program

Monday, 19 May 2014

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

Tuesday, 20 May 2014

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| 9 ⁰⁰ – 9 ³⁰ | DySoN 2014 Opening: Nigel Mason and Andrey V. Solov'yov |
| 9 ³⁰ – 11 ⁰⁰ | <u><i>Morning session I: Structure and dynamics of clusters, nanoparticles and biomolecules</i></u> Nigel Mason , The Open University, UK <i>Creating nanostructures with electrons and light</i> Eric Suraud , Universite Paul Sabatier, France <i>Clusters and molecules in extreme light</i> Julius Jellinek , Argonne National Laboratory, USA <i>Analysis of structural and dynamical complexities of finite heterogeneous systems</i> |
| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <u><i>Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i></u> Richard Palmer , University of Birmingham, UK <i>Atomic structure and dynamics of size-selected clusters and polyatomic molecules</i> Yuri Vainer , Institute of Spectroscopy RAS, Russia <i>Low-temperature spectral dynamics of single molecules in ultrathin nanofilms and subsurface layers of amorphous polymers</i> Michael Wilkinson , The Open University, UK <i>Two universalities in semiconductor physics</i> |
| 13 ⁰⁰ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 16 ⁰⁰ | <u><i>Afternoon Session I: Nanoscale insights in biodamage</i></u> Lenka Stefancikova , Université Paris Sud, France <i>Enhancement of medical radiation effects using nano-radiosensitizers: evidence of nanoscale phenomema</i> Pablo de Vera , Universitat d'Alacant, Spain <i>Cell irradiation with ion beams: realistic description of subcellular compartments</i> |

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| | Brenda Laster , Ben Gurion University, Israel <i>An innovative technique for preventing telomere elongation and its associated immortalization of cancer cells</i> |
| 16 ⁰⁰ – 18 ⁰⁰ | Coffee and poster session |

Wednesday, 21 May 2014

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| 9 ³⁰ – 11 ⁰⁰ | <u><i>Morning session I: Propagation of particles through medium</i></u> Hartmut Backe , Institute of Nuclear Physics, Germany <i>Channeling experiments at the Mainz Microtron MAMI</i> Andrei Korol , Goethe University, Germany <i>Simulation of radiation spectra from electron- and positron-based crystalline undulators</i> Vincenzo Guidi , Universita di Ferrara, Italy <i>Channeling of negatively charged particles</i> |
| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <u><i>Morning session II: Particle confinement phenomena</i></u> Jean-Patrick Connerade , Imperial College, UK <i>Selecting interesting atoms for quantum confinement</i> Andrea Mazzolari , Universita di Ferrara, Italy <i>Study of coherent interactions between a sub-GeV electron beam and a thin bent silicon crystal</i> Gennady Sushko , Goethe University, Germany <i>Simulation of electron, positron and muon channeling</i> |
| 13 ⁰⁰ – 13 ¹⁵ | Conference photo |
| 13 ¹⁵ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 18 ⁰⁰ | Castle visit |

Thursday, 22 May 2014

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| 9 ³⁰ – 11 ⁰⁰ | <u><i>Morning session I: Collision processes involving nanosystems</i></u> Bernd Huber , CEA-CIMAP, France <i>Energy and charge driven processes in molecular clusters: growth and reactivity</i> Olof Johansson , University of Edinburgh, UK <i>Angular-resolved femtosecond photoelectron spectroscopy of fullerenes</i> Florent Calvo , Université de Lyon 1, France <i>Evidence for broken ergodicity from the dissociation kinetics of binary clusters</i> |
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| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <p><i>Morning session II: Nanoscale insights in biodamage</i></p> <p>Eugene Surdutovich, Oakland University, USA <i>Multiscale approach to the physics of radiation damage with ions</i></p> <p>Stéphane Lucas, University of Namur, Belgium <i>Hadrontherapy: what can low energy particle accelerators bring to the field</i></p> <p>Ilya Fabrikant, University of Nebraska-Lincoln, USA <i>Electron-induced hydrogen loss in uracil and thymine molecules in a water cluster environment</i></p> |
| 13 ⁰⁰ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 16 ⁰⁰ | <p><i>Afternoon session I: Clustering and self-organization on the nanoscale</i></p> <p>Andrey Solov'yov, Goethe University, Germany <i>MBN Explorer: morphological transitions in nanostructures</i></p> <p>David Field, Aarhus University, Denmark <i>Spontelectrics: a new form of the solid state</i></p> <p>Arthur Reber, Virginia Commonwealth University, USA <i>Controlling band gap energy in nanoscale materials with cluster building blocks</i></p> |
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| 16 ³⁰ – 18 ⁰⁰ | <p><i>Afternoon session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i></p> <p>Gustavo Garcia, Instituto de Física Fundamental, Spain <i>Electron and positron scattering cross sections from clusters and condensed molecules</i></p> <p>Alexey Verkhovtsev, A.F. Ioffe Physical-Technical Institute, Russia <i>Electron production by carbon and noble metal nanoparticles in collision processes</i></p> <p>Lokesh Tribedi, Tata Institute of Fundamental Research, India <i>Probing mesoscopic objects with fast ions</i></p> |
| 19 ⁰⁰ - 22 ³⁰ | Conference Dinner |

Friday, 23 May 2014

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| 9 ³⁰ – 17 ⁰⁰ | “NAnoRADIation Processes (NARAP)” Workshop |
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Talks

Tu-I-1

CREATING NANOSTRUCTURES WITH ELECTRONS AND LIGHT

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The fabrication of nanostructures underpins the development of a range of technologies from the computer chip to medical implants. Traditionally plasma technology has been used to fabricate such structures with the surface being ‘etched’ to create the necessary components. However the ability of plasma technology to build truly nanoscale structures (<10nm) is in question with a limit of perhaps 20-30nm now being reached. Accordingly new methodologies that build from the ‘bottom up’ rather than ‘top down’ are being developed. These include the use of electrons to build structures through the irradiation of depositing material onto a substrate (Focused Electron Beam Induced Deposition (FEBID)) and the construction of structures using EUV light, both of these technologies are now entering a commercial phase. In this review I will discuss the advances of these techniques and also their limitations highlighting the need for a better understanding of the underpinning atomic and molecular processes.

Exploitation of the ability to manipulate individual atoms and molecules using Scanning Tunneling Microscopes (STMs) provides the ultimate solution of ‘single molecule engineering’ to build sub nm structures with controlled chemical and physical properties. I will review the current status of the field and discuss how (and if) such methodology can ever be transferred into a commercial tool.

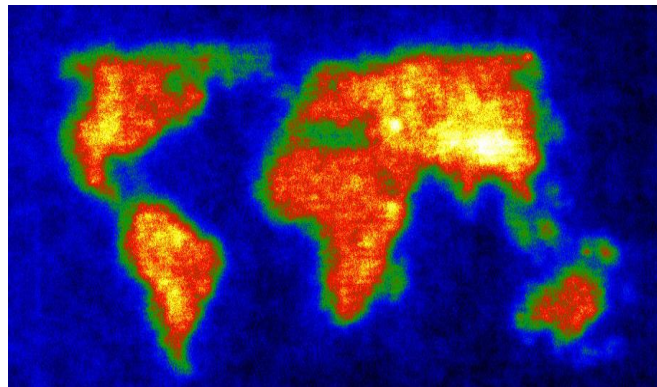


Figure 1: A nanoscale map of the world (width 230nm) 'built' using FEBID technology by Van Dorp [1].

REFERENCES

[1] F. Banhart, *"In situ Electron Microscopy at High Resolution"*, World Scientific, 2008, p. 244

CLUSTERS AND MOLECULES IN EXTREME LIGHT

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

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

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**ANALYSIS OF STRUCTURAL AND DYNAMICAL COMPLEXITIES
IN FINITE HETEROGENEOUS SYSTEMS**

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A number of descriptors to analyze structural and dynamical complexities in finite heterogeneous systems will be presented. Their utility will be illustrated through applications to bimetallic clusters.

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Tu-II-1

ATOMIC STRUCTURE AND DYNAMICS OF SIZE-SELECTED CLUSTERS AND POLYATOMIC MOLECULES

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Atomic manipulation is the extreme limit of nanotechnology. I will first discuss the manipulation of polyatomic molecules – notably chlorobenzene (C_6H_5Cl or PhCl) – anchored to a silicon surface, with a focus on new mechanisms [1] for single molecular manipulation via electron injection. Such mechanisms may (eventually) be relevant to chip-scale molecular manufacturing. I will report site-specific non-local atomic manipulation (leading to molecular desorption) of PhCl [2]: effectively this is 'remote control' of molecular manipulation. This non-local electron attachment mechanism is also thermally activated (barrier 0.4 eV) and suppressed by the proximity of the STM tip itself, both results explicable in terms of electron-driven excitation to an intermediate physisorbed state. Moreover we find that C-Cl bond *dissociation* in the molecule is also thermally activated [3], with an energy barrier of 0.8 ± 0.2 eV, which we correlate *thermal* excitation to the physisorbed (precursor) state of the molecule, where electron attachment occurs.

The controlled deposition of size-selected nanoclusters, assembled from atoms in the gas phase, is a novel route to the fabrication of surface features of size <10 nm [4]. Monodispersed, monometallic and bimetallic [5] cluster arrays represent new model catalysts [6] and a route to protein biochips [7]. Theoretical treatments of the atomic structure of clusters far outstrip direct experimental measurements. Here I show how the atomic structure of the deposited clusters is revealed experimentally [8] by aberration-corrected scanning transmission electron microscopy (STEM) in the high-angle annular dark field (HAADF) regime; we can “count” atoms [9] and thus obtain 3D information rather than just 2D projections. Results include mass spectrometry of passivated Au clusters [10], atomic imaging of Au adatom dynamics on the surface of Au_{923} magic-number nanoclusters [11], first atomic imaging of small Au clusters, notably Au_{55} and Au_{20} [12,13] and a method to explore the potential energy landscape of clusters, by the purposeful transformation of clusters under the e-beam to more stable configurations [14]. We hope these new data will help to enhance theoretical treatments of both cluster structure and dynamics, e.g., via refinement of empirical potentials.

Finally, a new kind of cluster beam source, designed to allow super-abundant generation of size-selected nanoclusters including binary systems, will be proposed.

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LOW-TEMPERATURE SPECTRAL DYNAMICS OF SINGLE MOLECULES IN ULTRATHIN NANOFILMS AND SUBSURFACE LAYERS OF MORPHOUS POLYMER

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Single molecule spectroscopy (SMS) opens up fundamentally new possibilities for obtaining information about the microscopic origin of the dynamical processes in disordered solids. We present the first results of our experimental studies of low-temperature dynamics of ultrathin nanofilms and subsurface layers of amorphous polymer via SMS. The system was ultrathin films of amorphous *polyisobutylene* (of thicknesses 5-300 nm) supported on microscopic glass substrate. The fluorescent *tetra-tertbutylterrylene* molecules were used as spectral nanoprobe. The aim of our research was to obtain information about temporal behavior of individual optical spectra of single fluorescent molecules introduced on the given region of the sample. For this purposes we developed a procedure for the controlled deposition of single molecules or solely upon the surface or into the subsurface layer of controllable depth (of nanometers and smaller) of films or into the whole volume of polymer films. In the case of molecules located directly on the surface, only broad-band fluorescence excitation spectra of ensemble fluorescent molecules were found. Individual zero-phonon lines (ZPLs) in optical spectra of single fluorescent molecules were never detectable. In the case of molecules incorporated into ultrathin subsurface layers the observed picture was completely different. At very small distances from the surface (< 1 nm), ZPLs became be detectable. The individual linewidths of ZPLs of fluorescent molecules near the surface were unusually large and strongly dependent on the distance from the surface. The temporal evolution of these spectra looked more random than in the case of molecules in the bulk of polymer. With increasing depth, the ZPLs become narrower and their temporal evolutions change to the behavior typical in the bulk. The thickness of a subsurface layer which demonstrates dynamical behavior different from the bulk of polymer under study was determined. In the case of polymer films doped in whole volume of the material it was found that certain portion of single molecules shows spectral evolution inconsistent with the standard tunneling systems model of glasses: their spectral lines were subject to irreversible jumps and continuous shifting, reflecting complex and irregular local dynamics in ultrathin polymer films. Percent of such “non-standard” molecules increased with decreasing film thickness. The possible mechanisms of the observed spectral dynamics of ultrathin amorphous polymer films will be discussed.

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TWO UNIVERSALITIES IN SEMICONDUCTOR PHYSICS

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I shall give theoretical explanations of two experimental observations of universal behavior in semiconductor systems.

The first concerns the dependence of photoconductivity G upon light intensity I . It is typically found that $G = I^\gamma$. Simple kinetic theory indicates that we should expect $\gamma = 1$ or $\gamma = 1/2$, but experimentally values close to $\gamma = 3/4$ or $\gamma = 2/3$ are often observed, with I varying over several decades. I shall present a new explanation for these universal exponents.

The second universality concerns exciton spectroscopy in heterostructures. The linewidth W of the absorption line and the Stokes shift S of the luminescence peak relative to the absorption peak are found to be related by $S/W = 0.6$ in most systems for which both values are published. This ratio is independent of the degree of disorder and of the composition of the semiconductors forming the heterostructure, with W varying over two decades. I shall also give a quantitative explanation of this result.

Finally I point out what these two phenomena have in common.

The results on photoconductivity are discussed in a recent paper, EPL **96**, 67007 (2011). The results on exciton spectra are much older. They were obtained with Fang Yang, E. J. Austin and K. P. O'Donnell, PRL **70**, 323 (1993).

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ENHANCEMENT OF MEDICAL RADIATION EFFECTS USING NANO-RADIOSENSITIZERS: EVIDENCE OF NANOSCALE PHENOMENA

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Radiotherapy is the most common therapeutic modality used to fight against cancer in about 50% of all cancer patients. However, traditional radiotherapy using photon beams has a significant lack of selectivity, provoking damage not only in abnormal cells but also in healthy tissue. Hence, the current challenge is to develop more efficient techniques and protocols to overcome these limitations. The use of hadron beams seems very promising due to better dose distribution (Bragg peak) allowing the deposition of maximum energy into a well-defined volume (zero dose deposition after the tumor). However, the damage produced in front of the tumor and in the path of the incoming particles is not negligible. In order to overcome this limitation, our group explores the possibility of combining hadrontherapy and nanomedicine to amplify the effects of fast ions interacting with amplifying agents into the tumor. High-Z atoms loaded compounds including nanoparticles (NPs), are promising agents able to enhance the radiobiological effect and thus the therapeutic index of radiotherapy.

The group has proved at molecular level (using plasmid DNA) and cellular level (on mice and human cell lines) that platinum [1, 2], gold and lanthanide based nanoparticles are efficient sensitizers when irradiated by high-energy photons and ion beams. In addition, microscopy experiments (TEM, DUV and confocal) show that the radiosensitization effect is due to the induction of nano-size radical clusters in the cytoplasm of the cancer cells, far from the nucleus. A multi-scale investigation protocol is now used to test different radiosensitizers with the perspective to elaborate an open database. The group is willing to collaborate with physicists and theoreticians to further elucidate and quantify the multi-scale processes proposed. These data are needed for the development of treatment planning and the development of new nanosensitizers.

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CELL IRRADIATION WITH ION BEAMS: REALISTIC DESCRIPTION OF SUBCELLULAR COMPARTMENTS

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Living cells are regarded as the ultimate biological target for radiation: traditionally, it was thought that the energy deposition by radiation in the cell nucleus leads to lesions in the DNA molecule, which can produce negative effects, such as mutations that have to be avoided in natural irradiation conditions (e.g., manned space missions), or positive effects in the case of radiotherapy, where the cell death is desired in order to eradicate tumors. Nonetheless, recent experimental evidence suggests that not only energy deposition in the cell nucleus can trigger the biological outcomes, but that also other parts of the cell, such as the mitochondria or the cell membrane, could be involved in radiation damage mechanisms [1]. Therefore, there is a need of theoretical models able of predicting the energy deposition in subcellular compartments, since obtaining this information experimentally is very difficult.

In this contribution we present an analytical model for the energy deposition and secondary electron production by ion beams in a cell model formed by cell nucleus and cytoplasm [2], which can be applied to the study of ion beam cancer therapy, one of the most promising radiotherapies nowadays [3]. The model is based on the continuous slowing down approximation for a simple analytical description of the ion beam propagation, and accounts for the production and transport of secondary electrons in micrometric scales. The energy loss of the ions and the electron production in realistic cell nucleus and cytoplasm are modeled within the dielectric formalism, which provides a suitable description of the electronic interactions in condensed phase targets, and with a semiempirical model recently developed by us, which allows predicting the secondary electron production in arbitrary biological materials [4]. The propagation of secondary electrons is accounted for analytically by using a spatially restricted linear energy transfer formula [5]. The model allows the analytical calculation of the energy deposition and number of ionizations produced in the different cell compartments by ion beam irradiation, representing a procedure faster than Monte Carlo simulations. Moreover, it makes use of realistic electronic interaction data for biological materials, which is a typical limitation for many theoretical approaches, where the biological target is usually regarded as liquid water.

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AN INNOVATIVE TECHNIQUE FOR PREVENTING TELOMERE ELONGATION AND ITS ASSOCIATED IMMORTALIZATION OF CANCER CELLS

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Photon Activation Therapy (PAT) is a long proposed radiotherapeutic modality [1] whose time has come to enter the nanomedicine arena. In PAT, high Z atoms are physiologically targeted to cancer cell DNA by tumor-seeking vehicles. Brachytherapy seeds, implanted directly into tumor, were proposed as the photon-emitting agents whose energies would induce a photoelectric effect at the K or L absorption edge of the high Z atom and elicit its emission of Auger electrons [2]. The low energy and short range of Auger electrons produces a dense and highly local ionization over a sphere of 25 nm in the DNA of cancer cells [3]. The DNA damage produced resembles high-LET damage and is non-repairable. Although the concept of PAT is highly enticing and based upon sound and proven physical principles, its success in the medical clinic has not been achieved. We attribute this failure to the inappropriate administration of the vehicles (drugs) that transport high Z atoms to tumor. When the drugs are introduced systemically, they are rapidly cleared from the body and the number of photon/high Z atoms interactions is significantly reduced.

We will demonstrate an innovative drug delivery technique that incorporates a drug within a biodegradable polymer and releases the drug in tumor over the long term (30 days). The rod-shaped polymer is inserted directly into tumor where the drug is released and inhibits the activation of the telomerase enzyme. Activation of the enzyme is a cancer cell survival mechanism because its actions sustain the length of DNA and confer immortality to the cancer cell. The drug also transports palladium (Pd) atoms to tumor cell DNA. Their continuous availability for emitting Auger electrons, induced by simultaneously implanted iodine-125 brachytherapy seeds, suggests that the realization of the PAT therapeutic modality may be imminent. In lieu of brachytherapy seeds, monochromatic photons from synchrotron radiation beams can also be used to induce a photoelectric effect in the continuously available Pd atoms.

We will demonstrate the effectiveness of the drug as a telomerase inhibitor and its therapeutic potential in PAT. We will emphasize the significance of binary systems that exploit a combination of radiation and pharmacology for cancer treatment within the purview of nanomedicine.

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CHANNELING EXPERIMENTS AT THE MAINZ MICROTRON MAMI

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At channeling the directions of charged particles are closely aligned with strings of atoms or crystal planes. Their motion is governed by many correlated collisions with the crystal atoms. As a result, the particles are steered along strings or planes. In the first part of the talk a pedestrian introduction to the phenomenon of channeling will be given.

The second part focuses on the experimental setup at the Mainz Microtron MAMI at which experiments by the Ferrara and Aarhus groups were performed to be presented in the session "*Propagation of particles through medium*" of this *DySoN Conference 2014*. The low emittance electron beam of MAMI is well suited to prepare a beam with small angular divergence which is mandatory for the mentioned channeling experiments. As an example, at beam energy of 600 MeV the vertical emittance amounts to 0.5π nm rad. At a typical beam spot size of $180 \mu\text{m}$ (1σ) in our experiments, the beam divergence results in only $2.8 \mu\text{rad}$ (1σ) which is small in comparison with the critical angle of $270 \mu\text{rad}$ for the (110) plane of silicon.

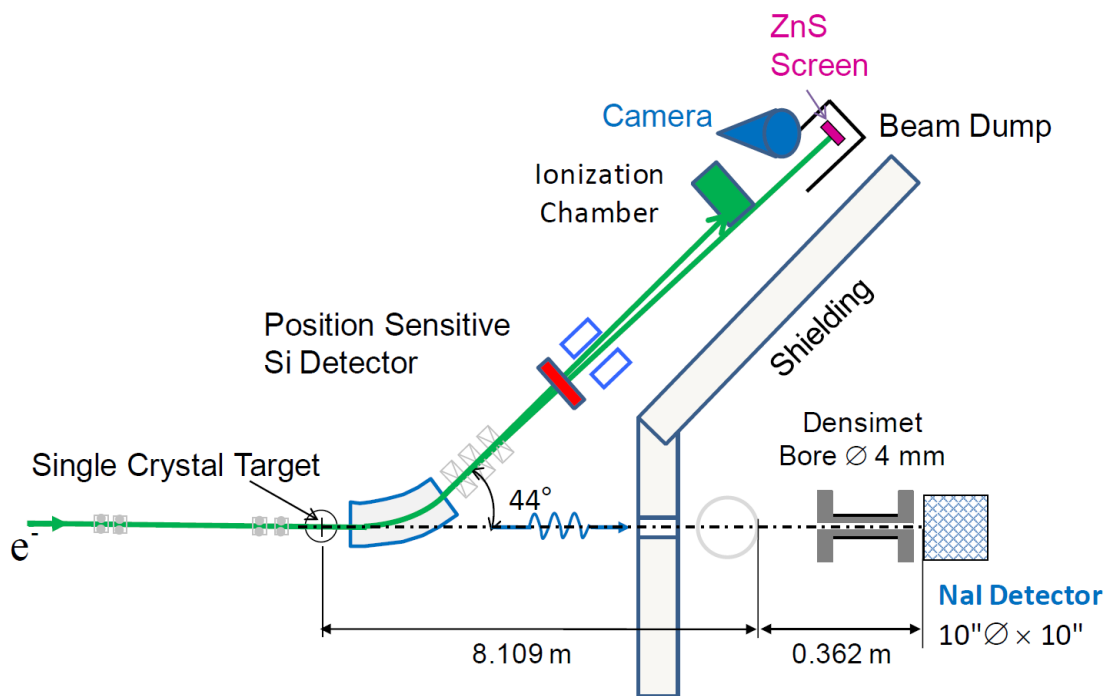


Figure 1: Typical experimental setup at MAMI to study channeling

The experimental setup at MAMI is shown in Figure 1. Single crystal targets are mounted on goniometers with which precise rotations around three axes and translations can be performed. Downstream the crystal target the beam is deflected horizontally by a 44° - bending magnet and thereafter vertically by a second 7.2° one. At the beam dump the beam spot can be observed by a camera detecting the emitted light from a ZnS screen. This way beam deflections at axial or planar

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channeling can be visualized. For more precise beam deflection studies a position sensitive detector has been employed with a spatial resolution of better than 10 μm which was placed 6.644 m downstream the target. Imaging properties of the 44° - bending magnet must be taken into account to obtain precise emission angles at the target. The ionization chamber serves as monitor counter for the detection of channeling. Electrons which have lost energy by emission of channeling radiation are deflected by the 44° - bending magnet towards the ionization chamber resulting in an increase of the signal height. Photon spectra are recorded with a 10" \varnothing – 10" length NaI detector, or with a Ge(i) detector with a bore of 7.8 mm \varnothing and 30 mm length. The photon beam from the target is collimated with apertures made either of lead or Densimet (density of 17.6 g/cm³, 92.5 % tungsten, 5 % nickel, 2.48 % iron) to accomplish nearly on-axis observation of the emitted radiation. The concrete shielding protects the radiation detectors from detection of bremsstrahlung radiation produced in the beam dump.

Besides axial channeling [1] in particular planar channeling phenomena have been studied at MAMI for silicon single crystals [2]. Recent experiments focus on radiation emission [3,4] and beam deflection studies [5] at periodically bent and curved crystals, respectively. In particular, beam deflection has been studied at (111) channeling by a 30.5 thick curved crystal with a bending radius of 33.5 mm [5].

The third part of this talk deals with very important prerequisites for experimental studies of undulator-like radiation in periodically bent crystals. This is the knowledge of the dechanneling length of electrons for the (110) crystallographic plane. Because of the fact that even for undistorted plane crystals only little is known experimentally, we have performed and recently reanalyzed dechanneling length measurements at various beam energies for plane crystals [4]. Both, radiation spectra as well as dechanneling length measurements at electron beam energies between 195 and 855 MeV feature quantum state phenomena for the (110) planar potential of the silicon single crystals [4] which enhance the dechanneling length.

Radiation emission spectra have been studied from a crystalline undulator at electron beam energies between 195 and 855 MeV [3,4]. The graded composition strained layer Si_{1-x}Ge_x undulator, epitaxially grown at the Department of Physics and Astronomy of the Aarhus University, had 4 periods with a period length of 9.9 μm and amplitudes between 2 and 4 Angstroms. All spectra taken at various beam energies at channeling in the undulating (110) planes exhibit a broad excess yield around the theoretically expected photon energies, as compared with a flat silicon reference crystal. Analysis with a simple analytical model suggests that the gross structure can be explained by synchrotron-like radiation emission component from small arc elements of the undulator. In order to explain the hump at the expected photon peak energies between 0.069 and 0.66 MeV energy, a coherent contribution must be added. A fraction of only about 2 % of the electrons which channel with a dechanneling length of 4.0 μm would explain the experimental observation. Why the coherent radiation component is so small is presently still an open question.

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SIMULATION OF RADIATION SPECTRA FROM ELECTRON- AND POSITRON-BASED CRYSTALLINE UNDULATORS

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The main phenomenon addressed in this work is the radiation formed in a Crystalline Undulator (CU) [1]. In this device, the electromagnetic radiation is generated by a bunch of ultra-relativistic particles channeling through a periodically bent crystalline structure. Such a system becomes a source of intensive radiation of the undulator type, and, under certain conditions, also a source of the laser light [1]. A CU-based laser could produce photons within the energy range from tens-hundreds keV up to MeV which is unachievable in the conventional FEL devices.

To simulate the motion of ultra-relativistic particles in oriented crystals we used the channeling module developed recently [2] within the MBN Explorer software package [3,4]. The general and universal design of the package allowed us to expand its basic functionality with introducing a module that treats classical relativistic equations of motion and generates the crystalline environment dynamically in the course of particle propagation.

The simulated trajectories were used further to calculate the spectral distribution of radiation $dE/d\omega$. At the Conference we present and discuss two sets of novel results obtained for the following two essentially different operational regimes of the CU device:

(1) Large-amplitude long-period regime [1] implies that the bending amplitude a is much larger than the interplanar spacing d and the period of bending λ_u exceeds greatly the period of channeling oscillations λ_{ch} . In this regime the peak of the undulator radiation is located at lower energies with respect to the peak of the channeling radiation. We will report the results obtained for 270-855 MeV and 10 GeV electrons and positrons channeling along Si(110) and Si(111) planes bent with the amplitude $a=4$ Å. The bending periods are 10 and 40 μm for the sub-GeV and 10 GeV projectiles, respectively.

(2) Small-amplitude short-period regime [5] is characterized by the opposite limits: $a \ll d$ and $\lambda_u \ll \lambda_{ch}$. As a result, the undulator peak is located beyond that of the channeling radiation. We will report the results corresponding to the bending parameters $a=0.2...0.6$ Å, $\lambda_u = 200...600$ nm and obtained for 270-855 MeV and 10 GeV projectiles channeling along Si(110).

The current theoretical results and the numerical data are highly relevant in view of the ongoing experiments with straight, bent and periodically bent crystals carried out with 195–855 MeV electron beams at the Mainz Microtron (Germany) facility [6] and with 1-20 GeV projectiles at the SLAC facility (USA) [7]. The crystalline undulators, used in the experiment, were manufactured in Aarhus University (Denmark) using the molecular beam epitaxy technology to produce strained-layer $\text{Si}_{1-x}\text{Ge}_x$ superlattices with varying germanium content.

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CHANNELING OF NEGATIVELY CHARGED PARTICLES

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The possibility to manipulate the trajectories of charged particle beams through coherent interaction of the particles with a bent crystal has fascinated the community of high-energy and accelerator physicists. In fact, the phenomena of channeling and of the recently discovered volume reflection appear to be promising techniques in this sense. The strong electric field experienced by a beam particle in proximity of an ordered structure of the atoms in a crystal exerts a strong confinement force onto the particle and may bound its trajectory to proceed parallel to a crystalline plane or an atomic string, which become preferential pathways in the crystal. As the crystal is being bent, the pathways are bent in turn and the particles are diverted towards a different direction with respect to incoming direction, i.e., beam steering is accomplished.

As far as positively charges are concerned, beam steering has progressed significantly over the years, boosted by the discovery of new phenomena such as multiple volume reflection in a bent crystal. Indeed, very little has been investigated concerning the steering of negatively charged particle beams via channeling in bent crystals because, unlike the positive particles, negative particles repeatedly oscillate across the nuclei of the crystal, leading to an increase of particle dechanneling about ten times larger than for positive charges. Yet, the possibility to master negatively charge particle beams via coherent interaction with crystals would lead to several interesting opportunities, spanning from halo collimation in future linear e^\pm colliders, to be the basis of a periodically bent crystal for miniature electron crystalline undulator.

In the last years, thanks to innovative techniques for crystals design and fabrication based on silicon micromachining techniques, it was possible to realize curved crystal, thin enough to avoid the loss of deflection efficiency caused by dechanneling, while maintaining the crystal structure perfectly intact. The realization of such thin bent crystals has opened the way to the investigation of all the orientational coherent interactions in bent crystals that are known for positively charged particles, to hold even for the case of negatively charged particles. Such a study was done in a very broad energy range, from sub-GeV at MAMI electron accelerator to hundreds of GeV at the SPS external lines with negative pions and electrons. Since dechanneling scales down with energies, the technology for bent crystal fabrication was pushed to its extreme limit, starting from the 2 mm bent crystals for CERN to arrive at the 30 μm bent crystals used in MAMI.

The campaign of measurements performed at CERN demonstrated the possibility to deflect ultra-high energy negative particles via either channeling or volume reflection in bent crystals [1]. Fig. 1a displays the deflected beam distribution vs. the misalignment angle between the beam of 150 GeV/c π^- and the bent crystal. One of the most important scientific results of the study performed at CERN was the determination of the dechanneling length of negative particles. Dechanneling is the process of exit of particles from channeling states due to collisions with electrons and nuclei that form the crystal lattice. The average length that a channeled particle crosses before its exit from planar or axial potential well is called dechanneling length. For the first time, a direct measurement of the

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dechanneling length of ultra-high energy negative particles was done thanks to the usage of a short bent silicon crystal [2]. It was also demonstrated the ability to steer negative particle beams through axial channeling regime with efficiency close to 100% [3]. In the case of axial alignment, it was also observed deflection of the particles in the direction opposite to the curvature of the crystal probably caused by multiple reflection of a volume of the particles on different crystallographic planes that intersect the axis of the curved crystal [4]. A particle that impinges onto the crystal in the vicinity of the axis is then reflected during its motion from several crystal planes, giving rise to a substantial increase in the deflection compared to the case of a single volume reflection.

A recent campaign of measurements performed at MAMI demonstrated that the same phenomena of channeling and volume reflection were observed either at 150 GeV or 855 MeV as highlighted by Fig. 1. The exploitation of the quasi-mosaic effect caused by the crystal anisotropy permitted to bent a crystal of 30 μm , whose length is of the order of the dechanneling length (20 μm) that was later measured directly with the same crystal [5].

Preliminary results of a new experiment at SLAC have shown that also in the intermediate energy range 3-10 GeV, properly sized bent crystals can effectively steer negative particle beams via either channeling or volume reflection.

In conclusion, we can state that coherent interactions in bent crystals can be profitably used for manipulation of negatively charged particle beams in a very broad range of energies that goes from hundreds MeV to hundreds GeV.

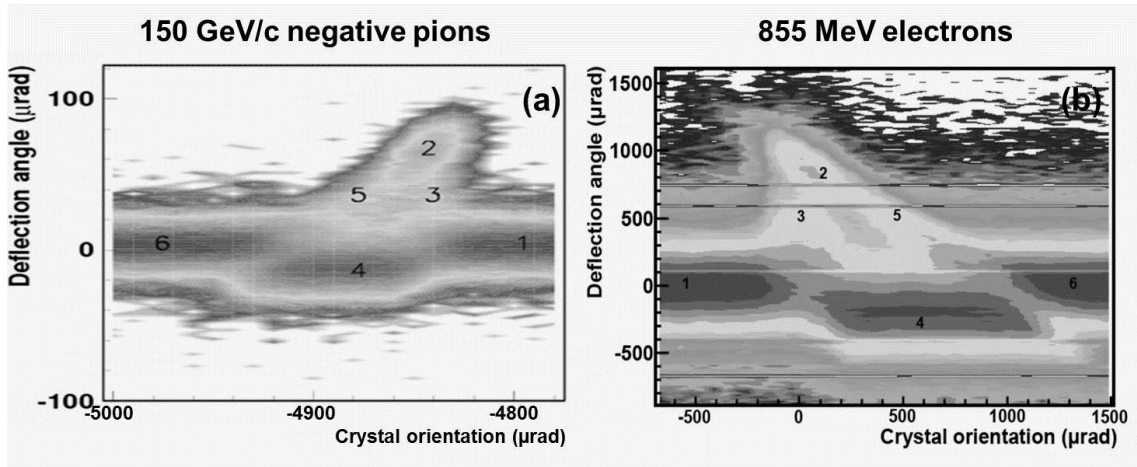


Figure 1: Deflected beam distribution vs. the misalignment angle between the beam and the bent crystal for 150 GeV/c π^- (a) and for 855 MeV e^- (b). Six different regions, corresponding to different interaction regimes, can be distinguished: (1) and (6) non-channeling; (2) channeling; (3) dechanneling; (4) volume reflection; (5) volume capture.

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We-II-1

SELECTING INTERESTING ATOMS FOR QUANTUM CONFINEMENT

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Originally, atoms confined in a volume of quantum size were a rather exotic subject, of study mainly for researcher seeking original solutions of the Schroedinger equation. Later, the subject of Quantum Confinement began to attract greater interest because of the experimental discovery of some unusual and beautiful structures which now serve as examples. However, before one can regard this area of research as significant, it is important to relate it to other subjects and to consider general questions to which methods developed for Quantum Confinement could provide novel answers. Indeed, it is desirable to put the questions first, and then consider what choices of atoms and confining cages should be made in order to answer them, both experimentally and theoretically. Some questions will be proposed, together with suggestions as to how they might be addressed in the context of Quantum Confinement. The aim will be to stimulate new directions rather than to dwell on existing examples.

STUDY OF COHERENT INTERACTIONS BETWEEN A SUB-GEV ELECTRON BEAM AND A THIN BENT SILICON CRYSTAL

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We report the observation of efficient steering of a sub-GeV electron beam by means of planar channeling and volume reflection in a bent silicon crystal. A 30.5 μm thick plate of (211) Si wafer was bent to cause quasi-mosaic deformation along the (111) crystallographic planes, which were used to steer the 855 MeV electron beam of MAMI accelerator. Experimental results resemble very much the achievements obtained in the hundreds-GeV energy range that, to date, is the only comparison term (see Fig. 1). On the contrary to the higher energy case, the rechanneling mechanism seems to play a crucial role in particles dynamics, as studied through Monte Carlo simulations, and hinders the spoiling of channeled particles. Obtained results allow for a deep understanding of the dynamics of sub-GeV electrons subject to coherent interactions in a bent silicon crystal. Moreover, we investigate also the emission electromagnetic radiation by 855 MeV electrons through coherent interactions in bent crystals. In more detail, we studied the influence of bending to radiation spectrum and investigated the e.m. radiation generation in volume reflection condition. The information extracted from this experiment, regarding both dynamics and radiation generation, can be exploited to investigate the possibility to use bent crystals to manipulate GeV particle beams or taken into account to properly design periodically bent crystals to be used as innovative and powerful sources of high intensity electromagnetic radiation.

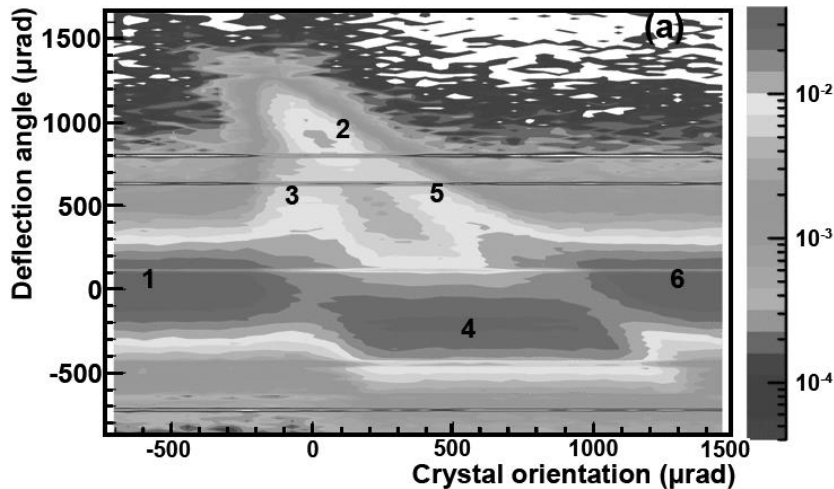


Figure 1: Deflected beam profile as a function of the misalignment angle between the electron beam and the crystal. Six different regions, corresponding to different interaction regimes, can be distinguished: (1) and (6) non-channeling; (2) channeling; (3) dechanneling; (4) volume reflection; (5) volume capture.

SIMULATION OF ELECTRON, POSITRON AND MUON CHANNELING

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We report results of simulation of axial and planar channeling of electrons, positrons and muons in straight [1] and periodically [2, 3] bent Si crystals. The calculations were done using direct calculation of trajectories of projectiles on atomic level using newly developed module for MBN Explorer software package [4]. The simulations were carried out by solution of relativistic equations of motion of projectile interacting with atoms of the medium with random sampling of initial direction of projectile and thermal vibration of atoms. Such model is not limited to specific structure of channels and direction within the crystal.

The analysis of trajectories allows us to study effects of channeling and rechanneling, calculate characteristic lengths of dechanneling, radiation spectra and angular distributions of different groups of particles. This approach allows direct comparison between different cases of channeling. The results of simulations obtained are in a good agreement with experimental data.

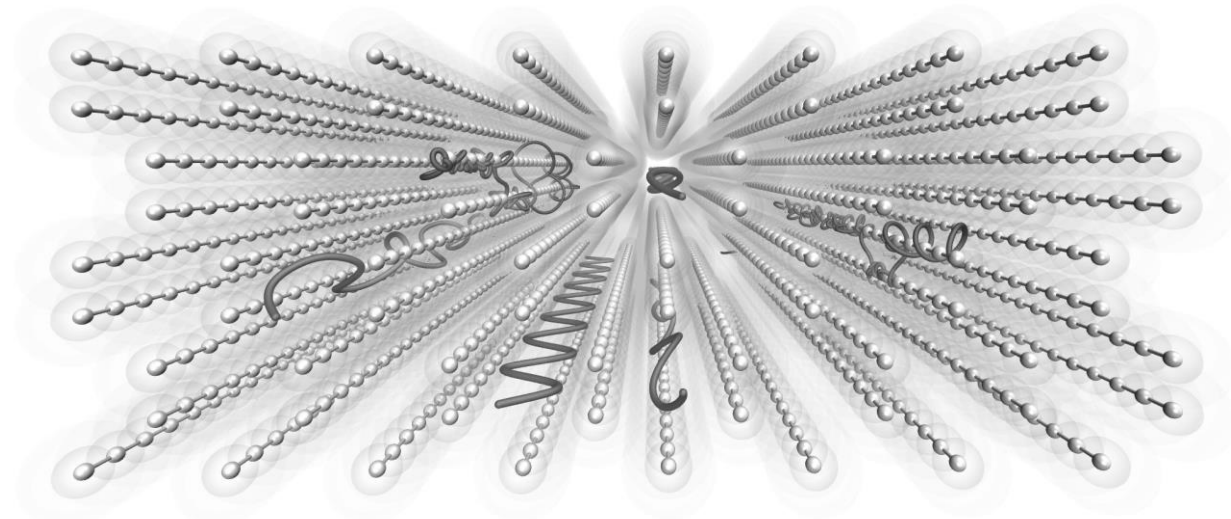


Figure 1: The examples of trajectories of 10 GeV electrons and positrons in axial channels in straight Si crystal. Axial strings of atoms in the crystal are schematically illustrated as well.

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Th-I-1

ENERGY AND CHARGE DRIVEN PROCESSES IN MOLECULAR CLUSTERS: GROWTH AND REACTIVITY

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Clusters of molecules are appealing systems to be studied as their structure and properties are governed by different types of molecular bonds. Whereas within individual molecules strong covalent bonds with binding energies of several eV dominate, the cluster-forming molecules are typically hold together by weak van der Waals forces or they present hydrogen-bonded systems with binding energies below 1 eV. Thus, they represent a weakly bound ensemble of more strongly bound systems. Nevertheless, these systems can withstand, on μs time scales, a large amount of internal energy, much larger than thermodynamic dissociation energies, or the Coulomb repulsion of several charges. These timescales allow to initiate chemical reactions in molecular clusters and to change binding conditions provided that reactive species are formed by transferring energy or charge to the system. In a second step, these species can react with other surrounding cluster constituents, given rise to molecular growth and modification.

Polycyclic aromatic hydrocarbon (PAH) molecules, fullerenes (C_{60}) as well as clusters of these molecules are highly abundant, both on earth and in space. However, their formation and in particular their growth and destruction pathways are not very well understood. Furthermore, the links between these two related classes of molecules remain unclear. Previously it has been shown that collisions between keV ions and isolated PAH molecules [1], isolated fullerene molecules [2], and clusters of fullerenes [3] can strongly enhance the reactivity of the individual molecules. In particular, non-statistical fragmentation has been shown to give highly reactive fragments and to be an important first step in such molecular fusion reactions [1-3]. The study of fullerene dimers [4] has sparked considerable interest in recent years as it is essential for the formation of fullerene polymers which may exhibit interesting electronic, magnetic and optical properties.

Here we report on the formation of covalently bound fullerene dimers C_{118}^+ and C_{119}^+ which are produced inside van der Waals (vdW) clusters of C_{60} molecules in collision with 22.5 keV He^{2+} ions, on the ion induced growth of pyrene molecules and on the behavior of mixed clusters consisting of PAH and fullerene molecules. The experiments have been performed at the low-energy ion beam facility of GANIL, ARIBE, in the framework of the Associated International Laboratory DYNAMO, created between the Universidad Autonoma de Madrid (group of F. Martin), the Stockholm University (group of H. Cederquist) and the AMA group of CIMAP in Caen.

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Th-I-2

ANGULAR-RESOLVED FEMTOSECOND PHOTOELECTRON SPECTROSCOPY OF FULLERENES

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The properties of photoexcited carbon nanoparticles are of interest for the development of organic opto-electronics and photovoltaic devices, where detailed knowledge of the electronic structure and photoinitiated dynamics of electrons is important. Fullerenes are ideal model systems to achieve a deeper understanding because their high symmetry and simple chemical composition simplifies theoretical modelling.

In this contribution, angular-resolved photoelectron spectroscopy has been used to study ionisation mechanisms of gas-phase fullerenes excited with fs laser pulses [1]. Efficient energy redistribution in gas-phase fullerenes after fs laser excitation leads to the production and decay of hot electrons. The high excitation energy absorbed from the laser pulse leads to the emission of thermal electrons in a process that is uncorrelated with the laser's electric field [2]. Electrons emitted during a time-varying electric field can gain a momentum "push" along the laser polarization direction, leading to an asymmetry in the angular-resolved electron kinetic energy distributions. This effect has been used to directly measure the timescales for thermal electron emission, which gives insights into electron-phonon coupling processes in carbon nanomaterials [3].

The photoelectron angular distributions have also been used to identify highly excited states in fullerenes with low angular momenta that are populated and efficiently ionized during the ca. 100 fs laser pulses [4]. These states are predominantly comprised of so-called superatom molecular orbitals (SAMOs), previously identified in scanning tunnelling spectroscopy studies by Feng *et al* [5]. The diffuse states can form nearly-free-electron bands in solids and are therefore of technological interest. The SAMOs have also been identified in C₇₀, C₈₂ and Sc₃N@C₈₀ [6]. It was found that thermal electron emission gradually dominates the photoelectron spectra for larger systems with lower symmetry.

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Th-I-3

EVIDENCE FOR BROKEN ERGODICITY FROM THE DISSOCIATION KINETICS OF BINARY CLUSTERS

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Although it is a fundamental assumption of statistical mechanics, ergodicity can hardly be proven in practical situations because one does not access statistical and time averages separately. In this contribution, we discuss a class of nanoscale systems for which the ergodic hypothesis turns out to break under appropriate choice of parameters, namely binary clusters of particles interacting through the simple Morse potential. Computational modeling of the out-of-equilibrium dissociation kinetics of those clusters is very sensitive to the equilibrium properties, especially in cases where the clusters exhibit a mixing phase transition. Sampling the equilibrium phase using dedicated Monte Carlo methods, the dissociation kinetics is found to depend significantly on the initial conditions, which indicates that dissociation can be much faster than global relaxation, causing in turn broken ergodicity. Further analysis reveals the conditions leading to such behavior and suggests possible experimental connections based on natural observables such as the branching ratio.

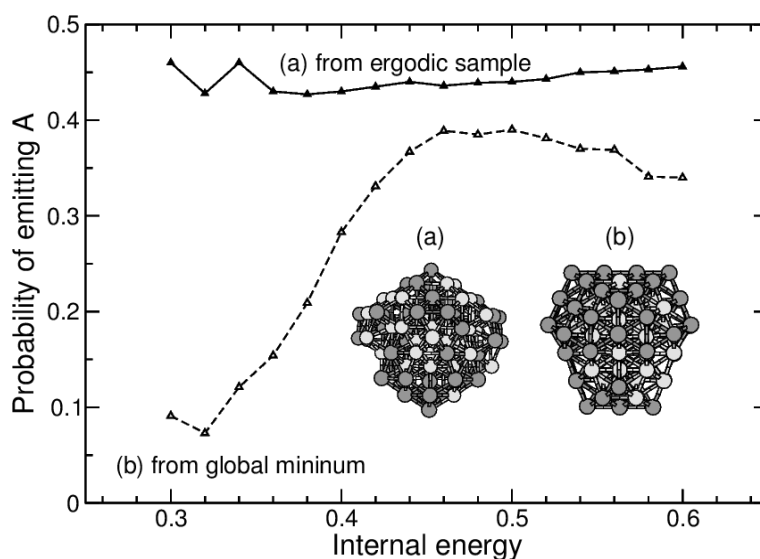


Figure 1: Probability of emitting a particle A (light grey) from the binary cluster $(AB)_{50}$ as a function of its internal energy, the cluster being prepared ergodically (a) or taken in its most stable structure (b). Global relaxation is enforced in the ergodic sample only.

Th-II-1

MULTISCALE APPROACH TO THE PHYSICS OF RADIATION DAMAGE WITH IONS

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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 application of ions interacting with biological targets. A number of important scientific questions, especially related to DNA damage assessment on the molecular level, have not yet been resolved. Therefore, 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 [1,2]. It is aimed at a phenomenon-based quantitative understanding of the scenario from the incidence of an energetic ion on tissue to the cell death. This method combines many spatial, temporal, and energy scales, and is therefore a truly multiscale approach. The multiscale approach raises questions about the nature of the effects that take place and lead to survival curves and the calculation of relative biological effectiveness 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 double strand breaks yield by secondary electrons, and the assessment of the complex DNA damage [2]. A special investigation was devoted to DNA damage as a result of thermo-mechanical effects caused by ions. These effects can be described as a dynamical change in temperature and pressure in the medium, due to ions passage, causing forces that may rupture bonds in DNA molecules. The understanding of such a possibility evolved from the estimates of the temperature increase in the medium as a result of ion propagation to the analysis of thermal and pressure spikes in liquid water and further to the analysis of the shockwave in the medium and its effect on biomolecules [3-5]. The latest research was devoted to the analytical analysis of different experiments and the development of the recipe for the phenomenon-based calculation of RBE. Such a recipe could be used in radiation optimization codes and other applications [2].

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Th-II-2

HADRONTHERAPY: WHAT CAN LOW ENERGY PARTICLE ACCELERATORS BRING TO THE FIELD

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Cancer is the leading cause of death in industrialized countries. One of the current treatment modality is radiotherapy. Even if most of the cancer cases candidates for radiotherapy are treated with sparsely ionizing radiation (like X-rays or ^{60}Co units), new modalities using protons or other heavy ions have emerged in the past decade.

Nowadays, about 100.000 patients have been treated with carbon or protontherapy systems. Although protontherapy and hadrontherapy are on the way to become treatments of choice, little data on cell survival after exposure to charged particles is available, especially at very low doses. For instance, protontherapy treatments are based on knowledge acquired with X-rays and the dose is scaled by a factor of 1.1. This approach oversimplified the effects, particularly at the end of the particle track. For hadrontherapy treatment, a very important feature is nuclear fragmentation: when heavy ions pass through an organ, even small sections for nuclear reactions produce a significant amount of lighter reaction products. This change in radiobiological efficiency between the primary ions like carbons and the lighter secondaries has to be studied in order to incorporate the effect in treatment planning.

Therefore, both for proton and higher ions based therapy the knowledge of cell survival data is a crucial issue to assess the radiosensitivity of a given cell line. Thus, fundamental studies are required to accurately determine radiosensitivity parameters for various cell lines and for various particles and energies and to examine molecular cell response pathways, which can be different when the radiation nature is modified. Such work can be performed by low energy particle accelerator that can be used to irradiate different cell lines with various particles, LET and dose rate: one can study the survival fraction and determine the RBE of a selected particle and cell line. Typical biological bioassays (cell viability, DNA damages and DNA synthesis, ...) are available specially to study a set of phenomena, called the non-targeted effects, that have been discovered recently and which challenges the idea that the only critical effect of ionizing radiation in the cell is the DNA damage and that less incident energy means less death, fewer DNA breaks and fewer mutations. Those effects are: adaptive response (AR), bystander effect (BE), genomic instability (GI), inverse dose rate effect (IDRE), low dose hyper-radiosensitivity (HRS).

In this lecture we will present a general view of the various setups that are used for in vitro radiobiology and we will discuss selected examples that are of interest for future ion based treatment protocols.

ELECTRON-INDUCED HYDROGEN LOSS IN URACIL AND THYMINE IN A WATER CLUSTER ENVIRONMENT

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Exposure of living cells to ionizing radiation leads to biological damage by both direct and indirect interaction with the cell components. During the last decade there has been increasingly stronger evidence that secondary electrons with energies below 20 eV have the capability of producing single and double strand breaks in DNA [1-2]. The exact mechanism of these strand breaks is still under discussion, but it is becoming increasingly apparent that dissociative electron attachment (DEA) processes are playing a decisive role in this damage.

The most abundant product of DEA to the building blocks (purines and pyrimidines) of DNA is the dehydrogenated closed-shell anion ($M-H^-$) [3], therefore a lot of effort was devoted to studies of the hydrogen loss due to DEA to uracil and DNA bases. In biological systems, it is important to know how this fundamental process is affected and modified in the presence of vital cellular components, in particular water [4].

In the present work we investigate theoretically low-energy electron-impact hydrogen loss due to DEA to the uracil and thymine molecules in a water cluster environment. Only the A' -resonance contribution, describing the near-threshold behavior of DEA, is incorporated. Calculations are based on the nonlocal complex potential theory and the multiple scattering theory, and are performed for a model target with basic properties of uracil and thymine, surrounded by five water molecules. The DEA cross section is strongly enhanced when the attaching molecule is embedded in a water cluster. This growth is due to two effects: the increase of the resonance lifetime and the negative shift in the resonance position due to interaction of the intermediate negative ion with the surrounding water molecules. A similar effect was earlier found in DEA to chlorofluorocarbons [5]. We conclude that the probability of the electron-impact bond-breaking in biologically-relevant molecules can be much higher than that measured or calculated for the pure gas phase.

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Th-III-1

MBN EXPLORER: MORPHOLOGICAL TRANSITIONS IN NANOSTRUCTURES

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MBN Explorer [1] is a multi-purpose software package designed to study structure and dynamics of molecular systems of various degrees of complexity. A broad variety of interatomic potentials implemented in the MBN Explorer allows one to simulate the structure and dynamics of different molecular systems, such as atomic clusters [2], fullerenes [3], nanotubes [4], metallic nanomaterials [5], proteins and DNA [6], crystals [7] composite bio-nano systems and nanofractals [8]. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and implemented multiscale features that make it applicable to really a broad range of problems involving complex molecular systems.

The talk will give an overview of the main capabilities of the package, highlight its computational efficiency and the case studies of thermally induced morphological transitions of nanofractals and other nanostructures based on kinetic Monte-Carlo simulations of atomic cluster deposition, nanofracture growth and evolution.

The professional version of MBN Explorer can be ordered via its website [9] upon the registration and acceptance the terms and conditions of the commercial license agreement. Currently, there are more than 1000 registered users of MBN Explorer, which is being under the permanent development conducted by the MBN Research Center in Frankfurt [10].

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Th-III-2

SPONTELECTRICS: A NEW FORM OF THE SOLID STATE

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When a film of material is laid down from the gas phase upon a cold surface, this film may spontaneously contain a substantial electric field, in excess of 10^8 V/m. This is called the ‘spontelectric effect’ and was first discovered in films of nitrous oxide [1]. An example is shown below for CF_3Cl , which shows a field of 4.25×10^7 V/m for deposition at 40K [2]. Higher temperature data are also shown.

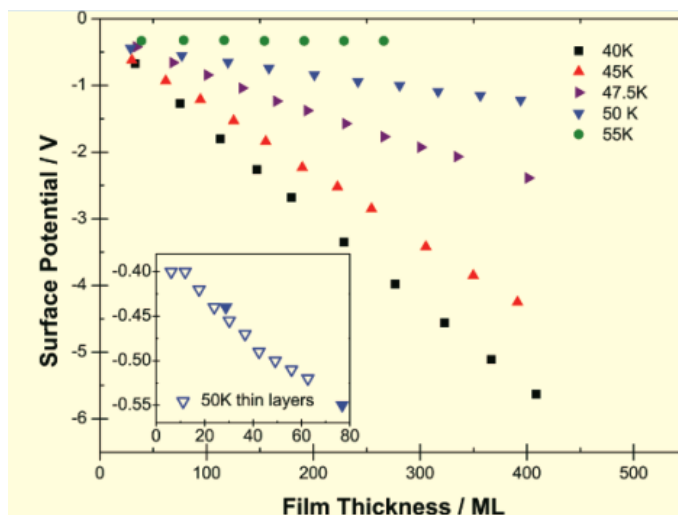


Figure 1: Surface potentials measured for films of CF_3Cl as a function of thickness in ML laid down at five different deposition temperatures. 55K data are included to show the absence of the spontelectric effect. The inset shows data at 50K for a lower rate of deposition

The structure of spontelectric films is neither strongly ordered with a repeating unit, as in a crystalline material, or completely disordered as in an amorphous solid. Spontelectrics, by contrast with all other known forms of the solid state, represent a degree of partial order associated with orientation of the dipoles of the constituent molecules engendered by non-linear and non-local phenomena [2,3]. Spontelectrics may be used to form films with nanostructured electric fields, both positive going, as in nitrous oxide, and negative going, as in CF_3Cl , and in principle make possible the formation of electrical nano-devices such as nano-traps.

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Th-III-3

CONTROLLING BAND GAP ENERGY IN NANOSCALE MATERIALS WITH CLUSTER BUILDING BLOCKS

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An exciting development in nanoscience is the formation of materials whereby atomic clusters serve as the building blocks. Since the properties of clusters change with size, composition and the charged state, cluster assemblies offer the attractive proposition of forming materials with novel combination of properties. Cluster solids can be stabilized either by using counter ions or via ligands to passivate the reacting species. The resulting assemblies allow the integration of multiple length scales into a hierarchical material and the emergent properties depend on the nature of the building blocks as well as the architecture of the assembled material as the solids combine intra-cluster, inter-cluster, linker-cluster, and ligand-cluster interactions, unavailable in conventional atomic solids.

The talk will first review our efforts in synthesizing cluster-based solids where the primitive motifs are the multiply-charged polyatomic anions, called Zintl anions. New building blocks can be formed by covalently linking multiple anions and the nature of the assemblies can be further controlled by extending the counteractions to include cryptated ions. Through variations of the anionic motifs and alkali/cryptated ions, it becomes possible to assemble the resulting solids in various architectures including zero, one, two, and three dimensional solids. In particular, I will present our results on the cluster-assembled materials derived from anionic As_7^{3-} combined with counteractions including alkali metals and cryptated K^+ ions, and building motifs that also involve Zintl ions covalently linked with Hg, Zn, Cd, Pd, etc. The talk will highlight how different cluster assemblies can be synthesized by using covalent linkers and assembling them with counteractions in various proportions. Taking the band gap energy of the resulting material as the property of choice, I will show that the energy bands in these cluster solids exhibit far less dispersion than in atomic solids and that the band gap energy can be controlled over a wide range.

The talk will also review two recent developments. The first involves ligated cluster assemblies involving metallic cores. In particular, I will present our results on assemblies with a bi-metallic core and the properties of the resulting material. The second involves our effort in developing air stable nano-materials. I will describe our recent success in synthesizing and characterizing three new alkaline earth Metal Organic-Frameworks (MOFs) and the origin of their differing band gap energies.

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Th-IV-1

ELECTRON AND POSITRON SCATTERING CROSS SECTIONS FROM CLUSTERS AND CONDENSED MOLECULES

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Clustering effects in the differential and integral electron and positron scattering cross sections have been investigated by calculating these magnitudes for different water cluster configurations (dimer, trimer and tetramer) as well as for fullerene (C₆₀).

By assuming that condensation effects can be described in terms of modifications of the single molecule electron or positron scattering cross sections induced by the surrounding molecules, effective data for liquid water is also provided. In the case of electrons, comparison with previous calculations in liquid water has been carried out through the inelastic mean free path, i. e. the mean length between successive inelastic collisions. Although a satisfactory agreement for high energies, above 100 eV, has been found, at lower energies some discrepancies remain and will be the subject of further investigations. As an example of modelling electron and positron interactions in soft matter, this set of data, complemented with other data that we have previously measured [1], has been used to simulate single electron tracks in liquid water by using our Low Energy Particle Track Simulation (LEPTS) code [2].

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ELECTRON PRODUCTION BY CARBON AND NOBLE METAL NANOPARTICLES IN COLLISION PROCESSES

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It is commonly understood nowadays that the vast portion of biodamage done by incident heavy ions is related, directly or indirectly, to the secondary electrons and free radicals produced in the process of ionization of the medium with ions [1]. Relative biological effectiveness of the ionizing radiation can be increased by injecting many-electron nanoparticles which play a role of sensitizers. At present, considerable interest is in using noble metal nanoparticles as sensitizers in cancer treatments with ionizing radiation [2, 3]. A very important fundamental problem closely related to the application of nanoparticle in cancer therapy is an adequate description of their dynamic response to the action of external fields.

A characteristic feature of metallic and, to some extent, carbon nanoparticles is a delocalization of the valence electrons, which can be excited collectively by an external electric field. Such excitations are represented as collective oscillations of delocalized electrons against the positively charged ions and are referred to as plasmons.

On the basis of the so-called plasmon resonance approximation (see, e.g. [4, 5] and references therein), we make estimates for the spectra of electrons generated by gold and carbon nanoparticles. The results of the present calculations are compared to those of model-based calculations [6] and Monte Carlo simulations for the case of a pure water medium. It is demonstrated that due to the prominent collective response to an external field, metallic and carbon-based nanoparticles may significantly enhance the production of secondary electrons in the medium in the energy range where collective electron excitation, which originate in noble metal and carbon nanoparticles, play a crucial role.

As an additional benchmark of the utilized approach, we have calculated photo- and electron impact ionization cross sections of carbon-based systems, namely fullerenes and polycyclic aromatic hydrocarbons (PAH). It is demonstrated that the results of calculations [7-9] for the C₆₀ fullerene as a case study are in good agreement with experimental data on photoionization [10] and electron inelastic scattering [5, 6]. Being a clear physical model, which describes collective electron excitations, the plasmon resonance approximation is proved to be a useful tool for interpretation of experimental results and making new numerical estimates.

Th-IV-2

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Th-IV-3

PROBING MESOSCOPIC OBJECTS WITH FAST IONS

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Collisional interactions with mesoscopic objects are useful to bridge the gap between gas atoms and bulk solids. The complex allotropes of carbon, such as, fullerenes, nanotubes and large organic molecules of biological (DNA bases) and astrophysical interest have been at the focus of recent atomic collision research. The interest in these systems arises from the necessity of understanding the influence of many-body nature on ionization. In a recent study we have shown that large ring-shaped organic molecules, such as, uracil have dramatically large cross section for forward electron emission and this behavior cannot be explained in terms of conventional ion-atom collision models. Similarly, the collective excitations in the polycyclic aromatic hydrocarbon (PAH) molecules found in the interstellar medium also influence their interaction with charged particles and photons. The structural complexity of these organic molecules and the lack of sophisticated theoretical framework are a major constraint to their understanding. This may be overcome to some extent by forging a synergy with large ordered molecules, like fullerene, which is known to show many-body correlation in their collision dynamics, through the exhibition of giant dipole plasmon resonance (GDPR).

The mesoscopic objects investigated here are fullerenes, uracil and coronene molecules. The secondary electron emission from bio-molecules is an important parameter to estimate the radiation damage caused by highly charged, energetic ions e.g., in hadron therapy. A large number of secondary electrons are produced along the track. Measurements providing double differential cross sections (in energy and emission angle) of secondary electrons (DDCS) provide stringent test to the theoretical models due to the complexity of the target molecule. The DDCS of secondary electron emission were measured for all three molecules in collisions with MeV bare C and O ions in the energy range of ~40-80 MeV and over a wide angular range i.e., between 30°-150° with respect to the incident beam direction. The detail energy and angular distributions show a dramatic difference with those for simple molecules like O₂ and N₂. The ab initio ion-atom model calculations based on the CDW-EIS models, although provide some gross features, fails to reproduce the unusually large forward-backward asymmetry. On the other hand, similar e-DDCS spectrum for the fullerene clearly manifests the existence of a “plasmon” peak which is enhanced in forward angles. The influence of such collective excitation in PAH molecule coronene (C₂₄H₁₂) could be seen to influence the forward backward asymmetry. A large enhancement of e-emission in forward emission can be related to the many-body effects, such as, collective excitation or size effect. In addition, the total ionization cross section shows a gradual variation in the q-dependence i.e. as $q^{1.0}$ (for C₆₀, coronene), $q^{1.5}$ (uracil) and $q^{2.0}$ (Ne and H₂O) for target Uracil, and These could provide some inputs for calculating the energy loss in condensed medium and models for radiation damage. The details will be presented.

Posters

CONFORMATIONAL EFFECT IN COLLISION DYNAMICS OF DNA BUILDING BLOCKS

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Action of radiations induces severe damage on biological medium. In addition to the primary radiation itself, important damage has been shown to be due to the secondary particles generated along the track after interaction of the ionizing radiation with the biological medium [1]. In particular, low-energy secondary ions have been widely investigated recently [2-4]. In such ion-biomolecule collisions, charge transfer and fragmentation mechanisms have to be considered [5]. From a theoretical point of view, the charge transfer process may be studied in the molecular framework and requires the determination of the potential energy surfaces of the different states involved in the reaction, as well as the non-adiabatic couplings between these levels. The dynamical treatment may be performed in a wide collision energy range using semi-classical methods.

Such an approach has been developed for the study of charge transfer between carbon ions and pyrimidine nucleobases, uracil, thymine, and halouracil targets. In such processes, radiosensitisation properties of the different targets have been pointed out as well as anisotropy and charge effects [7,8]. However it is important to analyze comparatively the behaviour of the different DNA building blocks. A complete study has been undertaken looking at the collision of isolated 2-deoxy-D-ribose in its furanose form with both protons and carbon ions [9]. The calculation has been performed in order to compare the sugar and nucleobases with regard to the charge, nature, orientation of the projectile ion. An analysis of the inner excitations is developed and comparison with experimental results is discussed [3,4]. The pyranose conformation of the sugar moiety corresponding to a six-membered ring geometry appears however the dominant form in gas phase experiments and consideration of the conformation of the sugar moiety is analysed [10,11].

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PHOTOIONISATION AND EXCITATION MECHANISMS OF FULLERENES AND HYDROCARBONS AFTER FEMTOSECOND LASER PULSE IRRADIATION

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Fullerenes are good model systems to study the excitation and ionisation mechanisms of complex molecules. Femtosecond photoelectron spectroscopy of fullerenes, like C₆₀ and C₇₀, revealed highly excited Rydberg-like states.¹ The photoelectron spectra (PES) showed a thermal electron background and a peak structure superimposed on it below kinetic energies corresponding to the photon energy.¹ The peak structure could be assigned to one-photon ionisation of diffuse low-angular momenta states, so-called superatom molecular orbitals (SAMOs) centred on the hollow fullerene core, based on photoelectron angular distributions (PADs) and TD-DFT calculations.¹ Further studies on the fullerene species C₈₂ and Sc₃N@C₈₀ showed PES and PAD with similar features.² The peaks become less prominent compared to the thermal electron background for increasing molecular size and decreasing symmetry and are almost absent for the endohedral species.² Therefore the thermal electron emission seems to be the main ionisation mechanism for larger and more complex molecules at these excitation conditions.² The relative photoionisation probabilities of the s-SAMO to p-SAMO were analysed for photon energies from 2-3.5 eV and showed good agreement with theoretical calculations.³

Quantum mechanical studies on a series of polycyclic aromatic hydrocarbons (PAH) revealed similar Rydberg-like molecular orbitals in analogy to the SAMOs in fullerenes and will be discussed. The binding energies of the s-state and the p_z-state show a decreasing trend with increasing molecular size.

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FEATURED TRENDS IN ELECTRON ELASTIC SCATTERING OFF ENDOHEDRAL FULLERENES

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Trends in electron elastic scattering off endohedral fullerenes $A@C_{60}$ in relation to the nature, size and spin of an encapsulated atom A are unravelled in a “zero-order” approximation. In the latter, (a) both the atom A and C_{60} cage are regarded as non-polarizable targets, (b) the C_{60} cage is modelled by an attractive potential well of inner radius r_0 , finite thickness Δ and depth U_0 , (c) electron correlation is ignored, (d) calculations are performed in a Hartree-Fock theory. The uncovered trends bear a semi-quantitative significance. Yet, they represent the most intrinsic features of $e + A@C_{60}$ scattering, since they are independent of secondary (finer) details of the C_{60} structure. In our study, $A = \text{Ar, Xe, Cr, Mn, Eu, Ba}$. In this abstract, we exemplify the discovered trends by results for $e + \text{Mn}@C_{60}$ scattering, see Fig.1. It is demonstrated that $e + A@C_{60}$ scattering can be noticeably weaker than scattering off an empty C_{60} cage; cp. $e + C_{60}$ with $e\uparrow\downarrow + \text{Mn}@C_{60}$ scattering, Fig.1. This happens when the encapsulated atom donates much of its electron density to the C_{60} cage; note how the Mn 4s-spin-up ($4s\uparrow$) and 4s-spin-down ($4s\downarrow$) orbitals are noticeably drawn into the C_{60} wall ($r \approx 5.3 - 8.2$ a.u.). Next, it is shown that, for such atoms, $e + A@C_{60}$ scattering can even be weaker than electron scattering off the isolated atom A itself, at certain electron energies; cp. $e\uparrow + \text{Mn}@C_{60}$ with $e\uparrow + \text{Mn}$ scattering. Moreover, it is found that if such atoms are, additionally, high-spin atoms then the C_{60} cage in $A@C_{60}$ becomes “spin-charged” itself; note the difference between the $\text{Mn}^{(6S)}@C_{60}$ $4s\uparrow$ and $4s\downarrow$ orbitals inside the C_{60} wall ($r \approx 5.3 - 8.2$ a.u.), Fig.1. The latter is shown to result in a noticeable electron spin-dependence of $e + A@C_{60}$ scattering, at certain energies; cp. $e\uparrow + \text{Mn}@C_{60}$ with $e\downarrow + \text{Mn}@C_{60}$ scattering, Fig.1.

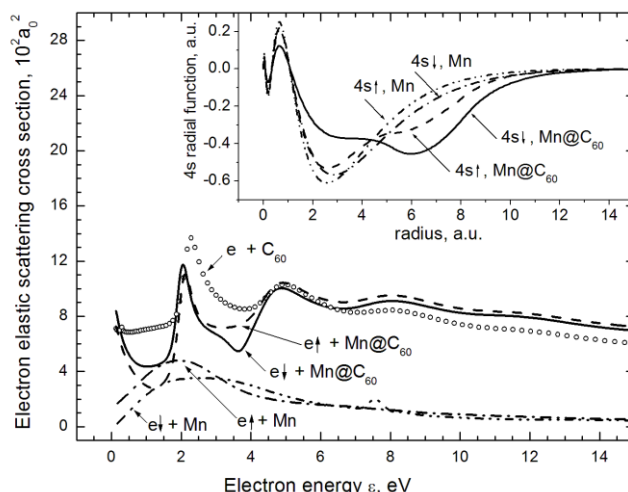


Figure 1: $e + C_{60}$, $e\uparrow\downarrow + \text{Mn}@C_{60}$ and $e\uparrow\downarrow + \text{Mn}$ electron elastic scattering cross sections, as marked. Inset: The $4s\uparrow\downarrow$ spin-orbitals of free Mn and $\text{Mn}@C_{60}$, as marked.

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ELECTRON LONG-WAVE BREMSSTRAHLUNG ON A@C₆₀ FULLERENES: THE INITIAL INSIGHT

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Spectral density $d\sigma/d\omega$ (ω is the photon frequency), angular asymmetry parameter β , as well the third Stock's polarization parameter ζ_3 of electron bremsstrahlung on endohedral fullerenes A@C₆₀ in relation to the nature, size and spin of an encapsulated atom A (A = Xe, Cr, Mn and Ba) are theoretically studied in a long-wave approximation ($\hbar\omega \ll$ electron energy). Furthermore, as in [1], (a) both the atom A and C₆₀ cage are regarded as non-polarizable targets, (b) the C₆₀ cage is modelled by an attractive potential well of inner radius R₀, finite thickness Δ and depth U₀, (c) electron elastic scattering phase shifts are calculated in a Hartree-Fock approximation. This is suitable for getting an initial insight into the subject. Obtained results, however, seem to reflect the most intrinsic features of e + A@C₆₀ bremsstrahlung, because they are independent of any finer details of the C₆₀ structure. It is demonstrated that $d\sigma/d\omega$, β and ζ_3 of a long-wave bremsstrahlung on A@C₆₀ (i) are oscillatory functions of electron energy, (ii) may differ markedly from those for bremsstrahlung on empty C₆₀ and (iii) become electron-spin-dependent when A is a high-spin atom (such as, e.g., the Mn atom whose spin S = 5/2); see Fig.1 for illustration.

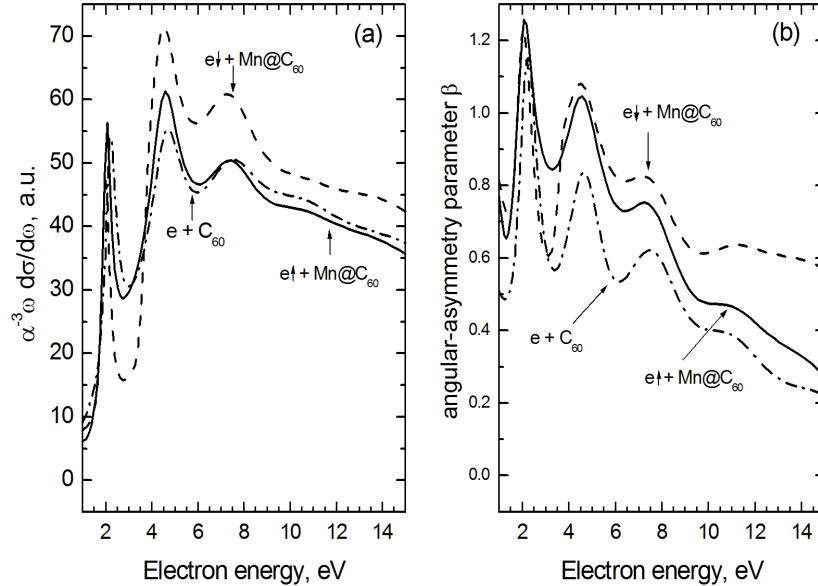


Figure 1: (a) $\alpha^{-3}\omega(d\sigma/d\omega)$ and (b) parameter β of electron bremsstrahlung on C₆₀ and Mn@C₆₀ versus electron energy. $\alpha=1/137$, arrows $\uparrow\downarrow$ mark electron spin polarizations.

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RADIATION INDUCED PROCESSES IN CLUSTERED BIOMOLECULES AND NEUTRAL BEAM CONTROL

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Radiation induced processes in biomolecules have been investigated intensively recently, notably in order to better understand the fundamental processes that can initiate DNA lesions [1]. While studies of isolated molecules generally provide the clearest data interpretations, equivalent measurements on hydrogen-bonded complexes enable closer analogies to be drawn with biological environments where different unimolecular or intermolecular reactive pathways can be significant.

By comparing dissociative ionization by electron impact (EI) and UV multi-photon ionization (MPI) of isolated and clustered nucleobases, we have obtained evidence for isomeric transitions in neutral electronic excited states. In particular, a new fragment ion ($C_3H_4N_2O^+$) has been observed from gas-phase uracil by 2-photon absorption at photon energies below 5.29 ± 0.06 eV (Fig. 1) [2]. The threshold agrees closely with the minimum calculated activation energy (5.25 eV, CASSCF) for a ring opening conical intersection from the lowest-lying $^1\pi\pi^*$ state to a $^1\sigma(n-\pi)\pi^*$ closed shell state [3]. Clustering with water suppresses the $C_3H_4N_2O^+$ channel, indicating that the hydrogen-bonded environment stabilizes uracil with respect to excited state ring opening [3]. We will also report progress in the development of experiments to analyze low energy electron interactions with selected neutral isomers and clusters [4].

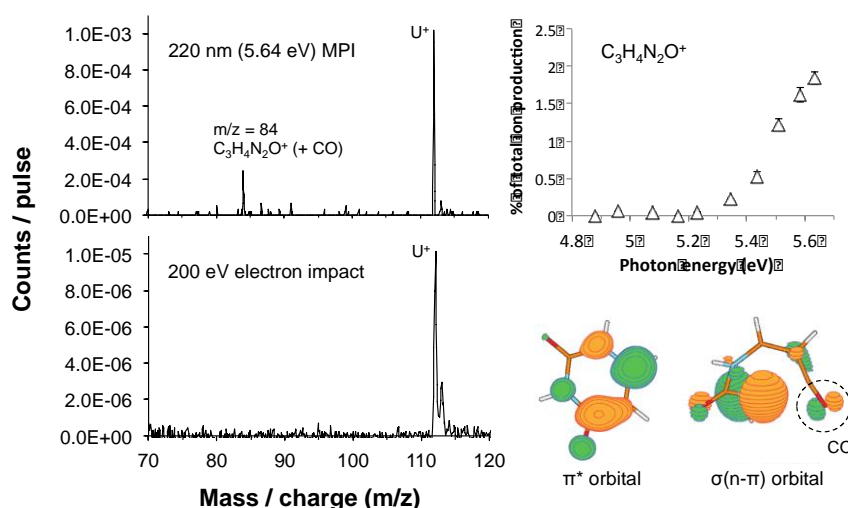


Figure 1: (Left) Comparison of MPI and EI mass spectra for uracil [2]. (Top right) Photon energy dependence of $C_3H_4N_2O^+$ production from uracil by MPI [2]. (Bottom right) The two orbitals [3] involved in the ring-opening excitation discussed above.

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MOLECULAR-DYNAMICS SIMULATION OF MARTENSITE-AUSTENITE TRANSITION IN NICKEL-TITANIUM NANOPARTICLES

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The structural transition from lower-symmetry martensite to higher-symmetry austenite is crucial for the shape-memory effect in distinct crystalline solids [1]. In particular for the widely used nickel-titanium alloy, a satisfactory theoretical description of this cooperative process on the microscopic scale is lacking. In this work, we explore the thermally induced transition from monoclinic martensite to cubic austenite in free equiatomic nickel-titanium nanoparticles by means of molecular-dynamics simulations using a many-body potential. For spherical particles with 8472 to 39349 atoms, and radii from 3 nm to 5 nm respectively, we complement the investigation of a recently proposed model [2] by looking at structural parameters as well as specific heats. Notably, we approximate the low-temperature specific heat based on the classical simulations. On the one hand, we confirm features like the size-dependent scaling of transition temperatures and surface nucleation as a trigger of the martensite-austenite transition. On the other hand, by considering slower heating and by performing annealing runs, we reveal the relaxation from martensite to distinct austenite ground-state lattices.

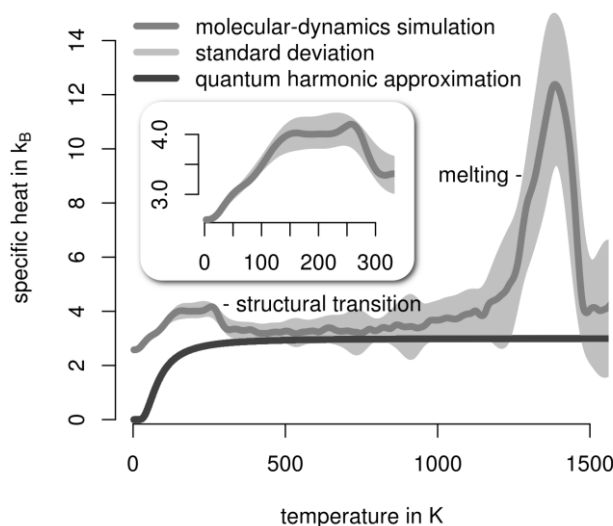


Figure 1: Specific heat for nickel-titanium nanoparticle with radius $R=3$ nm. The graph of the harmonic approximation is estimated from MD velocity data. *Inset*: Magnification of the martensite-austenite transition.

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CAGE EFFECTS ON CORE-EXCITED FREE, CLUSTERED AND ENCAPSULATED MOLECULES

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Molecular electronics is the subject of intriguing changes taking place when a molecule happens to be confined in a cage. Special emphasis is put on core-to-valence transitions embedded into the core ionization continuum of SF₆ confined in fullerene cages such as C₆₀, C₂₄₀ and C₅₄₀. X-ray absorption and inner-shell photoionization spectra are regarded as a basic probe of the cage effects. Their origin is being attributed mainly to (i) changes in molecular dynamics [1,2], (ii) electron elastic and inelastic scattering at the cage [2,3] and (iii) intermolecular interaction and dynamic polarization of the cage [4]. These cage phenomena are discussed in more detail within the quasiatomic approach and the double-barrier-optical potential model [2,5].

Spectral distribution of oscillator strength for X-ray transition near the *shape, confinement* and *window-like* resonances in X-ray absorption and inner-shell photoemission from the caged molecules are computed and analyzed. These resonances are originated from the interference of the primary photoelectron wave with the scattered waves on atoms embodied in the confined molecule and the cage and assigned respectively with the quasibound states spatially localized within the inner and external wells as well as the interstitial region. The shape and window-like resonances are revealed in S 1s and 2p-to-continuum transitions in SF₆@C_{60,240,540}. The confinement resonances are revealed in Ar 1s transitions in Ar@C₆₀. Dynamical aspects connected with the photoelectron trapping time and core-hole lifetime are discussed. Recoil dynamics of the confined molecule is also examined. Special emphasis is put on the photoelectron – valence electron interaction resulting in appearance of the confined cation in the positively charged cage, e.g. SF₆⁺@C₆₀⁺ and Ar⁺@C₆₀⁺. Perspectives in applications of the cage effects for deeper understanding of elementary processes occurring in biological, complex composite systems and pores are discussed.

The work is supported by the RFBR grant 12-02-00999, and SPBU grant 11.38.638.2013.

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SELF-TRAPPING PHENOMENA IN PHOTOEMISSION FROM FREE AND CONFINED MOLECULES

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Shape resonances and multielectron excitations play dominating role in the near-edge x-ray absorption of nanoobjects. The latter are usually originated by the conjugate shake up mechanism. The former are associated with temporary trapping of the photoelectron within the finite size potential (pseudopotential) barrier and subsequent tunneling of the photoelectron through the barrier into the continuum. Spectral distribution of oscillator strength for the shape resonance transitions are reasonably described as a convolution of asymmetric and symmetric Lorentzian and Gaussian line shapes [1]. The widths of the Lorentzian contributions are responsible for the resonance lifetime connected with the photoelectron trapping time and the core-hole lifetime. The experimental data analysis [1] evidences that the trapping time is usually much shorter than the core-hole lifetime.

We show that the photoelectron – valence electrons interaction that accompany the photoelectron tunneling through the barrier, leads to self-trapping of the photoelectron within the valence-excited-photoion and invokes the specific distortion of the shape resonance. The self-trapping mechanism is examined in detail by considering the C 1s $\Sigma \rightarrow \sigma^*\Sigma$ shape resonance in CO. The shape resonance demonstrates an anomalous behavior (see, Fig.1) with the low-energy side (298 – 302 eV). The nature of the anomaly is unknown. There are substantial difficulties with its understanding as it superimposes with the triplet and singlet 2h – 2e excitations $2\sigma(\text{C}1s)^{-1}5\sigma^{-1}2\pi^1 n/\sigma^1$ in the $\Sigma \rightarrow \Pi$ channel [2]. We assign here this anomaly to the coupling of the photoelectron elastic and inelastic scattered waves on valence electrons, namely with changes in the amplitudes of elastic scattered waves near the inelastic thresholds. We mainly concentrate on the interval 297 – 305 eV where the $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^2$ and $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^1 n/\sigma^1$ excitations couple with the $\sigma^*\Sigma$ shape resonance.

The C 1s hole creation σ^\oplus (Fig.1) and single-hole ionization σ^+ cross sections for the $\Sigma \rightarrow \Sigma$ transition are computed taking the triple convolution approach [1], the VDFN model [3] and the optical potential concept [4]. By comparing the computed and the experimental [2,5] cross sections we conclude that the recapture of the C 1s photoelectron by the remaining photoion, which leads to the formation of the $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^2$ (Σ) and $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^1 n/\sigma^1$ (Σ) states explains the anomalous behavior of the σ^* -shape resonance. The $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^1 n/\sigma^1$ (Σ) excitation is associated with the intense vibrational transitions and results in the additional phase shift of the elastic scattered waves and the shoulder at 300 – 302 eV (Fig.1). The $2\sigma(\text{C}1s)^{-1}1\pi^{-1}2\pi^2$ (Σ) excitation centered at photon energy ~ 298 eV refers to fast molecular dissociation with the yield of neutral C and O atoms. Fig. 1 presents the C 1s (Σ) $\rightarrow \sigma^*$ (Σ) shape resonance computed by neglecting the inelastic scattering of the C 1s photoelectron on the valence electrons (dashed line) and taking the self-trapping of the photoelectron (solid line). The comparison of the curves with the experimental spectra indicates an important role of the self-trapping phenomena on the C 1s photoemission in the $\Sigma \rightarrow \Sigma$ channel.

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In contrast to the conjugate shake-up mechanism dominating in the $\Sigma \rightarrow \Pi$ channel, the self-trapping mechanism works in the $\Sigma \rightarrow \Sigma$ channel resulting in appearance the new $2h - 2e$ excited molecular Σ -states and substantial changes in the intramolecular interference of the primary and scattered photoelectron waves. It is shown that the $2h - 2e$ excited Σ -states induce either the fast molecular dissociation or the population of high vibrational levels.

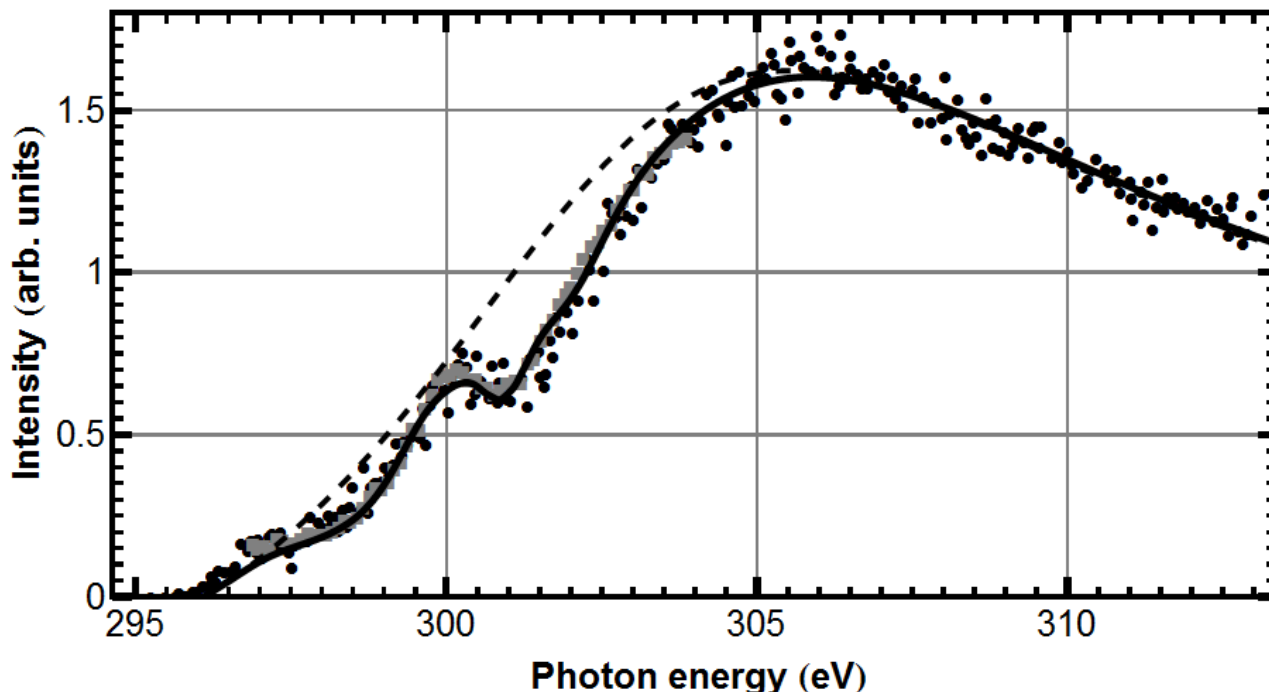


Figure 1: The experimental C 1s (Σ) \rightarrow σ^* (Σ) shape resonance in the fixed-in-space CO is displayed by black and grey symbols taken from the works [2] and [5] respectively. The computed shape resonance: without the photoelectron – valence interaction – dashed line and with the account of the self-trapping mechanism – solid line.

The important role of the self-trapping mechanism in spectral dependence of photoemission from atoms and molecules confined in fullerene shells are also examined and discussed.

The work is supported by the RFBR grant 12-02-00999, and SPBU grant 11.38.261.2014.

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THE USE OF NANODRUGS TO IMPROVE THE HADRON THERAPY

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Radiotherapy based on the use of high energy photons (X-rays or γ -rays) is the most common approach in clinical settings. However, its implementation is limited by the tolerance of healthy tissue. Therefore, it is of major interest the development of new techniques and clinical protocols. Due to the ballistic effect and energy deposition of charged particles in depth, the hadrontherapy (proton or carbon ions) is considered as one of the most promising techniques for cancer radiation therapy. However, it remains restricted by the side effects caused by the dose deposited at the entrance of the track. To overcome this limitation, our work aims at developing new high-Z atom based nanoparticles (HZ-NPs) and studying their amplification effect when medical ion beams are used. From biomolecules to cells, our group has shown the potentialities of platinum [1][2], gold and gadolinium based nanoparticles to intensify biological damage. The amplification effect of HZ-NPs has been explained as due to early stage mechanisms of electronic activation and emission, which take place at molecular level and produce a nanoscopic perturbation (complex damage). To better understand the role of these molecular scale processes in living cells, it is necessary to characterize the uptake and localization of nanoparticles in cells (by TEM, DVU and Confocal microscopy), to evaluate their toxicity and, in parallel, to model the interface NP-biological environment to get new insights into the possible dose enhancement mechanisms. In this work, the synthesis and characterization of different HZ-NPs with variable size and composition will be presented. Their stability in relevant culture media, toxicity in human cancer cells and amplification effect will be discussed.

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DNA RADIO- AND PHOTSENSITIZATION WITH PLATINUM-BROMINE COMPOUNDS

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One of the major goals of modern radiotherapy is to develop methodologies which increase cellular DNA damage in tumor cells using lower radiation doses such that damage to healthy cells is reduced and side effects on patients are mitigated. Among the most successful methods adopted today is the introduction of a radiosensitizer into tumor, such a treatment has been shown to be particularly beneficial in the treatment of neck, lung, pancreas or stomach cancers [1]. However the mechanisms by which such radiosensitization occurs are still unclear but recent research has highlighted that low energy electrons, which are the most abundant species created during high energy irradiations, may be as efficient in causing damage to biomolecules and DNA in particular [2], as the incident radiation itself. Such secondary particle damage can be initiated by other types of ionizing radiation, such as X-rays or γ -rays. Accordingly a wide range of radiosensitizing chemicals are being investigated, among which platinum-containing ones have been found to be the most successful [3], [4]. It has been shown that such compounds coordinate themselves to nitrogen atoms of purines in DNA helix [3]. One of the most widely used cancer therapy drugs is cisplatin, which apart from being a very efficient chemotherapeutic drug, toxic to living cells [5], can be also used as a potential source of secondary particles emitted by high energy irradiation, mainly low energy electrons and radicals. This property of cisplatin has been investigated recently and an increase in single (SSBs) and double strand breaks (DSBs) formation was reported [6]. The enhancement of DNA damage upon resonant X-ray radiation in presence of platinum-derived complexes due to the Auger effects has been widely investigated [7], [8], showing that DNA damage increases upon Pt adducts. Apart from platinum-containing drugs [9], brominated compounds [10, 11] were also found to be efficient radio- and photosensitizers in clinical radiotherapy. Therefore, an even more efficient drug may be developed if it contains both platinum and bromine.

We had performed X-ray and UV light irradiation of plasmid DNA in presence of platinum and/or bromine compounds in order to assess the photo- and radiosensitization capabilities of these compounds. In present investigations we have used plasmid DNA pBR322 to monitor effectiveness of chosen compounds in inducing strand breaks. Samples were incubated in presence of several potential radiosensitisers: platinum (II) bromide, hydrogen hexabromoplatinate (IV), hydrogen hexahydroxyplatinate (IV), sodium hexahydroxyplatinate (IV), cis-diamminedichloroplatinum (II) and cis-diamminedibromoplatinum (II). It was found that platinum (II) bromide can greatly increase

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the levels of single- and double-strand break formation observed in the irradiated samples with respect to the samples containing platinum as a radiosensitizer only [12], possessing no chemotherapeutic activity. In addition, this compound induced no photosensitivity in samples irradiated with UV light. The process we observe can be explained by DEA to PtBr₂ at low energies, creating a bromine anion and thus further damage to DNA [13]. The suggested drugs exhibit much higher level of radiosensitivity than widely used cisplatin and thus are good candidates for cancer treatment.

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MBN EXPLORER: A UNIVERSAL TOOL TO STUDY COMPLEX MOLECULAR STRUCTURE AND DYNAMICS

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MBN Explorer [1] is a multi-purpose software package designed to study structure and dynamics of molecular systems of various degrees of complexity. A broad variety of interatomic potentials implemented in the MBN Explorer allows to simulate the structure and dynamics of different molecular systems, such as atomic clusters [2], fullerenes [3], nanotubes [4], metallic nanomaterials [5], proteins and DNA [6], crystals [7] composite bio-nano systems and nanofractals [8,9]. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and implemented multiscale features that make it applicable to really a broad range of problems involving complex molecular systems.

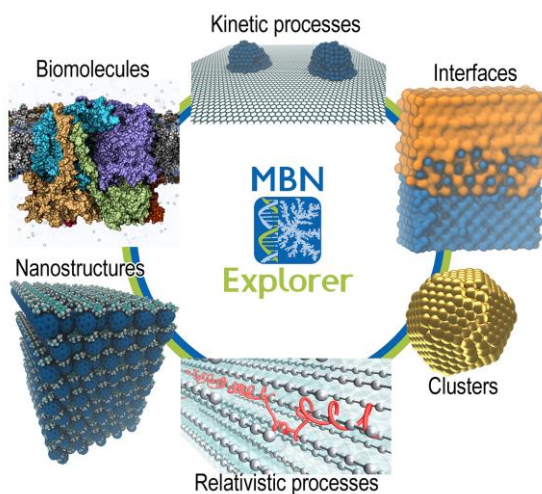


Figure 1: Illustration of different application areas of MBN Explorer [1].

The poster will give an overview of the main capabilities of the package and will highlight a number of recent case studies carried out with the use of MBN Explorer some of which are illustrated in Figure 1.

The professional version of MBN Explorer can be ordered via its website [10] upon the registration and acceptance the terms and conditions of the commercial license agreement. Currently, there are more than 1000 registered users of MBN Explorer, which is being under the permanent development conducted by the MBN Research Center in Frankfurt [11].

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MBN EXPLORER: SIMULATION OF CHANNELING PROCESSES OF CHARGED PARTICLES IN STRAIGHT, BENT AND PERIODICALLY BENT CRYSTALS

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MBN Explorer [1,2] is a multi-purpose software package designed to study structure and dynamics of molecular systems of various degrees of complexity. A broad variety of interatomic potentials implemented in the MBN Explorer allows to simulate the structure and dynamics of different molecular systems, such as atomic clusters [3], fullerenes [4], nanotubes [5], metallic nanomaterials [6], proteins and DNA [7], crystals [8] composite bio-nano systems and nanofractals [9,10]. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and implemented multiscale features that make it applicable to really a broad range of problems involving complex molecular systems.

The poster will give an overview of recent studies on motion of ultra-relativistic particles in oriented crystals carried out with the use of MBN Explorer [8,11-15]. The special module was developed that implements dynamic generation of the crystalline environment medium and solves three-dimensional relativistic equations of motion in order to calculate trajectories of projectiles in crystals.

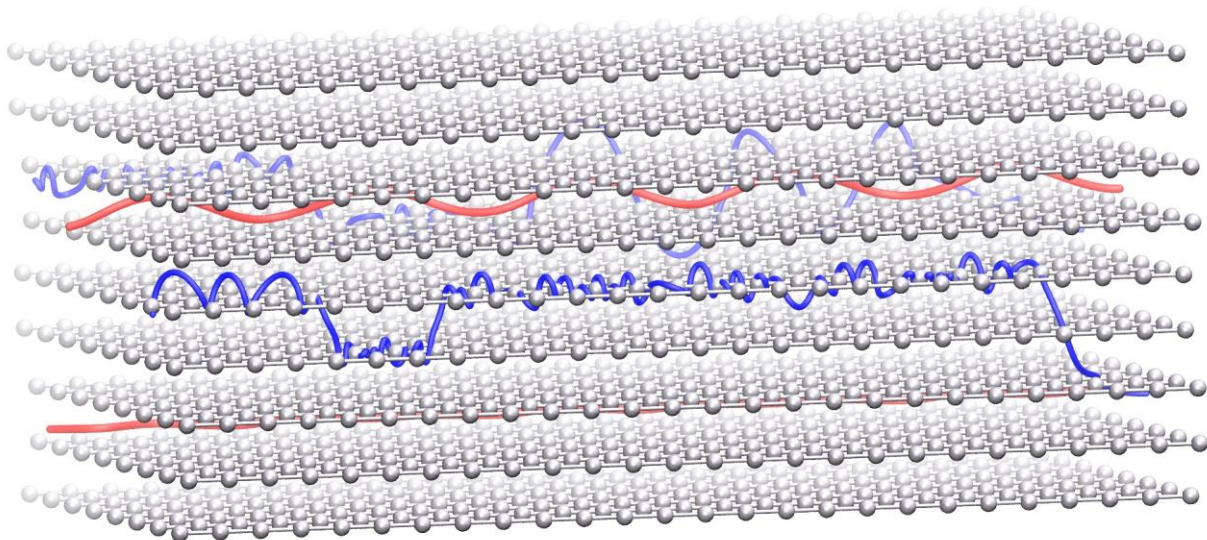


Figure 1: Illustration of axial channeling trajectories of 10 GeV electrons and positrons in Si crystal. The atoms of Si are shown schematically in a different scale.

This approach allows efficient direct comparison of different cases of channeling as well as flexibility in considering various types of crystals, projectiles, incident direction of the beam, its energy and other parameters imposed by experimental setup. The MBN Explorer package was

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applied to studying of channeling effect in straight [8,11], bent [12-14] and periodically bent crystals in planar [12,15] and axial cases [15]. The analysis of simulated trajectories allows one to calculate the radiation spectrum, dechanneling length and the fraction of channeling particles.

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PHOTOIONIZATION OF FULLERENES AND OTHER CARBON-BASED NANOSCALE SYSTEMS

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Photoionization of fullerenes as well as other atomic clusters and nanoscale systems involves a number of prominent phenomena, which have been studied by means of various theoretical methods. Being by its nature a quantum phenomenon, the photoionization process can be described within the *ab initio* framework based on the time-dependent density functional theory (TDDFT) [1]. However, it is well established that photoionization of nanoscale carbon systems, fullerenes in particular, as well as various metallic clusters and nanoparticles, takes place through collective excitations of delocalized valence electrons, called plasmons, induced by an external electric field. The plasmon excitations correspond to oscillations of the electron density with respect to the positively charged ions. Such collective excitations, appearing in many-electron systems, are well known in classical electrodynamics and are described in classical physics terms (Refs. [2, 3] and references therein).

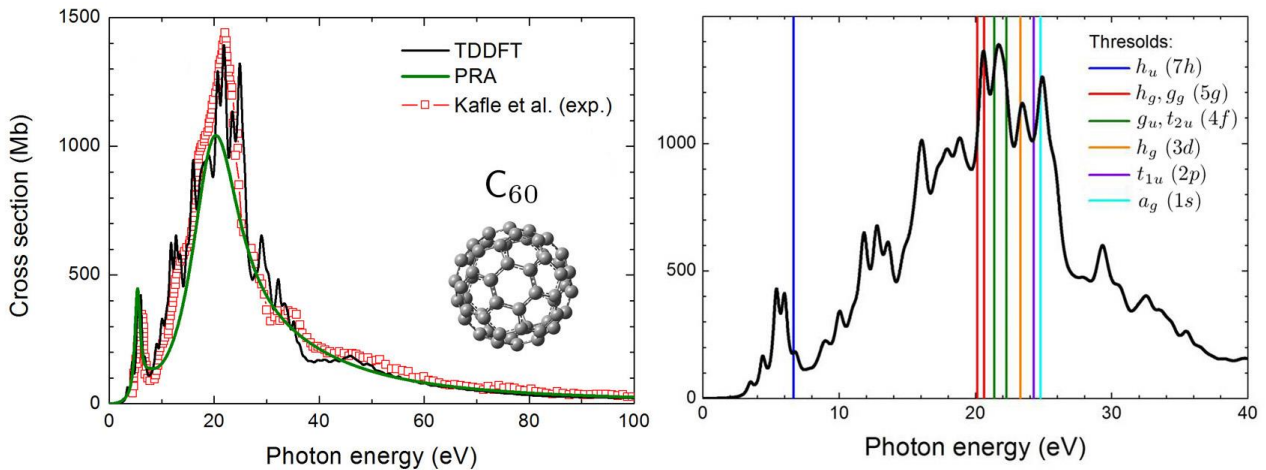


Figure 1. Left panel: The photoabsorption cross section of C_{60} calculated within the TDDFT method (thin solid curve) and the plasmon resonance approximation (thick solid curve). Theoretical curves are compared to the experimental data compiled by Kafle et al. [6]; Right panel: Ionization thresholds of the HOMO (h_u) as well as of a number of innermost valence orbitals of C_{60} .

Considering photoionization of the C_{60} fullerene as a case study, we elucidate the contributions of various classical and quantum physics phenomena appearing in this process. Comparing the TDDFT results with those based on the plasmon resonance approximation (Refs. [2-4] and references therein), we map the well-resolved features of the photoabsorption spectrum of C_{60} to single-particle and collective excitations which have a different physical nature [5]. It is demonstrated that the peculiarities arising in the photoionization spectrum of C_{60} atop the

dominating plasmon excitations have the quantum origin. In particular, we demonstrate that a series of individual peaks can be assigned either to the optically allowed discrete transitions or to the ionization of particular molecular orbitals of the system (see Figure 1).

A similar method, based on the comparative analysis of the *ab initio* and model-based approaches, is utilized to study the photoionization spectra of other carbon-based nanoscale systems, such as polycyclic aromatic hydrocarbons (PAH) [7] and more complex structures like carbon buckyonions (see Figure 2). In particular, TDDFT-based calculations of the photoionization spectrum of the $C_{60}@C_{240}$ buckyonion revealed the absence of strong plasmonic couplings between individual fullerenes which were proposed earlier on the basis of the jellium-model approach [8].

The results of the *ab initio* and model-based calculations are found to be in close mutual agreement and correspond well to the available experimental results on photoionization of fullerenes and PAHs (Figures 1 and 2). The developed methodology is proved to be an efficient and reliable tool for the calculation and analysis of ionization spectra of complex molecular systems.

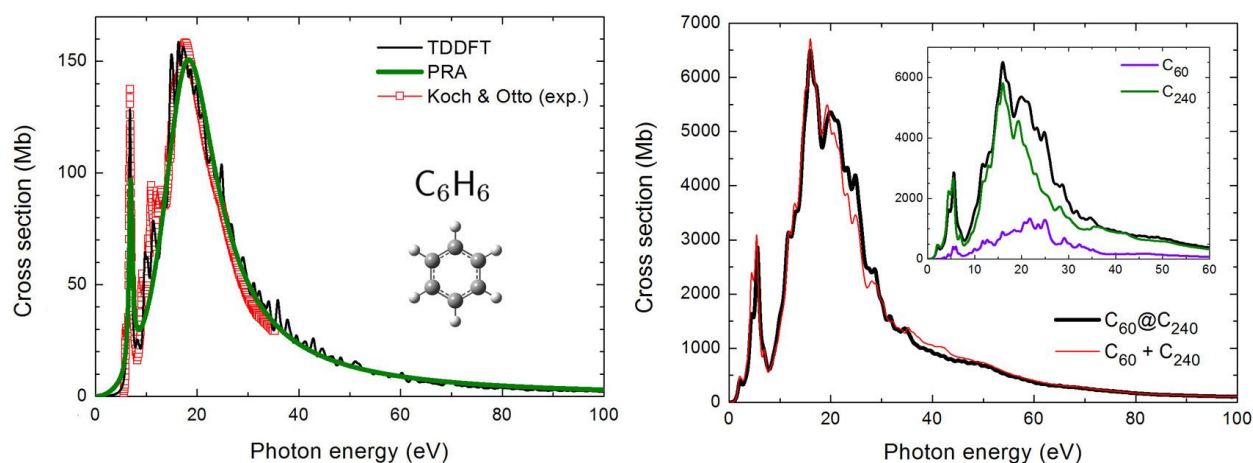


Figure 2. Left panel: The photoabsorption cross section of the benzene molecule calculated within the TDDFT method (thin solid curve) and the plasmon resonance approximation (thick solid curve). Theoretical curves are compared to the experimental data [9]; Right panel: The photoabsorption cross section of the $C_{60}@C_{240}$ buckyonion (thick solid curve) and the sum (thin curve) of the spectra of isolated C_{60} and C_{240} (shown in the inset) calculated within the TDDFT method.

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For notes

For notes

Monday, 19 May 2014

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

Tuesday, 20 May 2014

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| 9 ⁰⁰ – 9 ³⁰ | DySoN 2012 Opening: Nigel Mason and Andrey V. Solov'yov |
| 9 ³⁰ – 11 ⁰⁰ | <i>Morning session I: Structure and dynamics of clusters, nanoparticles and biomolecules</i> Nigel Mason Eric Surraud Julius Jellinek |
| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <i>Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i> Richard Palmer Yuri Vainer Michael Wilkinson |
| 13 ⁰⁰ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 16 ⁰⁰ | <i>Afternoon Session I: Nanoscale insights in biodamage</i> Lenka Stefancikova Pablo de Vera Brenda Laster |
| 16 ⁰⁰ – 18 ⁰⁰ | <i>Coffee and Poster Session</i> |

Wednesday, 21 May 2014

| | |
|-------------------------------------|--|
| 9 ³⁰ – 11 ⁰⁰ | <i>Morning session I: Propagation of particles through medium</i> Hartmut Backe Andrei Korol Vincenzo Guidi |
| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <i>Morning session II: Particle confinement phenomena</i> Jean-Patrick Connerade Andrea Mazzolari Gennady Sushko |
| 13 ⁰⁰ – 13 ¹⁵ | Conference photo |
| 13 ¹⁵ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 18 ⁰⁰ | Castle visit |

Thursday, 22 May 2014

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| 9 ³⁰ – 11 ⁰⁰ | <i>Morning session I: Collision processes involving nanosystems</i> Bernd Huber Olof Johansson Florent Calvo |
| 11 ⁰⁰ – 11 ³⁰ | Coffee break |
| 11 ³⁰ – 13 ⁰⁰ | <i>Morning session II: Nanoscale insights in biodamage</i> Eugene Surdutovich Stéphane Lucas Ilya Fabrikant |
| 13 ⁰⁰ – 14 ³⁰ | Lunch |
| 14 ³⁰ – 16 ⁰⁰ | <i>Afternoon session I: Clustering and self-organization on the nanoscale</i> Andrey Solov'yov David Field Arthur Reber |
| 16 ⁰⁰ – 16 ³⁰ | Coffee break |
| 16 ³⁰ – 18 ⁰⁰ | <i>Afternoon session II: Structure and dynamics of clusters, nanoparticles and biomolecules</i> Gustavo Garcia Alexey Verkhovtsev Lokesh Tribedi |
| 19 ⁰⁰ – 22 ³⁰ | Conference banquet |

Friday, 23 May 2014

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| 09 ³⁰ – 17 ⁰⁰ | “NAnoRADIation Processes (NARAP)” Workshop |
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