4th International Conference *"Dynamics of Systems on the Nanoscale"*

Häcker's Grand Hotel, Bad Ems, Germany
October 03 - 07, 2016

DYSON 2016

Book of Abstracts

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Preface

The Fourth International Conference “Dynamics of Systems on the Nanoscale” (DySoN 2016) will be held in Bad Ems, Germany during October 3-7, 2016 at the historical Häcker’s Grand Hotel.

The DySoN conference has been built upon a series of International Symposia “Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale (ISACC)” (see www.isacc-portal.org). During these meetings it has become clear that there is a need for an interdisciplinary conference covering a broader range of topics than just atomic cluster collisions, related to the Dynamics of Systems on the Nanoscale. Therefore, in 2010 the ISACC International Advisory Committee decided to launch a new conference series under the title “Dynamics of Systems on the Nanoscale”. The first DySoN conference took place at the National Research Council, Rome, Italy in 2010; the second conference was held in St. Petersburg, Russia in 2012; the third one was held in Edinburgh, UK in 2014. DySoN 2016 is the fourth conference in this series.

The DySoN 2016 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, nanostructures, ensembles of nanoparticles, nanomaterials, 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 bio-technology, 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 nanoscale? Are these principles classical or quantum? How does function emerge at the nano- and mesoscale in systems with different origins? Which 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, theoretical and applied aspects of these problems will be discussed at the conference. Particular attention will be devoted to dynamical phenomena and many-body effects taking place in various MBN systems on the nanoscale, which include problems of structure formation, fusion and fission, collision and fragmentation, surfaces and interfaces, collective electron excitations, reactivity, nanoscale phase and morphological transitions, irradiation driven transformations of complex molecular systems, biodamage, channelling phenomena and many more.

DySoN 2016 aims also at highlighting the breakthroughs achieved within the currently running COST Action CM1301 CELINA – “Chemistry for ELectron-Initiated Nanolithography” and the project FP7-ITN-ARGENT-608163 – “Advanced Radiotherapy, Generated by Exploiting Nanoprocesses and Technologies”. The latter project inherited and extended the scopes of the recently ended COST Action “Nanoscale insights into ion-beam cancer therapy” (Nano-IBCT) towards the understanding of nanoparticle impacts on biological systems and related biomedical

applications. Therefore, DySoN 2016 will continue traditions of the earlier Nano-IBCT Conference series.

Also, the mini-workshop “Periodically bent crystals for crystalline undulators” held within the HORIZON 2020 RISE-PEARL-690991 project will be linked to DySoN 2016. The research areas represented by the mentioned European projects overlap strongly with the Topical Areas of the DySoN Conference.

Finally, DySoN 2016 will provide a platform to host discussions about current and future research challenges and initiatives within the DySoN Conference Topical Areas. 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 Häcker's Grand Hotel, located in Bad Ems, Germany.

Bad Ems is a small town on the river Lahn, which was considered in 17th-19th centuries as one of Germany's most famous bathing resorts and became the summer residence of various European monarchs and artists.

Conference Reception

The conference reception will take place on Monday, October 3 from 19^{00} to 21^{00} and will be located in the hotel.

Conference Dinner

The conference dinner will take place on Thursday, October 6, in the restaurant Concordiaturm Bad Ems (http://www.concordiaturm-badems.de/) from 19^{00} to 22^{30}. A transfer from the hotel will be organized.

Conference Tour

On Wednesday, October 5, a guided tour along the historical center of Bad Ems will be organized. During this tour, the participants of DySoN 2016 will have an opportunity to learn more about the history of this place. The tour will start at 16^{30} and will last for two hours.

DySoN 2016 Proceedings

Proceedings of the DySoN 2016 Conference will be published in the dedicated Topical Issue "Dynamics of Systems on the Nanoscale" of the European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics. Participants of the conference are coordinally invited to submit a contribution to this Topical Issue. Submission deadline is December 30, 2016.

Training Course on Multiscale Modeling of MBN Systems

DySoN 2016 will be followed with the training course on multiscale modelling of Meso-Bio-Nano (MBN) systems, their structure and dynamics, by means of MBN Explorer and MBN Studio – the powerful and universal software, being developed by MBN Research Center. The course will take place on October 8-9 at MBN Research Center in Frankfurt am Main.

Information on the registration, scope and schedule of the training course can be found at the following webpage: http://mbnresearch.com/tutorial-5-scope.

All the DySoN participants who express interest in attending the course are asked to register at the dedicated webpage (http://mbnresearch.com/tutorial-5-registration) and contact members of MBN Research Center for more information.

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Sponsors

The conference is held under the auspices of the following sponsors:

- MBN Research Center, Frankfurt am Main, Germany
- HORIZON 2020 RISE-PEARL-690991
- FP7-ITN-ARGENT- 608163
- Springer

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DySoN Conference Webpage

Updated information on the conference is available at the following internet address:
www.mbnresearch.com/dyson-2016

Conference Program

Monday, 03 October 2016

12^{00} - 16^{00}	Participants registration
14^{00} - 14^{45}	**DySoN2016 Opening** **Andrey V. Solov'yov**, MBN Research Center, Frankfurt am Main, Germany *Multiscale modelling of Meso-Bio-Nano systems with MBN Explorer: biomedical and nanotechnology applications*
14^{45} - 16^{15}	*Afternoon session I: Structure and dynamics of clusters, nanoparticles and biomolecules* *Chair: Nigel J. Mason* **Eric Suraud**, Universite Paul Sabatier, Toulouse, France *Dissipation in clusters and molecules* **Julius Jellinek**, Argonne National Laboratory, Lemont, USA *Solving the problem of anharmonic densities of states* **Kit Bowen**, Johns Hopkins University, Baltimore, USA *Dipole bound anions, quadrupole bound anions, and double Rydberg anions*
16^{15} - 16^{45}	**Coffee break**
16^{45} - 18^{45}	*Afternoon session II: Nanoscale phase and morphological transitions* *Chair: Shiv N. Khanna* **Nigel J. Mason,** Open University, Milton Keynes, UK *Exploring morphology and chemical synthesis in ices and thin films* **Michael Moseler**, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany *Mechanically driven phase transitions and the formation of tribomaterial nanolayers* **Florent Calvo**, University Joseph Fourier - Grenoble 1, France *Evidence for non-statistical behavior in the collision-induced fragmentation of water clusters* **Thomas Schlathölter**, Zernike Institute for Advanced Materials, University of Groningen, the Netherlands *Radiation damage on the molecular level: from free oligonucleotides to DNA origami*
19^{00} - 21^{00}	**Welcome Reception**

Tuesday, 04 October 2016

9^{30} - 11^{00}	*Morning session I: Multiscale physics of radiation damage processes* *Chair: Andrey V. Solov'yov* **Eugene Surdutovich**, Oakland University, Rochester, USA *Multiscale approach to the physics of ion-beam cancer therapy: from prediction to experiment* **Pablo de Vera**, Queen's University Belfast, UK *Molecular dynamics insights into the biological effects of shock waves induced by ions* **Alexey Verkhovtsev**, Instituto de Física Fundamental, CSIC, Madrid, Spain *Predictive assessment of biological damage due to ion beams*
11^{00} - 11^{20}	**Coffee break**
11^{20} - 13^{00}	*Morning Session II: Biomedical applications of radiation* *Chair: Eugene Surdutovich* **Steffen Greilich,** German Cancer Research Center (DKFZ), Heidelberg, Germany *Assessing microscopic energy-deposition pattern in ion-beam therapy using fluorescent nuclear track detectors*

	Martin Falk, Institute of Biophysics of the CAS, Brno, Czech Republic *The biological mechanism of metal nanoparticle-mediated radiosensitization* **Malgorzata Smialek**, Gdansk University of Technology, Gdansk, Poland *Oligonucleotide-modified nanoparticles for cancer therapy* **Ilko Bald,** Institut für Chemie - Physikalische Chemie, Universität Potsdam, Germany *Probing low-energy electron induced DNA damage using DNA nanostructures and metal nanoparticles*
13^{00} - 14^{30}	**Lunch**
14^{30} - 16^{30}	*Afternoon session I: Nanostructured materials* *Chair: Michael Moseler* **Richard Palmer**, University of Birmingham, Birmingham, UK *Fulfilling Feynman's vision: arranging the atoms in size-selected clusters and a route to manufacturing* **Simon Connell**, University of Johannesburg, Republic of South Africa *The search for diamond crystal undulator radiation* **Victor Balykin**, Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Russia *Giant optical nonlinearity of a single plasmonic nanostructure* **David Field**, Aarhus University, Aarhus, Denmark *Spontaneously electrical solids*
16^{30} - 17^{00}	**Coffee break**
17^{00} - 18^{30}	**Poster session** and **H2020-RISE-PEARL** management board meeting

Wednesday, 05 October 2016

9^{15} - 10^{45}	*Morning session I: Surfaces and interfaces* *Chair: Florent Calvo* **Wolfgang Ernst**, Graz University of Technology, Graz, Austria *Surface deposition of metal clusters and nanowires formed in superfluid helium droplets* **Yuri Vainer**, Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Russia *Anomalous spectral dynamics in ultrathin subsurface layers and nanofilms of amorphous polymer* **Nouari Kebaili**, Laboratoire Aime Cotton, CNRS, Orsay, France *Preformed clusters deposition: a probe for surface states characterization*
10^{45} - 11^{10}	**Coffee break**
11^{10} - 12^{50}	*Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules* *Chair: Julius Jellinek* **Rodolphe Antoine**, University Lyon 1, France *Optical properties of silver and gold quantum clusters: playing with colors and photons* **Michael Beuve**, Université Claude Bernard Lyon 1, Lyon, France *Nanox, a multi-scale model to predict biological effects and hadrontherapy* **Elette Engels**, School of Physics, University of Wollongong, Australia *Synchrotron microbeam radiation therapy: enhancement with high-Z nano-structured ceramic particles* **Vadim Ivanov**, Peter the Great St. Petersburg Polytechnic University, Russia *Ab initio calculations of potential and electron density distribution of C_{60}^{+}, C_{60} and C_{60}^{-}*
12^{50} - 13^{00}	**Conference photo**
13^{00} - 14^{30}	**Lunch**

14^{30} - 16^{00}	*Afternoon Session I: Electron transport in molecular systems* *Chair: Bernd Huber* **Kurt Stokbro**, QuantumWise A/S, Copenhagen, Denmark *First principles simulation of electron transport across a metal-insulator interface* **Vincenzo Guidi**, Universita di Ferrara, Italy *Gas sensing via chemoresistive effect in nanosizes semiconductors* *Conference discussion* **Jean-Patrick Connerade**, Imperial College, London, UK *From nuclear to meso systems: how small is simple and how large is complex?*
16^{30} - 18^{30}	**Conference tour**

Thursday, 06 October 2016

9^{30} - 11^{00}	*Morning session I: Propagation of particles through medium: H2020 RISE-PEARL Project* *Chair: Simon Connell* **Andrei Korol**, MBN Research Center, Frankfurt am Main, Germany *Investigation of channeling and crystalline undulators with MBN Explorer* **Hartmut Backe**, Institute of Nuclear Physics, Johannes Gutenberg University, Mainz, Germany *Channeling experiments with electrons at the Mainz Microtron MAMI* **Ulrik Uggerhøj**, Aarhus University, Aarhus, Denmark *Radiation phenomena at high energies in crystals*
11^{00} - 11^{30}	**Coffee break**
11^{30} - 13^{00}	*Morning Session II: Collision processes, fusion, fission, fragmentation* *Chair: Eric Suraud* **Franco Gianturco**, University of Innsbruck, Innsbruck, Austria *Coulomb crystals in cold traps: chemical reactors and probes for quantum dynamics* **Bernd Huber**, CEA-CIMAP, Caen, France *Energetic processing of carbon-containing nanopartciles by ion collisions* **Jorge Kohanoff**, Queen's University Belfast, UK *Excess electrons and holes in irradiated systems: from DNA to nuclear waste forms*
13^{00} - 14^{30}	**Lunch**
14^{30} - 16^{00}	*Afternoon session I: Propagation of particles through medium: H2020 RISE-PEARL Project* *Chair: Andrei Korol* **Werner Lauth and Hartmut Backe**, Institute of Nuclear Physics, Johannes Gutenberg University, Mainz, Germany *Status report of undulator experiments at the Mainz Microtron MAMI* **Laura Bandiera**, Istituto Nazionale di Fisica Nucleare (INFN), Ferrara, Italy *Bent crystals as a tool for electron beams manipulation* **Andrea Mazzolari**, Universita di Ferrara, Italy *Recent developments in manufacturing of crystalline undulators*
16^{00} - 16^{30}	**Coffee break**
16^{30} - 18^{15}	*Afternoon session II: Modelling of nano- and biomolecular systems* *Chair: Florent Calvayrac* **Enrico Bagli**, Istituto Nazionale di Fisica Nucleare (INFN), Ferrara, Italy *The DYNECHARM++ toolkit for the simulation of the particle interaction with crystals* **Ulf Saalmann**, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany *Dynamical coupling of electrons and ions in X-ray-induced dynamics*

	Masato Nakamura, Nihon University, Funabashi, Japan *Stability and fragmentation of multiply charged van der Waals clusters* **Alexey Verkhovtsev, Kaspar Haume, Pablo de Vera** (ESRs of FP7-ITN-ARGENT Project and MBN Research Center, Frankfurt am Main) *Recent updates of the RADAM (Radiation DAMage) database*
19^{00} - 22^{30}	**Conference Dinner**

Friday, 07 October 2016

9^{15} - 11^{00}	*Morning session I: Clusters and nanoparticles: structure, reactivity and catalysis* *Chair: Jean-Patrick Connerade* **Shiv N. Khanna**, Virginia Commonwealth University, Richmond, USA *Effect of support in reducing sintering, improving catalytic activity, and stabilizing magnetic order in deposited clusters* **Andrew Wheatley**, University of Cambridge, UK *Improving the photocatalytic potential of nanostructured tin oxide* **Florent Calvayrac,** Institut des Molecules et Materiaux, Universite du Maine, Le Mans, France *Structure, magnetism, thermal and optical properties of some functionalized iron oxide nanoparticles and clusters of medical and industrial interest* **Hisato Yasumatsu**, Cluster Research Laboratory, Toyota Technological Institute, Chiba, Japan *Size dependence of catalytic CO-oxidation driven by uni-sized Pt clusters directly bound to Si surface through steady-state and transient measurements*
11^{00} - 11^{30}	**Coffee break**
11^{30} - 12^{50}	*Morning session II: Irradiation driven transformations of complex molecular systems* *Chair: Jorge Kohanoff* **Katrine Aalbæk Jepsen**, University of Southern Denmark, Odense, Denmark *Recognition of DNA-UV damage by repair enzymes* **Christian Kexel**, MBN Research Center, Frankfurt am Main, Germany *Molecular simulation of interstellar ice surfaces* **Kaspar Haume,** Open University, Milton Keynes, UK *Transport of secondary electrons from gold nanoparticles through PEG coating*
12^{50} - 13^{00}	**Conference Closing**
13^{00} - 14^{30}	**Lunch and Departure**

Overview of Abstracts

Talks

Posters

Talks

Mo-I-1

Multiscale Modelling of Meso-Bio-Nano (MBN) Systems with MBN Explorer: Biomedical and Nanotechnology Applications

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MBN Explorer [1] is a multi-purpose software package designed by MBN Research Center team to study structure and dynamics of molecular systems of various degree 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, fullerenes, nanotubes, metallic nanomaterials, proteins and DNA, crystals, composite bio-nano systems and nanofractals, see [2] and references therein. 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 the description of many very different MesoBioNano (MBN) systems.

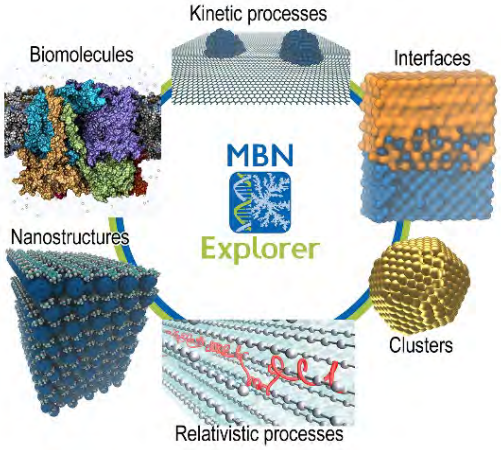

Figure 1: Illustrative examples of MesoBioNano systems structure and dynamics of which were unravelled with MBN Explorer [1].

The talk will give an overview of the main features of the package and will highlight a number of recent case studies of structure and dynamics of MBN systems carried out with the use of MBN Explorer, some of which are illustrated in Fig. 1, being in the core of the currently running FP7 HORIZON 2020 European Projects.

In particular, the multiscale approach to the molecular level assessment of radiation damage in biological targets, being elaborated with the use of MBN Explorer, was designed for the qualitative and quantitative descriptions of the effects that take place when energetic ions interact with living tissues [3]. A road towards the quantitative understanding physical aspects of ion-beam cancer therapy on the molecular level revealed that this problem has many temporal, spatial, and energy scales, while the main events leading to the cell death happen on a nanometer scale [4]. The multiscale approach [3] allows also to evaluate radio-sensitisation effects caused by metal nanoparticles and other radio-sensitising molecular species [5]. This work is especially active now within the currently running European project ITN-ARGENT [6].

European COST Action 'Chemistry for ELectron-Induced Nanofabrication' (CELINA) [7] explores the Focused Electron Beam Induced Deposition (FEBID), a very promising direct deposition technique for nanofabrication, for producing free-standing 3D structures of sub-10 nm size. To study the irradiation driven modifications of chemical transformations of complex molecular systems a new molecular dynamics (MD) approach for computer simulations has been suggested [8,9]. The approach is based on the idea that irradiation induced quantum transformations can be treated as random, fast and local processes involving small molecules or molecular fragments. In this way the quantum transformations, such as molecular bond breaks, creation and annihilation of dangling bonds, electronic charge redistributions, changes in molecular topologies, etc., could be

incorporated locally into the molecular force fields that describe the classical MD of complex molecular systems under irradiation. The irradiation driven molecular dynamics (IDMD) designed for the molecular level description of the irradiation driven chemistry has been implemented in the MBN Explorer software package [1] and successfully applied for the description of the FEBID process [9].

The HORIZON 2020 PROJECT RISE-PEARL project "Periodically Bent Crystals for Crystalline Undulators" [10], started in January 2016, aims at advancing the technologies for manufacturing of high quality Periodically Bent Crystals (PBCr). The PBCr developed in the course of this project will be utilised for the construction of novel light sources of high-energy ($h\nu \geq 100$ keV up to GeV range) monochromatic electromagnetic radiation by means of a Crystalline Undulator (CU). The experimental and technological part of this project will be accompanied by the complimentary advanced theoretical research utilising modern theoretical, computational and modelling methods and high performance computing techniques. PEARL will focus on whole complex of the important technological, experimental and theoretical problems aiming to achieve the major breakthrough in this important research area. The PEARL research programme is highly collaborative, strengthening the ongoing, international collaborative research in several EU and non-EU countries. This talk will provide an overview of achievements of the newly emerging technology for the intensive sources of monochromatic high energy radiation in which properties of the high quality periodically bent crystalline structures play an important role and to demonstrate the advanced capabilities of MBN Explorer to simulate the CU light sources, their characteristics and all the related phenomena.

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Mo-I-2

Dissipation in Clusters and Molecules

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Mean field provides an essential starting point to understand the dynamics of numerous many-body systems ranging from nuclei to molecules, clusters and nano structures. Beyond structural or low energy properties, the analysis of dynamical processes, especially beyond the linear response domain requires the account of correlations beyond mean field, especially incoherent ones. The topic has been widely explored in nuclear dynamics with major efforts devoted to the development of semi-classical approximations, leading to Boltzmann type kinetic equations [1]. Recent developments in laser technology now allow to analyse in some detail the response of clusters and molecules in short intense laser fields which typically lead to dissipative effects, beyond meand field. Semi-classical approaches have also been explored in the field [2] but are restricted to simple metals at sufficiently high excitations, which represents a strong limitation. There is thus a growing interest in the inclusion of dissipative features in current mean field theories in the case of electronic systems. The underlying mean field theory is here provided by Density Functional Theory (DFT) in its simplest Local Density Approximation (LDA), which is recognized as a robust and flexible approach for such systems, at least at moderate excitations [2,3].

We discuss in the present work some extensive studies we have led to include incoherent correlations on top of Time Dependent LDA or Time Dependent Harthree Fock (TDHF) approaches which represent archetypical approaches in the time domain. We briefly discuss available methods such as Trajectory Surface Hopping [4] and Time Dependent Current Density Functional Theory [5]. We next propose two alternative routes. We propose a quantum Relaxation Time Ansatz (RTA) providing an approximate quantum kinetic treatment [6] and a stochastic extension of mean field, know as Stochastic TDHF [7]. The RTA has allowed us to access realistic laser irradiation scenarios and study the impact of dissipation on electron emission in moderate size clusters. The STDHF approach is much richer but still at a more schematic level. We have explored it in simple molecular systems and been able to analyse its capabilities in detail [8,9].

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Mo-I-3

Solving the Problem of Anharmonic Densities of States*

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New dynamics-based methodologies for computation of classical and quantum vibrational densities of states of arbitrarily anharmonic systems will be presented and their utility illustrated through applications to atomic clusters.

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Mo-I-4

Dipole Bound Anions, Quadrupole Bound Anions, and Double Rydberg Anions

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In this talk, we will present the anion photoelectron spectra of several newly discovered dipole bound anions, quadrupole bound anions, and a double Rydberg anion, all delocalized electron systems. Two different formation mechanisms were used to form the dipole bound anions, i.e., nozzle-ion and Rydberg electron transfer. The quadrupole bound anions were made by Rydberg electron transfer, and the double Rydberg anion was made via laser vaporization. The capabilities of our new Rydberg Electron Transfer-Photoelectron Spectrometer will be illustrated and discussed.

Mo-II-1

Exploring Morphology and Chemical Synthesis in Ices and Thin Films

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The structure and chemical reactivity of atomic and molecular species in thin films and ices is important in a range of natural and technological phenomena. The morphology of molecular ices in the InterStellar Medium (ISM), where they are formed on the surface of micron sized dust grains comprised of carbon and silicon, is believed to play a crucial role in the synthesis of molecules that underpin planet formation and create the physical/chemical conditions under which prebiotic molecules form in turn influencing the development of life itself. The chemical reactivity within and on surfaces of thin films determine the creation of nanostructures either by etching and erosion of by irradiation and underpins modern plasma and nanotechnology industry. Similarly understanding the adhesion and effects of irradiation of (bio)molecular coating on nanoparticles is playing a key role in development of next generation radiotherapy (as discussed elsewhere in this meeting). Therefore, a complete study of the morphology of such ices and thin layers and how it depends on deposition conditions is necessary. Similarly studies of chemical synthesis within the ice during deposition and under irradiations (UV, electrons and ions) are vital if we are to understand and (in modern technology) control the surface chemistry.

In this talk I will review the results of current experiments exploring the morphology and chemical reactivity within ISM ice mimics and discuss how the deposition and reactivity in thin films underpins the future implementation of Focused Electron Beam Induced Deposition (FEBID) as a commercial method for construction of nanostructures. The need for detailed simulation to complement and explain these experimental studies will be highlighted. In both cases evidence will be given that reveal that often the molecules in the surface exist in clusters whose structure strongly influence the mobility of fragments produced during irradiation. The temperature of the ice/thin film will be shown to strongly influence the both the products of the local chemistry and the rate of synthesis. The morphology of the ice is will also be shown to change rapidly when different mixing ratios of nascent deposition species are selected though to date this is neither understood nor predictable from simulations. Future research directions will be discussed and methods for developing new insights into such ices and thin films reviewed.

Mo-II-2

Mechanically Driven Phase Transitions and the Formation of Tribomaterial Nanolayers

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Elevated stresses and shear rates in the buried interface between two sliding bodies drive chemical reactions and the formation of exotic phases that are not accessible by conventional thermo-chemistry. The resulting tribomaterials are essential for the function of tribological systems in academic and industrial applications. Experimental studies of tribomaterials are still restricted to an ex-situ characterisation by highly resolved TEM and spectroscopic techniques allowing only for speculations about the underlying processes. This contribution will present examples for a complementary approach that employs atomic scale models and simulations to elucidate the mechano-chemistry in sliding contacts and mechanisms that govern the formation of tribomaterials in metals [1], ceramics [2] and carbon hard coatings [3-7]. For some cases the impact of the tribomaterial on friction and wear will be discussed.

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Mo-II-3

Evidence for Non-Statistical Behavior in the Collision-Induced Fragmentation of Water Clusters

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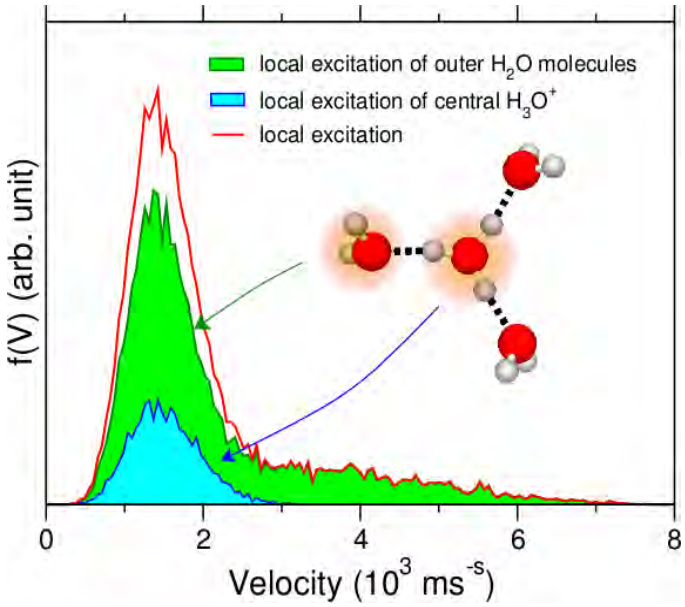
The fragmentation of mass-selected, protonated water clusters containing between 1 and 10 molecules and induced by the collision of a fast impinging argon atom has been studied both experimentally and by means of computer simulations. A coincidence time-of-flight technique combined with velocity map imaging provides unambiguous event-by-event characterization of fragment velocities in which the total number of fragments can be counted. The experimental velocity distributions feature a dominant peak that corresponds to statistical evaporation in a conventional thermal decay mechanism. However, another distinct feature is also observed at higher velocities, with a marked dependence on cluster size.

In order to interpret the measurements, molecular modeling of the dissociation process has been carried out assuming either complete statistical redistribution of the excitation energy, or a more local excitation on individual molecules, or even on specific vibrational modes. In this purpose molecular dynamics simulations employing different force fields have been used along protocols as similar as possible to the experimental situation. The calculated velocity distributions of the evaporated molecules indeed show significantly different features depending on the statistical nature of the dissociation, non-ergodic dissociations having a specific signature when the excitation is local. By varying the temperature but keeping the internal energy of the excited system as fixed, the relative importance of non-statistical effects can also be affected, which further highlights the key role of thermalization (or lack thereof) and finite size on the nanoscale dynamics of protonated water clusters.



Mo-II-4

Radiation Damage on the Molecular Level: From Free Oligonucleotides to DNA Origami

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Over the last decade, radiation damage to DNA model systems, ranging from gas-phase DNA building blocks [1] and their clusters [2] over gas-phase oligonucleotides [3] to plasmid DNA in solution [4] or deposited on surfaces [5] has been studied with great interest. It has for instance been demonstrated that deoxyribose is much more sensitive to ionization than nucleobases for gas phase single molecules as well as for entire oligonucleotides [1,3]. Also the damage-increasing action of radiosensitizers has been observed on all levels of complexity [4,5]. However, despite the wealth of strong experimental and theoretical data, there still is controversy regarding the relevance of these data for the understanding of radiation damage in living systems. One of the key arguments against the relevance of gas phase systems and plasmids is their lack of complexity as compared to DNA in biological systems.

In my presentation, I will show new examples on how specific radiation induced mechanisms can be investigated in the gas phase and how more complex DNA structures in the condensed phase can be used for radiation damage studies.
i) In DNA an initial excitation, i.e. an electron-hole pair, can migrate long distances before it reaches a site where it manifests as damage. Recent theoretical studies support the concept, that DNA contains sacrificial guanine-rich sites able to trap excitations and protect sensitive DNA regions from damage, with the human telomere sequence TTAGGG being a particularly efficient trap [6]. We have studied soft X-ray photoionization and photofragmentation of gas-phase deprotonated oligonucleotides TTAGGG-CCGCCG close to the C, N and O K-edges. Besides non-dissociative electron detachment, the formation of negatively charged fragments is observed, most of which originate from scissions in the telomere GGG region. Furthermore, we find that DNA damage is generally suppressed for photoabsorption in the nucleobases.
ii) We are currently investigating DNA origami [7] as a target for condensed phase irradiation studies. DNA origami has a much more complex 3D structure than the conventionally used plasmid DNA and is arguably better suited in particular for studying direct DNA damage.

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Tu-I-1

Multiscale Approach to the Physics of Ion-Beam Cancer Therapy: From Prediction to Experiment

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A multiscale approach to the physics of radiation damage with ions (MSA) has been developed in order to relate the biological damage as a result of irradiation with ions to physical, chemical, and biological effects [1]. This relation is usually achieved by obtaining of the dependence of probability of cell-survival or other biological effects on the dose deposited in the target. In the case of ions, however, the dose is not the only physical parameter related to radiation. In order to understand and even more so to quantitatively predict the biological outcome of irradiation with ions, the scenario that leads to biodamage has to be studied analytically.

Over years, the MSA has addressed a number of effects starting with ion propagation in tissue, features of the depth-dose profile with a Bragg peak, production of secondary electrons as a result of ionization of tissue, transport and energy loss by these electrons along with other reactive species, the radial dose distribution around each ion, formation of wave fronts around the ions' paths and consequent propagation of cylindrical shock waves, etc., etc [1, 2]. On the other side, the models of radiation damage as a result of action of secondary electrons, other reactive species, or stresses due to shock waves were explored.

Recently, it has become possible to join the whole multiscale scenario in a recipe for calculating the survival probability [1]. This recipe has been tested on plasmid DNA and most recently on a number of cell lines [3]. A number of DNA lesions have been analyzed and a criterion for lethal damage has been suggested and tested. A variety of experimental results such as survival probabilities of plasmid DNA lesions, cell survival curves, enzyme repair foci, etc., have become the field of either improving the MSA or testing its predictions. More experiments are being designed.

The phenomenon-based MSA is a unique method in its inclusiveness, versatility, and integrity. While it is looking forward to becoming practical for clinical planning of ion-beam therapy, a similar approach to the analysis of radiation damage with nano-particles as sensitizers is being developed.

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Tu-I-2

Molecular Dynamics Insights into the Biological Effects of Shock Waves Induced by Ions

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The interaction of energetic ions with biological systems in the nanometer scale is a topic of great interest, not only for the fundamental study of the dynamics of these systems under irradiation itself, but also for their applications. Energetic ion beams are being used in the advanced type of radiotherapy known as ion beam cancer therapy, and the improvements of this technique might arise from a basic knowledge of the nanoscale processes governing its mechanism. The multiscale approach to ion beam cancer therapy developed over the last years [1] has revealed a possible new mechanism of DNA damage not considered before: the ion induced shock waves [2]. Shock waves might arise due to the large amounts of energy deposited by ion beams in a few nanometers around the ion's path, as a consequence of the propagation of the large number of low energy electrons ejected. This produces a heating of the water surrounding the ion's path, what prompts the hydrodynamics response of the medium in the form of a strong explosion [2].

The evolution and effects of such shock waves can be conveniently studied by means of classical molecular dynamics simulations [3, 4]. These effects include the distortion and thermo-mechanical damage of biomolecules by the high pressures developed during the shock wave (see Fig. 1), as well as the propagation of reactive chemical species by the wave front, a mechanism faster than diffusion. The present contribution reviews recent advances on the simulation of the biological effects of ion-induced shock waves, by the use of the multiscale approach [1] to set up its initial conditions and the MBN Explorer code [5] to simulate the damage of DNA.

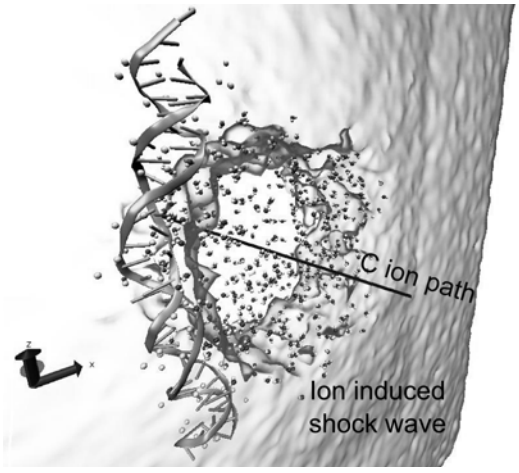

Figure 1: DNA molecule affected by a carbon ion induced shock wave in the Bragg peak region (adapted from Ref. [4]).

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Tu-I-3

Predictive Assessment of Biological Damage due to Ion Beams

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We present recent achievements in validation of the Multiscale Approach (MSA) to the physics of radiation damage with ions (see [1] and references therein). An analytical recipe for the assessment of biological damage, developed using the phenomenon-based MSA, has been applied to numerous experiments, where survival curves were obtained for different cells and irradiation conditions [2].

The phenomenon-based MSA can quantitatively predict macroscopic biological outcomes in ion-beam cancer therapy through accounting for the relevant physical and chemical effects arising on the nanometer scale due to the interaction of ions with the biological medium. Contrary to other, in essence empirical methods for evaluation of macroscopic effects of ionizing radiation, which rely on the linear-quadratic model, the MSA predicts the biodamage based on the effects related to ionization of the medium, transport of secondary particles, chemical interactions, thermo-mechanical pathways of biodamage, and heuristic biological criteria for cell survival [1].

Capability and predictive power of the MSA has been demonstrated recently by an extensive comparison with experimental data for numerous mammalian cancerous and normal cell lines, irradiated with protons and heavier ions at different values of linear energy transfer [2]. This method can be applied to evaluate survival of repair-efficient cells [2, 3], whose survival probability as a function of deposited dose is different from "normal" cells. The analysis performed for cells irradiated under aerobic and hypoxic conditions allows us to conclude that the MSA can also describe phenomena, such as oxygen enhancement ratio, which are related to different concentration of oxygen in the irradiated cells [4].

The advantages of the method allow one to extend it to many other cell lines, different cell phases, irradiation conditions (e.g., in the presence of radiosensitizers [5]) and make predictive evaluation of radiobiological effects.

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Tu-II-1

Assessing Microscopic Energy-Deposition Patterns in Ion-Beam Therapy Using Fluorescent Nuclear Track Detectors

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Single crystalline Al_2O_3:C,Mg-based fluorescent nuclear track detectors (FNTDs) show transformation of color centers when exposed to ionizing radiation. The resulting fluorescence signal is dependent on the local energy deposition. It can be read-out by confocal laser scanning microscopy yielding three-dimensional information on energy distribution with submicrometer resolution [1]. Radiotherapy with ion beams can be beneficial compared to X-rays for a number of tumor entities due to an inverse depth-dose profile and hence better dose conformality. Also, ions show an enhanced biological effectiveness as a result of their highly localized energy deposition. Our group has been investigating the use of FNTDs for ion beam therapy [2]. More specifically, we study the quantification of the energy loss spectrum of mixed ion fields as an input parameter for radiobiological models and assays.

Heterogeneity in energy deposition patterns is thereby found on two scales: firstly, for ion heavier than protons, the energy imparted – and the radiation quality - within cell nuclei can vary significantly. The major part of this variation can be assessed using FNTDs as a substrate for cell survival assays [3]. Secondly, the stochastical energy loss along particle tracks on the scale of nuclei can be measured in FNTDs with optical sections as thin as 1 µm. Studying a set of 70 detectors irradiated with monoenergetic ion beams (^{1}H, ^{4}He, ^{12}C, and ^{16}O with energy loss in alumina between 1.5 and 150 keV/µm) we found the resulting relative energy loss fluctuation to range from approx. 40% (for fast protons) to below 10% (for slow oxygen). In addition, no dependence of particle charge was observed [4].

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Tu-II-2

The Biological Mechanism of Metal Nanoparticle-Mediated Radiosensitization

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Though radiotherapy is being used to treat a substantial fraction of tumors, still a tumor targeting by radiation can be improved. Metal nanoparticles are preferentially sequestered by tumors and are capable of locally escalating the radiation dose; hence, they promise to function as new tumor-cell radiosensitizers, potentially improving the specificity and efficiency of radiotherapy at the same time (and sometimes also diagnostics; theranostics). Importantly, even though physical processes mediating the radiation dose amplification by nanoparticles have been already well described, cellular structures aimed by nanoparticles remain unknown. Currently, it looks paradoxical that while the DNA molecule in the cell nucleus is a critical target for radiation, nanoparticles were reported to be localized restrictedly in the cell cytoplasm [1,2]. The biological mechanism of cell radiosensitization by (cytoplasmic) nanoparticles and the role of the nuclear DNA damage in this process thus remain elusive.

In this work [2], we studied the effect of 3 nm-gadolinium based nanoparticles (GdBNs) on the induction and repair of DNA double-strand breaks (DSBs) in the nuclear DNA of U87 tumor cells irradiated with γ-rays. To address the question, we used currently the most sensitive method of DSB detection, based on high-resolution confocal immunofluorescence microscopy with two independent DSB markers, γH2AX and 53BP1. Equivalent data for Au and Pt nanoparticles are just being analyzed.

Under conditions where GdBNs amplify the radiation effects, they remain localized in the cytoplasm and influence DSB induction and repair only insignificantly [2]. GdBNs and potentially other nanoparticles (of defined parameters) thus seem to radiosensitize cells through a still unknown cytoplasmic event that is independent of the nuclear DNA breakage. Colocalization of GdBNs with the lysosomes but not mitochondria [1,2] then suggests the former organelles as a potential extranuclear target for the (studied and other?) nanoparticles.

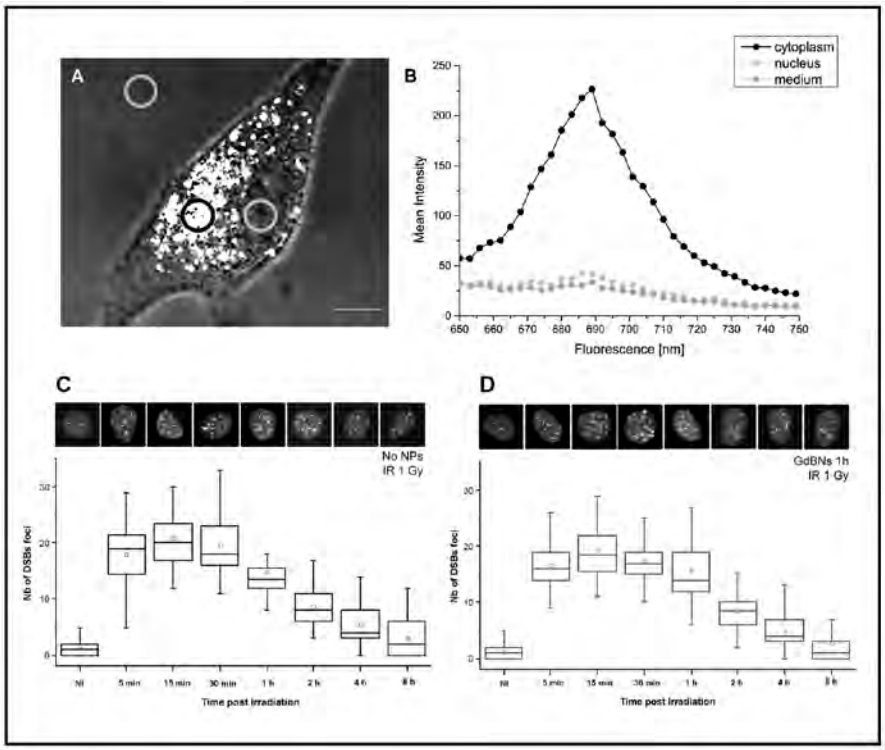

Figure 1: **A.** Localization of GdBN-Cy5.5 (white) nanoparticles (1 mM NPs for 16 h incubation) in U87 cells. A correlative fluorescence confocal image and transmission light image. The scale bar = 10 μm. **B.** Fluorescence emission spectra of the indicated regions (cytoplasm, nucleus, plain medium). **C+D.** Distribution of γH2AX/53BP1 (DSB) foci numbers per nucleus in irradiated U87 cells **(C)** never incubated with GdBNs and **(D)** incubated with 1 mM GdBNs for 1 h. The illustrative images of nuclei (composed of 40 superimposed confocal slices 0.2 μm thick) are shown for each period of time post-irradiation; γH2AX+53BP1, white; chromatin, grey; non-irradiated controls = NI. Adapted from Ref. [3]. For the image in colours see [3].

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Tu-II-3

Oligonucleotide-Modified Nanoparticles for Cancer Therapy

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In developed countries cancer is now the second most common form of death after cardiovascular disease. In Europe in 2012 approximately 3.45 million new cases were diagnosed and 1.75 million deaths were attributed to cancer [1], therefore the development of new methodologies for cancer treatment are a high priority. Approximately half of patients receive radiotherapy as part of their cancer treatment, indeed this type of therapy is second only to surgery in the treatment of cancer. However, radiotherapy is limited by the side effects it induces in the surrounding healthy tissues and/or the damage it can cause to vital organs (e.g. the kidney and brain). Several new approaches that enhance radiosensitivity within tumours have been proposed [2–6], methods that have the potential to provide a major impact on the delivery of radiotherapy to patients allowing lower doses to be applied with the same tumour mortality.

Two of the most promising approaches are hadron- and nanoparticle-enhanced therapies, which allow the tumour to be directly targeted allowing both lower doses to be applied and reducing damage to neighbouring healthy tissue and cells. Hadron therapy using protons and carbon ions is now used in several medical centres worldwide. Nanoparticle therapy (NPT), while still in formative stage (early clinical trials), is showing promising results and it is expected that, in future, a combination of hadron and NPT will be the preferred (non-surgical) treatment.

In this paper we would like to present our recent findings on the influence of the oligo-modified gold nanoparticles on the survival rate of skin cancer cells upon X-ray irradiation.

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Probing Low-Energy Electron Induced DNA Damage Using DNA Nanostructures and Metal Nanoparticles

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High-energy radiation is routinely used to treat cancer in combination with radiosensitizing therapeutics. The treatment relies on an accurate modeling of DNA radiation damage, which is to a large extent ascribed to the indirect damage by low-energy electrons [1]. To accurately quantify DNA strand breakage induced by low-energy electrons in terms of absolute cross sections for DNA strand breakage we have developed an approach using AFM analysis of target DNA arranged on DNA origami platforms [2-6]. In this way we can effectively study the dependence of DNA strand breakage on the sequence [3] and assess the effect of radiosensitizers used or proposed for cancer radiation therapy, such as 2-Fluoroadenine (^{2F}A) [6]. The incorporation of ^{2F}A into DNA results in an energy dependent and enhanced strand breakage (Figure 1).

Furthermore, we use gold nanoparticles (AuNPs) as a source of low-energy electrons in aqueous solutions. We study the decomposition of the DNA/RNA nucleobases thymine (T) and uracil (U) and the radiosensitizer 5-bromouracil (BrU) in close vicinity to AuNPs, which are irradiated with a laser matching the surface plasmon resonance of the AuNPs. The induced damage of nucleobases is analyzed by UV-Vis absorption spectroscopy and surface-enhanced Raman scattering (SERS).

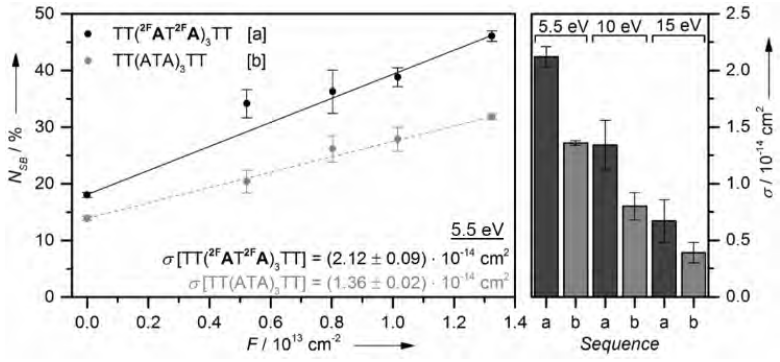

Figure 1: Left: Fluence dependence of strand breakage of two oligonucleotide sequences at 5.5 eV electron energy. Right: Comparison of the absolute strand break cross sections σ at 15 eV, 10 eV and 5.5 eV. Figure taken from Ref. [6].

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Tu-III-1

Fulfilling Feynman's Vision: Arranging the Atoms in Size-Selected Clusters and a Route to Manufacturing

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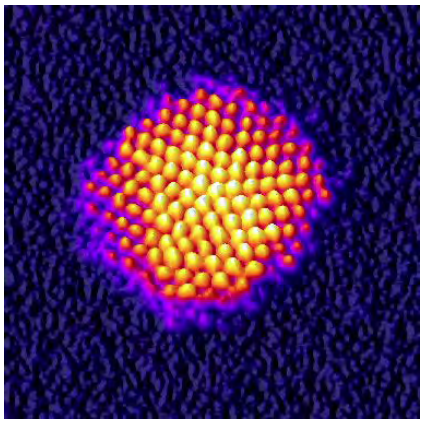
In his famous 1959 lecture "There's plenty of room at the bottom" Nobel Laureate Richard Feynman expressed a vision of making materials by arranging the atoms. Atomic clusters were one of the systems in his thoughts. In this talk I will explore how far we have come in realising the route to new functional materials based on deposition of size-selected atomic clusters with 3D structural control [1,2].

The talk will include a discussion of new efforts to scale-up dramatically the rate of cluster generation, which promise significant future impact. We can now report a cluster beam current of 10 microamps, 4-5 orders of magnitude above a conventional cluster source, with our "Matrix Assembly Cluster Source" (MACS) [3]. I will discuss various applications in catalysis (with first experimental results for cluster-powders) as well as metrology and biomedicine.



On the fundamental side one current frontier is the question of the *metastability* of the clusters themselves. New techniques like aberration-corrected scanning transmission electron microscopy (ac-STEM) are only now being applied to soft-landed, size-selected clusters [4-9]. Dynamical manipulation experiments, which probe the transformation of metastable isomers into more stable configurations, reaction-exposure experiments, which probe the response of the nanocluster structures to real catalytic conditions [10], and thermal heating experiments, which probe clusters surface melting, will be treated. Such experiments constrain computational models and are readily extendable to other sizes and cluster materials including binary systems [11]. The image shows one frame from a dynamical STEM video of an $Au_{923\pm23}$ cluster.

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Tu-III-2

The Search for Diamond Crystal Undulator Radiation

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The successful experimental realization of crystal undulator radiation requires a crystal with undulating lattice planes and of very high structural quality (no extended defects). The undulations may be realized by a superlattice that can be produced in diamond (the preferred material) using spatially periodic concentration graded doping with boron during synthesis. Few GeV positrons represent a preferred beam for the channeling in the undulating crystal channel (high symmetric direction). The critical angle for channeling is then about 80 μrad. Typical beams available are of the order of mm diameters. The constraints on the integrity of the undulator are therefore severe. One requires a uniformity of undulation amplitude and period as well as a maximum local strain in the lattice (apart from the undulations) approaching 10^{-6}, in a plane sample of several mm side and towards 1 mm thickness for the undulating part. This paper discusses the progress towards the diamond crystal undulator, as established by advanced X-ray diffraction imaging techniques. Several positron beam facilities are available for testing, and a recent test at the T9 Beamline of the Proton Synchrotron at CERN is discussed.

Tu-III-3

Giant Optical Nonlinearity of a Single Plasmonic Nanostructure

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Plasmonic nanostructures allows for light concentration into a size considerably smaller than the light wavelength. This has found practical applications in many fields, such as photodetection, photovoltaics, optical microscopy with a nanometer resolution, biosensors, optical nanolithography, etc. The nonlinear optical properties of nanostructures allow one to considerably extend their applications due to the harmonics generation by the nanostructures, two-photon excited luminescence and nonlinear four-wave mixing.

Due to a strong light absorption by metals, it is believed that plasmonic nanostructures cannot be used for generating intensive radiation harmonics in the UV spectral range. We present results of investigation of the nonlinear optical interaction of laser radiation with a single gold nanostructure in the geometry of the Split-Hole Resonator (SHR) [1-3] under the-state-of-the-art experimentally realized conditions. Several multipole plasmon resonances can simultaneously be excited in the SHR nanostructure. A strong nonlinear optical interaction at the frequencies of these resonances that leads to (i) the second-harmonic generation, (ii) the third harmonic generation (THG), and (iii) the light generation at mixed frequencies. The THG near field amplitude reaches 0.6% of the fundamental frequency field amplitude, which enables the creation of UV radiation sources with a record high intensity. The UV THG may find many important applications including biomedical ones (such as cancer therapy).

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Tu-III-4

Spontaneously Electrical Solids

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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. The field can be in excess of 10^8 V/m. This is called the 'spontelectric effect' and was first discovered in nitrous oxide laid down at low temperature [1]. This effect appears to be very widespread and requires no special procedure to create. The structure of such films is neither strongly ordered with a repeating unit, as in a crystalline material, or completely disordered as in an amorphous solid. Spontelectrics represent rather a degree of partial order due to alignment of the dipoles of the constituent molecules [1-8]. I will describe how the phenomenon may be studied using both direct measurements of surface potentials and through the vibrational Stark effect. Spontelectrics are quite distinct from ferroelectrics and represent the first fundamentally new spontaneously electrical solids discovered since the 1920s. I will describe the non-linear and non-local properties of spontelectrics using methyl formate and other species as examples, showing that spontelectrics may have counterintuitive properties such as an apparent increase in dipole order with increasing temperature of deposition. I may also touch upon astrophysical applications of solid CO on grains in space and implications for star formation.

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We-I-1

Surface Deposition of Metal Clusters and Nanowires Formed in Superfluid Helium Droplets

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Superfluid droplets of 10^4 to 10^7 helium atoms (He_N) are doped with foreign atoms or molecules that move freely in or on the droplets and may form complexes in this cold environment [1]. In our labs, large Cu; Ag, Au, and Ni aggregates of different morphology are generated in helium droplets [e.g. 2, 3] and their landing on a solid substrate has been modelled in a molecular dynamics simulation [4]. Employing different pick-up cells for doping the droplets (see Fig. 1), nanowires and core-shell clusters with one metal surrounding a core of a different species can be created.

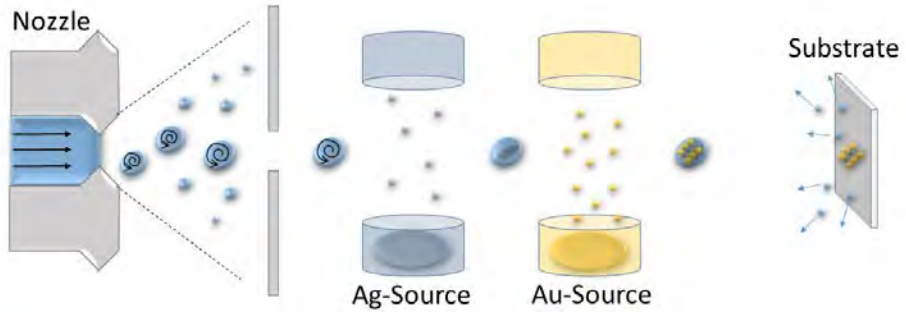

Figure 1: Sketch of the experimental set-up, see Ref. [7] for details.

After surface deposition on various types of substrates, they are removed and taken to the neighbouring electron microscopy facility [5, 6]. A vacuum transport chamber helps to avoid contamination. Analysis using a scanning transmission electron microscope with atomic resolution including tomographic reconstruction results in 3-dimensional images of the particles. Element specific methods like energy-dispersive x-ray spectroscopy (EDXS) and 2D electron energy-loss spectroscopy (EELS) identify the conditions for generating single or double core clusters [7]. As it turns out, the temperature of the substrate [6] and the doping rate [8] have an important influence on the final cluster or wire structure. Our systematic studies will help to provide recipes for the creation of tailored nanoparticles.

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We-I-2

Anomalous Spectral Dynamics in Ultrathin Subsurface Layers and Nanofilms of Amorphous Polymer

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The surface plays an important role in many physical properties of nanoobjects. In spite of extensive research, our knowledge about the surface processes and their contribution to properties of nanoobjects is very limited. One of the reasons is that most of experimental methods yield information averaged over a microscopically large volume of a sample. Furthermore, most of methods have access to the surface only, while surface properties are determined by processes in subsurface layer as well.

We developed a method that allows to investigate local dynamics in ultrathin subsurface layers of solids on nanolevel. It is based on introducing single fluorescent molecules (SMs) in the desired place of the sample and the detection of individual phonon-less optical spectra of these molecules. The aim of our research was to obtain information about local dynamics in ultrathin nanofilms and subsurface layers of amorphous polymers. One of the purposes was to determine experimentally the thickness of a subsurface layer where local parameters differ from those in the bulk volume. For our studies we chose polyisobutylene with high molecular weight $M = 4.2 \times 10^6$ g/mol, the internal dynamics of which is well described by the standard tunneling model of low-temperature glasses. Zero-phonon spectral lines of SMs and their temporal evolution (spectral histories) provided us valuable information about low-temperature dynamics of polymer in nearby vicinity of the probe molecule. We developed an experimental procedure that allows to deposit fluorescent probe molecules or directly upon the surface or into the near-surface layer of polymer on controllable depth in ~ 0.5 nm steps. The measurements were performed at T = 4.5 K.

One of the key results was that no zero-phonon lines were observed closer than 0.5 nm to the polymer surface. Only broad-band fluorescence emission was detected in this case. It was found that in polymer films thinner than 50-100 nm and in subsurface layers in depths shallower than 20 nm the spectral dynamics deviates from those deep in the bulk. Less than 5 nm deep, the zero-phonon line widths increase rapidly, whereas the number of detected molecules decreases. The spectral histories of SMs introduced in ultrathin films and subsurface layers of polymer also demonstrate more random behavior than histories of SMs doped in bulky material. Additionally to reproducible jumps of zero-phonon line frequencies, caused by flipping two-level systems, irreproducible jumps and drifts of zero-phonon line frequencies were observed.

The obtained results clearly demonstrate the existence near the surface of polymer sample ultrathin layer with faster and richer than in the case of bulky material dynamics. Possible physical reasons of the observed phenomena are discussed.

We-I-3

Preformed Clusters Deposition: A Probe for Surface States Characterization

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One of the main targets of nanophysics is the development of controlled, reproducible and industrially transposable, nanostructured materials. The precondition to any technological improvement supposes the comprehension of the basic mechanisms controlling the nano-architectures, which are definitely linked to the interaction between the elementary building block and the substrate. An interesting step in the elaboration process consists of using preformed nanoparticles as elementary building blocks instead of atoms or molecules. In this case, the nanostructures obtained by preformed clusters deposition on surface have shown that the morphology of islands grown on surfaces from soft-landed preformed clusters depends on the nature and temperature of the substrate, on the nature, size and flux of the clusters. Depending on these parameters, compact shapes or dendritic ones are obtained for instance (see for example [1-3]). The control of the morphology of the final island is possible, giving access to morphology filters. It is also possible to control nanostructures organization by calibrating surface defects leading to nucleation guides.

It emerges also, as the mobility of deposited clusters is highly influenced by the surface electronic and topological properties, then nanostructures obtained can also be seen as characteristic signature of local surface structure. Using the clusters as local probes for surface characterisation is one of the main raised questions here. For instance, the diffusion and/or nucleation of clusters on polycrystalline surfaces are influenced by the orientation of the crystal grains and the existence of grain boundary, and then imaging the obtained nanostructures would give us a map of crystal information. Determination of the position of defects and their nature can be reached through its influence on clusters mobility and nucleation. Mechanical field can also impact clusters mobility and then can be revealed through obtained nanostructures imaging. This makes possible the analysis of surfaces, like graphene for instance, at intermediate ranges between atomic and macroscopic scale. It would also enhance the signature of phenomenon at characteristic length comparable to the probe size, and restrict the analysis only to the surface itself, with no impact of probe penetration length like in other kind of surface analysis, electron diffraction or spectroscopy namely. This alternative use of clusters deposition as probe for surface states characterization appears as an attractive and remarkable tool.

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We-II-1

Optical Properties of Silver and Gold Quantum Clusters: Playing with Colors and Photons

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Atomic clusters of metals are an emerging class of extremely interesting materials occupying the intermediate size regime between atoms and nanoparticles. Nonlinear optical (NLO) characteristics of atomically precise clusters of gold and silver revealed remarkable features. The two-photon absorption cross section of protected noble metal nanoclusters is several orders of magnitude larger than that of commercially-available dyes. However, the fundamental photophysical mechanisms underlying those two-photon processes in ligand protected clusters with few metal atoms are not fully understood yet.

Theoretical models to explain the experimental observations will be introduced and the possibility to deduce the key ingredients to propose new classes of nanoclusters with large NLO efficiency will be discussed. Additional case studies, from small liganded clusters to large particles will be presented to emphasize their NLO properties making them promising candidates for various imaging techniques such as fluorescence microscopy or Second-Harmonic Generation microscopy.

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We-II-2

Nanox, a Multi-Scale Model to Predict Biological Effects and Hadrontherapy

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The number of facilities that offer tumor treatment with particle therapy has been increasing substantially over the past decades. Ions are known for their enhanced effectiveness in killing tumor cells when compared with protontherapy. Such a characteristic is quantified through the RBE (relative biological effectiveness), which is a complex function of multiple parameters like cell line, cell cycle stage, radiation quality and irradiation conditions. Therefore, determining the value of RBE for every scenario is a challenging task that requires modeling to comply with the demands of a clinical environment.

We developed a new model: nanox^{TM} (NAdosimetry and Oxidative stress). The nanox^{TM} model takes as input dosimetry quantities at multi-scale, starting from nanoscale, but also the production of radicals induced by water radiolysis. The cell survival predicted by Nanox^{TM} for V79 cell line was compared to experimental results for photons, protons and carbon ions, and even others like argon ions. A good agreement was found in all cases. In particular, the model is able to describe the effectiveness of ions, including the overkill effect at higher LET values. Moreover, Nanox^{TM} can reproduce the typical shoulder in cell survival curves. This was possible due to the introduction of the “non-local” events, through the chemical dose, which varies with LET. It is worthwhile to note that such results were obtained through the adjustment of a reduced number of free parameters.

Synchrotron Microbeam Radiation Therapy: Enhancement with High-Z Nano-structured Ceramic Particles

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Microbeam radiation therapy (MRT) implements a high-dose, spatially-fractionated kilovoltage x-ray treatment regime for deep-seated tumour targeting [1] while sparing normal tissue [2]. With the high-dose requirement for effective radioresistant tumour treatment [3], MRT can improve the prognosis, but the treatment is not completely optimized due to the large dose gradient from the peak (in-beam) to the valley (between successive microbeams). High-Z nanoparticles (NPs) enhance the dose delivered by radiotherapeutic treatments, in particular for kilovoltage X-rays [3]. Novel ceramic NPs have oxygen activation sites that allow better targeting of desirable properties such as cell-specificity, radioprotection, drug attachment, and toxicity [4]. This research investigates synchrotron MRT treatment enhancement with nano-structured ceramic particles, in particular a non-toxic Ta_2O_5 NP [4], through simultaneous experimental and simulation studies.

Geant4 [5,6] simulations investigated the physical dose enhancement due to Ta_2O_5 NPs in a local population of cells (Figure 1) exposed to monoenergetic microbeams (30-200 keV), based on two Ta_2O_5 NP configurations observed *in vitro* (Fig. 1 insets). The NP geometry was chosen to reflect the microscopic observations of Ta_2O_5 NPs in tumorous 9L and normal healthy MDCK cells.

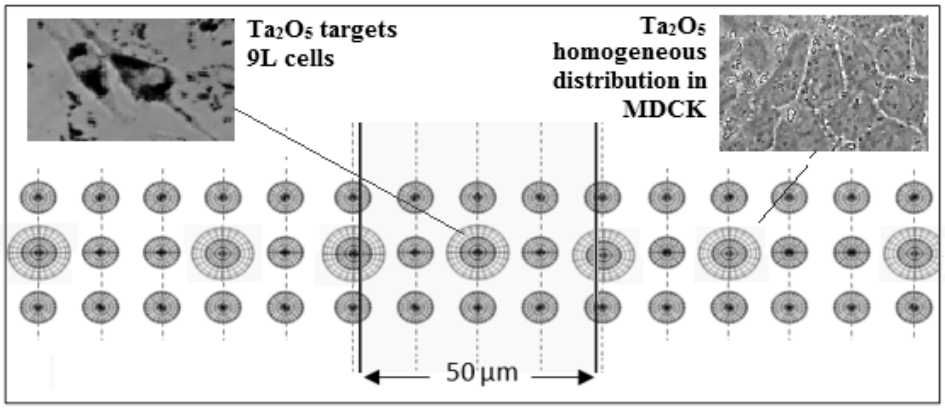

Figure 1: Cell population set-up with Ta2O5 NPs modelled as a 3 µm shell around the cells or as a homogeneous NP distribution, noted from experimental observation of 9L and MDCK cell lines respectively.

Experimental measurements with Ta_2O_5 NPs were made at the Imaging and Medical Beamline (IMBL), located at the Australian Synchrotron. Radioresistant tumorous 9L gliosarcoma and

healthy Madin Darby Canine Kidney (MDCK) cells were exposed to 0.4 Gy in the valley between microbeams due to 50µm wide 400µm spaced X-ray microbeams, with mean energy of 44 keV, and produced by a 1.4 T wiggler field. Ta_2O_5 NPs were added to cells in T12.5cm^2 flasks 24 hours before 90-100% confluence. Cells were irradiated in T12.5cm^2 flasks, while embedded in a 20 cm x 20 cm x 12 cm solid water phantom (RMI-457) with the cells at 2.5 cm depth. Clonogenic assays were used to interpret cell survival.

The experimental results indicate that Ta_2O_5 NPs increase the efficiency of MRT for 9L gliosarcoma only, compared to MDCK, as shown in Figure 2(A). While the 9L cell is generally more radioresistant than MDCK, the effect of the NP improves the treatment and selectivity of MRT toward tumour cells. The congregation of the Ta_2O_5 NPs around the 9L cell nuclei is likely responsible for the physical dose enhancement more localized within the 9L cells.

Figure 2(B) shows the dose enhancement produced by Ta_2O_5 NPs congregating around cell nuclei in a low energy microbeam (50 keV), as shown in Figure 1. The simulation study indicates a greater coverage of physical dose enhancement from the microbeam peak and into the valley region with the NPs. The frequent NP "shells" in and out of the microbeam produce localized increases in the physical dose and high LET secondary electrons in the low kilovoltage photon field. In the valley, significant dose enhancement ratios of 35 times that of water (without NPs) were observed, indicating better tumour dose coverage is possible. These results may indicate why the response of 9L gliosarcoma with NPs is elevated with respect to the homogeneous NP distribution of MDCK, providing further evidence that targeted ceramic NPs can optimize tumour control in MRT.

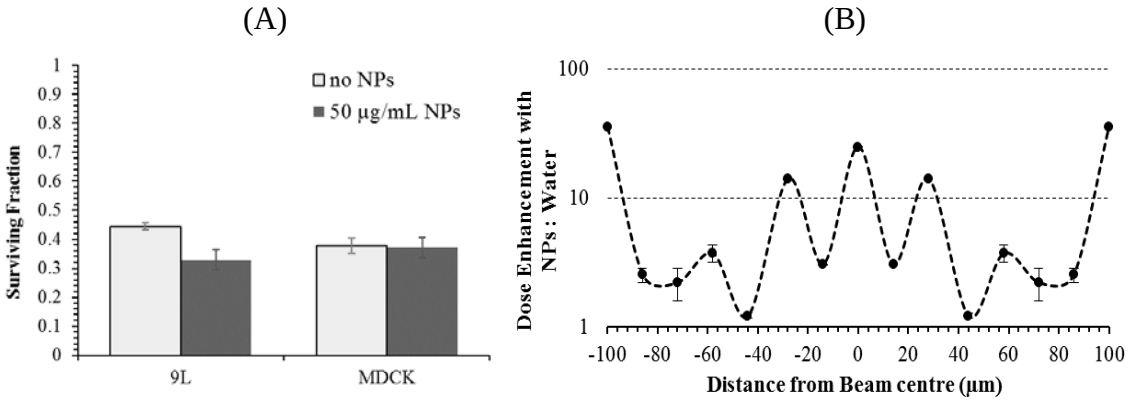

Figure 2: Surviving fraction produced with and without 50 µg/mL of Ta_2O_5 NPs in 9L and MDCK (A), and the Geant4 study results of physical dose enhancement produced by the NPs modelled, in Fig. 1, after the configuration observed in 9L (B).

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We-II-3

Ab initio Calculations of Potential and Electron Density Distribution of C_{60}^+, C_{60} and C_{60}^-

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In this work, we present the model pseudopotentials of the neutral fullerene C_{60} and its ions C_{60}^+ and C_{60}^- for applications in molecular dynamics simulations. The proposed model uses the electronic charge densities determined from ab-initio calculations.

This study is of interest because of the application point of view, because these novel materials are the most promising in the field of artificial photosynthesis, non-linear optics and the preparation of photoactive films and nanostructures. All the ab-initio computations are performed with the FireFly quantum-chemistry package [1]. The initial optimization of the neutral and ionic C_{60} structure was realized through the semi-empirical PM3 approach [2]. The resulting geometry is used as a zero-order approximation in final optimizations at the different levels of theory. To see the role of many-electron correlations we start from the calculations within the Restricted Open-shell Hartree-Fock (ROHF). Then two DFT-based treatments have been chosen. The first choice is the combination of the Slater exchange and the Vosko-Wilk-Nusair correlation functional (SVWN) [3], which is a typical DFT-based approach within the Local Density Approximation (LDA). The second choice is the hybrid Becke-Lee-Yang-Parr three-parameter (B3LYP) density functional treatment [4], including the HF-type exchange and exchange-correlation functionals formulated within the Generalized Gradient Approximation (GGA). In current calculation, we use the B3LYP-D3 approach [5] which takes into account the attractive dispersion corrections to the DFT treatment.

Electronic densities are calculated using the structures optimized at the different levels of theory. By averaging the resulting electrostatic potential over the spherical angles, the radial dependence of the effective pseudopotential is determined for neutral C_{60} and its ions C_{60}^+ and C_{60}^-. The influence of the electronic correlation, included via the B3LYP-D3 approach on the optimized cluster structures and the resulting pseudopotential, is manifested in the slight increase of the average fullerene radius (about 0.05 a.u. for C_{60}^- and 0.15 a.u. for C_{60}^+) in comparison with the ROHF results. The pseudopotential depth changes also with the inclusion of the correlations: the depth becomes smaller for C_{60}^- and increases in C_{60} and C_{60}^+. Although these changes are rather small in comparison with total potential depths, it leads to significant rearrangement of single-electron spectrum. Calculations show also that there is no essential difference between results obtained within B3LYP/6-31G(d) and B3LYP-D3/6-31G(d) treatments. Since the sharp shape of potential leads to very high sensitivity of the electronic level position, even this small discrepancy should be treated carefully.

The effective pseudopotentials for neutral C_{60} and ionic C_{60}^+ and C_{60}^-, calculated with B3LYP-D3 approach are compared in Figure 1. The C_{60}^- pseudopotential clearly manifests two different types

of interaction between a fullerene anion and an external electron: The strong attraction close to a radius of fullerene's anion and the weak repulsion outside and inside of fullerene cage. The trade-off between repulsion and attraction gives rise to the formation of weak barriers for any negative projectile particle and can lead to an increase of probability for the projectile to "getting stuck" on the fullerene cage. The numerical analysis shows that the pseudopotential behavior fits well with the 1/R law at the radial distance about 10.3 a.u. For the neutral fullerene and positive ion, the pseudopotential has the attractive character at all distances. The position of potential minimum is slightly increasing from C_{60}^{+} to C_{60}^{-} while the depth is becoming smaller as expected. Coulombic behavior of pseudopotential for positively charged fullerene starts from distance about 9.5 a.u.

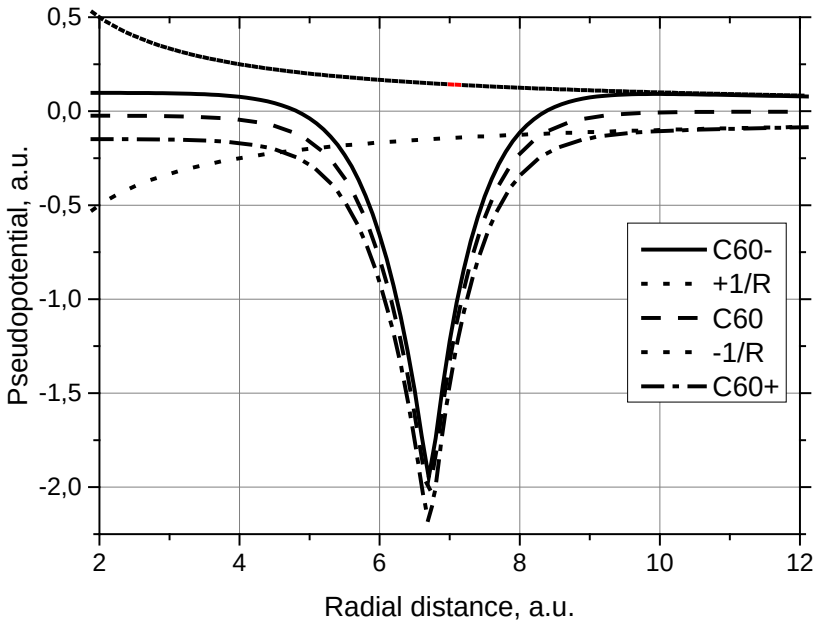

Figure 1: Pseudopotentials of C_{60}^{-}, C_{60} and C_{60}^{-}, obtained from ab-initio calculations within the B3LYP-D3/6-31G(d). Coulomb potentials are shown for comparison with asymptotic behavior of pseudopotentials.

Finally, the resulting effective pseudopotential is fitted to a simple analytical form which can be applied in further classical and quantum molecular dynamics of fullerene-based compounds.

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We-III-1

First Principles Simulation of Electron Transport Across a Metal-Insulator Interface

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The physics at metal-semiconductor contacts are important for a large number of applications. Historically, their microscopic understanding has been hampered by the inability of traditional analytical and numerical methods to fully capture the complex physics governing their operating principles. Atomistic electronic structure calculations have traditionally used the slab approximation, however, as will be shown in this presentation, the slab approximation provides a poor model of the interface. Here we introduce an atomistic approach based on density functional theory and non-equilibrium Green's function, which includes all the relevant ingredients required to model realistic metal-semiconductor interfaces and allows for a direct comparison between theory and experiments via I-V bias curves simulations. We apply this method to characterize an Ag/Si [1] and a gold-pentacene [2] interface both relevant for photovoltaic applications. Among other things we study the rectifying-to-Ohmic transition as function of the semiconductor doping.

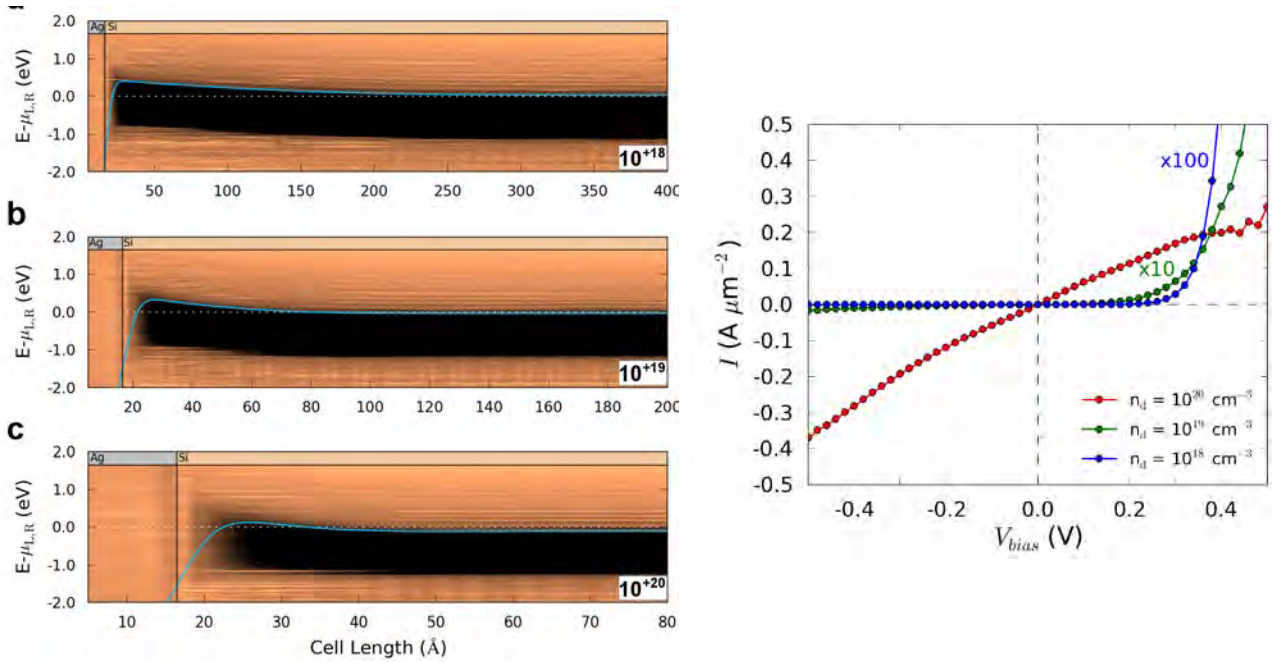

Figure 1: (Left) First principles simulation of the Schottky barrier at an Ag-Si interface as function of the doping of the Silion. From top: doping level 10^{18} cm^{-3}, 10^{19} cm^{-3} and 10^{20} cm^{-3}. (Right) I-V characteristics of the 3 systems. From Ref. [1].

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We-III-2

Gas Sensing via Chemoresistive Effect in Nanosizes Semiconductors

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The great challenge of low-dimensional nanostructured materials lies in the control of their properties by the morphology and the grain size, which combines bulk and surface effects [1, 2]. One-dimensional (1D) nanostructures are ideal for investigating the dependence of electrical transport, mechanical and optical properties on size and dimensionality [3], i.e., lower turn-on voltage for field emitters, higher efficiency for solar cells, better electrochemical performance for lithium-ion batteries and enhancement of thermoelectric figure of merit. Two-dimensional (2D) nanostructures, i.e., nanosheets, nanoplates, and nanowalls, are suggested to be ideal components for nanoscale devices used in data storage, nanoswitches and biological sensors, due to their nanometre-scale thickness, high surface-to-volume ratio, and fascinating photocatalytic and optical activities [4]. In the last years, the variable features of colloidal nanocrystals, such as their size-dependent electronic, optical, magnetic, mechanical and chemical properties, which cannot be obtained in their bulk counterparts, have attracted the attention of researchers [5]. In particular, within colloidal semiconductors, metal chalcogenide nanocrystals have been extensively investigated due to their size-dependent photoemission characteristics and quantum confinement effects [6]. Among these nanocrystals, metal oxides have gained a significant role in technology development due to their exceptional skills, which allow exploring new application fields, such as optical, electronic, optoelectronic and biological domains. In particular, the application in which metal oxides have been widely used is chemoresistive gas sensing. The performance of sensors based on metal oxides depends crucially on their dimensions, morphology (Figure 1), composition and surface activity. Among the several parameters that influence the sensing properties of a metal oxide, the potential barrier at the interface between grains is a major physical quantity [7]. Indeed, in this sense, the broad assortment of one-, two- and three-dimensional metal-oxides nanostructures has been a precious source for gas sensors technology, which owes its constant development to the requirements of physical, chemical and biological detection systems [8, 9].

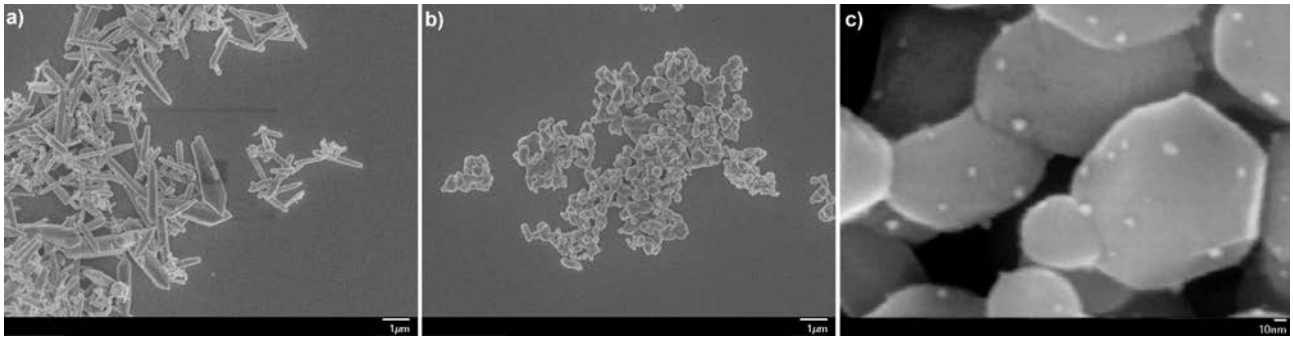

Figure 1: SEM images of a) nanorods, b) nanoparticles, and c) gold nanoclusters decorated ZnO powders.

However, there are different types of nanostructured materials that may be very good candidates to be further investigated in the chemoresistive gas sensing field, i. e., metal sulfides. Indeed, by using

these materials (Cds, SnS_2 in Figure 2), we expect an improvement from an energy consumption point of view, both in thermal and photo-activation modes, due to their lower band-gap than for metal-oxide semiconductors. This means that the activation of intrinsic surface reactions occurs at lower working temperatures, and then minor power supply is necessary. Due to this advantage, we were motivated in the search for potential improved performance in terms of selectivity and stability. The absence of oxygen in the crystal lattice of metal sulfides leads to a different catalytic mechanism on the surface reaction with respect to metal oxides. In addition, this absence may solve the constant drift of the signal suffered by metal oxides and ascribed to the in/out diffusion of oxygen vacancies, which alters the doping level [10, 11].

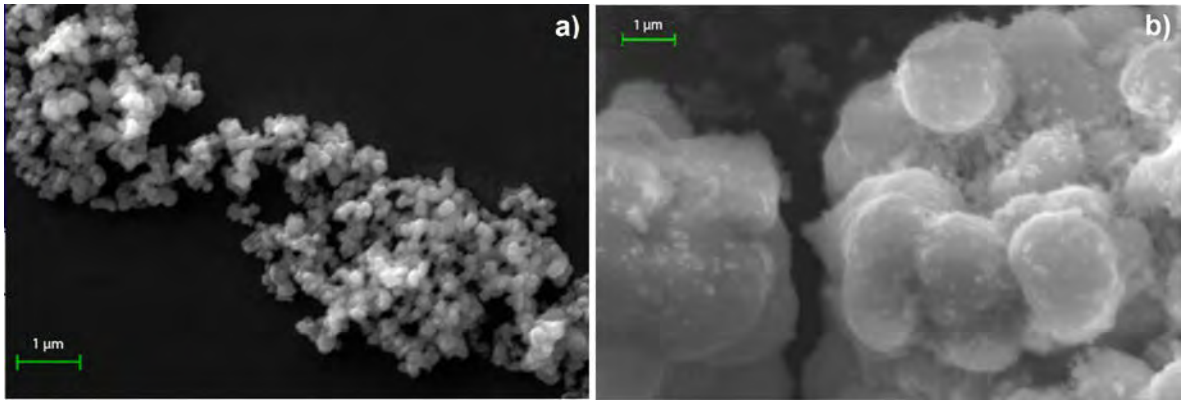

Figure 2: SEM images of a) CdS, and b) SnS_2 nanopowders.

Recently, organic-inorganic hybrid nanocomposites have quickly gained a prominent position in the gas sensing field. For example, due to its excellent electrical, mechanical and thermal properties chemically modified graphene has been extensively studied as sensing film. So far, the research focused on graphene and graphene-based materials has led to an extensive assortment of highly performing devices, including Functionalized Graphene Oxide (FGO) and its reduced counterpart (rFGO). Modified graphene oxide (GO) has shown good sensing performance, which are critically important to design a commercially viable gas sensing system. In this advent, several approaches are employed to improve the interactions between FGO layer and the gaseous molecules.

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We-III-3

From Nuclear to Meso Systems: How Small is Simple and How Large is Complex?

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Ever since quantum mechanics (QM) was 'invented' (I use this phrase because 'discovery' is connected with certainty, and certain aspects of QM do remain obscure) the question has arisen of some kind of frontier separating 'small' systems, to which QM must be applied, from large ones, for which classical physics is a more natural and simpler choice. Indeed, in some presentations of QM, most notably that of Landau and Lifshitz, classical physics is regarded as essential to underpin QM, and the Correspondence Principle, which moves across this frontier, becomes the basic tool to identify QM operators.

From the start, the question arose: are there also other boundaries where qualitative changes occur? Schrödinger himself asked the question: what is life? and put it in a context of size. One may think of a virus, which can be the smallest living system, and an inorganic cluster, which can be of similar size, so the issue is more involved than merely a question of scale. It has become customary in such cases to look towards complexity as holding a possible key.

Another point is a dynamical one, and relates to the manner in which the system is probed. In Nuclear scattering, for example (the nucleus being a 'small' system in this context) one would like to use the observed scattering spectrum to deduce the potential from which a particle was scattered and hence probe the structure. However, a limitation is set by the de Broglie wavelength of the scattered particle. If the scale size of the (short range) scattering potential is of the order or smaller than the de Broglie wavelength of this scattered particle, then nothing can be deduced about the structure of the potential, because any short range potential, by adjusting its strength, will give a low energy scattering spectrum equivalent to any other. Thus, for 'small' systems, the inverse scattering problem can be solved, but for 'large' ones, it cannot. Here the words 'small' and 'large' mean something different, since we are always in the context of Nuclear physics.

In a completely different context (optics) we can replace the scattered particle by light and the scatterer by an obstacle placed in the beam. The transition then becomes the boundary between geometrical and physical optics, where the critical size is now related to the wavelength of the photons.

The issue of complexity is somehow tied in with the transition from quantum to classical, according to an issue first raised in a famous question by Einstein to Bohr: how can one quantise orbits which, in classical physics, never close (chaotic orbits)? This issue arises in Atomic Physics: the question becomes: as n, the principal quantum number of an atomic system is increased, i.e. one tends towards towards large sizes, does one recover all of classical physics or only a part? This question is not really answered today. That is why, in atomic physics, much effort (experimental as well as theoretical) has been devoted to studying the transition from simple to complex orbits for classically non-integrable systems. This is yet another transition.

The transition from nano to meso systems in cluster physics seems to raise similar issues of size. Is there a physical criterion to decide at what point complexity becomes of over-riding importance? Are we dealing with a real boundary, or only with our relative inability to calculate? Is there just one kind of complexity or are there many, and what kind of complexity is then at issue in real cases? Does the transition from nano to meso provide us with yet another boundary to be considered in going from the quantum to the classical limits? Does each situation define its own boundaries?

Comparing some of the other cases listed above, which rest on rather simple physical criteria to define the different ranges, the situation in nano- and meso- physics seems rather less definite. The purpose of the present contribution is not to present results but rather to stimulate discussion around the issue and, perhaps, lead to new thoughts around the questions raised.

Th-I-1

Investigation of Channeling and Crystalline Undulators with MBN Explorer

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The main phenomenon addressed is the motion of particles and 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 855 MeV and 10 GeV electrons and positrons channeling along Si(110) and diamond (110) planes bent with various amplitudes and bending periods.

(2) Small-amplitude short-period regime [5] is characterized by the opposite limits: $a << d$ and $\lambda_u << \lambda_{ch}$. 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=0.1-0.9 Å, λ_u = 200-600 nm and obtained for 855 MeV [6] and 20-35 GeV [7] projectiles channeling along Si(110) and diamond (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 and with 20-35 GeV projectiles at the SLAC facility (USA).

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Th-I-2

Channeling Experiments with Electrons at the Mainz Microtron MAMI

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A very important prerequisite for experimental studies of undulator-like radiation in periodically bent crystals is the knowledge of the dechanneling length. Because of the fact that even for electrons channeling in undistorted plane crystals only little is known experimentally, dechanneling length measurements have been performed at the Mainz Microtron MAMI at various beam energies between 195 and 855 MeV [1]. The low emittance electron beam of MAMI is well suited to prepare a beam with small angular divergence which is mandatory for conclusive experiments of this type. As an example, at a beam energy of 600 MeV the vertical emittance amounts to 0.5 π nm rad. At a typical beam spot size of 180 µm in our experiments, the beam divergence results in only 2.8 µrad (1 σ) which is small in comparison with the critical angle of 270 µrad for the (110) plane of silicon.

Measurements have been performed for electrons channeling in the relevant (110) crystallographic plane of silicon single crystals as function of the crystal thickness with the intensity of channeling radiation or bremsstrahlung as signals [1]. Alternatively, the angular distribution of electrons initially trapped in the (111) plane of a bent silicon single crystal contains also information on the dechanneling length [2]. Measurements with the latter method at beam energies in the multi-GeV range exhibit a surprising small dechanneling length [3].

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 which enhance the dechanneling length. However, a model-independent measurement of the dechanneling length is not a simple task. Various model assumptions in the analysis procedure, the role of rechanneling, the crystal thickness, statistical errors, and various definitions of the dechanneling length will be scrutinized in order to enable eventually a comparison of experimental results with three-dimensional simulation calculations on the basis of, e.g., the MBN Explorer package [4, 5].

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Th-I-3

Radiation Phenomena at High Energies in Crystals

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Utilizing the relativistic invariance of the parameter $\chi=\gamma E/E_0$, ultrarelativistic particles in strong crystalline fields E of the order 10^{11} V/cm enable investigations of processes in fields of the order the QED critical field $E_0=m^2c^3/e\hbar=1.32\cdot10^{16}$ V/cm ($B_0=4.41\cdot10^9$ T) in the particle rest frame. In the framework of the CERN NA63 experiment we have obtained experimental results on e.g. quantum synchrotron radiation emission, trident production and coherent pairs in such fields, as well as observing effects related to the mesoscopic photon formation zone. Apart from their relevance to astrophysical emission processes as e.g. taking place at neutron stars, and relevance to the fields encountered in heavy ion collisions, these studies are important for the design of the interaction point of future high energy colliders. Secondly, many of the processes studied are relevant in the context of intense laser fields, as e.g. aimed to be investigated at the Extreme Light Infrastructure (ELI). Processes in specially manufactured crystals with single or multiple bends have also been studied using high energy particles, lately also at SLAC.

Th-II-1

Coulomb Crystals in Cold Traps: Chemical Reactors and Probes for Quantum Dynamics

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Ion traps are the core technology utilized to con_ne charged particles over a long period of time, allowing further application of different cooling techniques [1,2] and the manipulation of single molecules on the quantum level. The well-established technique of buffer-gas cooling is the only method so far that has led to the production of translationally as well as internally cold molecular ions to the few-kelvin range.

Experiments attempting to reach these temperatures by buffer gas cooling have found that although the molecular motion and rotation are quickly cooled to the cryogenic temperature, in some cases the molecular vibration relaxes at impractically long timescales.

For this kind of problems theory can provide important information to overcome some of the experimental limitations and to explain the behavior of specific systems. Modeling the molecular de-excitation under physical conditions of ion traps by accurate quantum calculations has helped to identify a specific class of systems that exhibit efficient ro-vibrational cooling [3,4]. At present, cold molecular ions are at the center international research because its applications go beyond the study of chemical reactions; they are also important in fundamental precision measurements [5] and quantum information processing [6].

In this talk I shall endeavour to show that highly sophisticated experimental results in cold ion traps under the above conditions can be explained and modelled very accurately by combining high-level structural calculations of the interaction forces and quantum dynamical methods to describe the collisional energy exchanges [7,8].

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Th-II-2

Energetic Processing of Carbon-Containing Nanoparticles by Slow Ion Collisions

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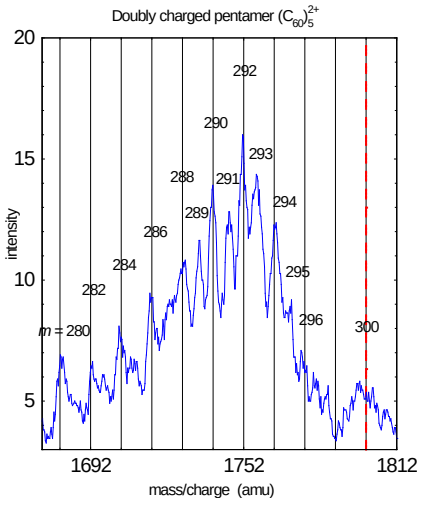
Fullerenes and polycyclic aromatic hydrocarbon (PAH) molecules and clusters have been shown to be frequently present in space. Their energetic processing in environments like supernova shocks, interstellar winds or in the atmospheres of planetary systems by collisions with photons, electrons and ions plays an important role in their destruction by fragmentation processes. Thus larger dust or grain particles can be reduced in size and form smaller particles like PAHs (top-down mechanism). On the other hand, these interactions for examples with PAH molecules or clusters may also produce reactive species which can aggregate and thus may contribute to the formation of small grain particles (bottom-up approach).

In this work we present results on ion-induced fragmentation and on bond-forming reactions inside of pure clusters consisting of coronene molecules ($C_{24}H_{12}$) or fullerene molecules(C_{60}) as well as in mixed clusters containing both species. In each case collisions with 22.5 keV He^{2+} and 3 keV Ar^{+} ions have been performed. For the first projectile the interaction is dominated by electronic excitation processes whereas in the second case nuclear collisions are predominant. This leads to very different final ion distributions.



Mass spectrum of the doubly charged pentamer; the number of C-atoms m=300 corresponds to the van der Waals cluster $(C_{60})_5^{2+}$

In the case of collisions with $(C_{60})_n$ clusters, the He^{2+} projectile leads mainly to ionized van der Waals clusters with the exception of the covalently bound species C_{119}^{+} [1]. On the contrary, collisions with Ar^{+} projectiles result dominantly in the production of covalently bound cluster ions, which are characterized for doubly and triply charged clusters by much lower appearance sizes. As shown in the Figure for the doubly charged pentamer, these systems have lost several C-atoms due to knockout processes. The number of lost atoms is found to be much lower than previously reported in experiments using fs-laser irradiation.

Similar results are obtained in mixed clusters where covalently bound systems $(C_{60})_mCor_n^{+}$ are formed. These studies show that nuclear collisions allow to produce efficiently reactive species inside van der Waals clusters by local relatively low energy deposition occurring at short time scales (fs) well below the dissociation time of the excited cluster (~10^{-12} s).

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Th-II-3

Excess Electrons and Holes in Irradiated Systems: From DNA to Nuclear Waste Forms

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The initial stage of the irradiation process, both via energetic particles or electromagnetic radiation, consists of ionizing the material generating secondary electrons and holes. These species diffuse through the sample experiencing inelastic collisions with the medium until they find an opportunity to react, producing chemical modifications that can lead to various types of damage. In the case of biological matter, damage to the genetic component (DNA) may cause the arrest of the cell cycle. It is linked to diseases like cancer and constitutes the basis for radiotherapies. But materials are subject to ionizing radiation in many other areas, such as radiation detectors, electronic devices in spacecrafts and satellites, structural components in nuclear power plants, and nuclear waste forms encapsulating disposed radioactive fuel and contaminated components. While the type of damage and its consequences depend on the specific material and application, the underlying physics is quite similar, and it is related to the fate of secondary electrons and holes.

We have studied the problem of electron and hole localization and chemical reactivity in a variety of systems of interest using electronic structure calculations and first-principles molecular dynamics simulations (FPMD). Here we will present results for strand breaks in DNA due to low-energy electrons in the condensed phase, which is representative of the physiological environment. We will show that there are a variety of protection mechanisms that are not present in gas phase models, which are important to assess the feasibility of strand breaks [1-5]. We will also discuss recent results for the localization of electrons and holes in $Mg(OH)_2$ (brucite), which is one of the main phases in the UK nuclear waste inventory, and cement that is the most common material used for the immobilization of nuclear waste. In both cases we will show that electrons tend to localize in interstitial regions while holes are generally located in OH groups, and discuss the implications. FPMD simulations are used to examine the initial stages of the radiolytic road to hydrogen gas production.

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Th-III-1

Status Report of Undulator Experiments at the Mainz Microtron MAMI

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The possibility to produce undulator-like radiation in the hundreds of keV up to the MeV region by means of positron channeling is well known [1]. However, the demonstration and utilization of such devices hampers from the fact that high quality positron beams in the GeV range are not easily available, in contrast to electron beams. It was suggested that by means of planar channeling of ultrarelativistic electrons in a periodically bent single crystal the production of undulator-like radiation should also be possible.

In recent years, experiments have been performed at the Mainz Microtron MAMI to explore the radiation emission from epitaxially grown strained layer $Si_{1-x}Ge_x$ undulators at electron beam energies between 270 and 855 MeV. Clear enhancements of intensities were observed in the energy region where the undulator radiation is expected. However, a peak could not be observed, which may be due to imperfections of the $Si_{1-x}Ge_x$ undulators [2,3].

Recently, new technics for the preparation of boron doped diamond crystals have been developed. A crystal undulator with 4-periods and a period length 4.9 µm in the [110] direction has been produced on a high quality diamond backing with a thickness of 100 µm. The concentration of the boron has been varied between $7 \cdot 10^{20}$ and $1.6 \cdot 10^{21}$ atoms/cm^3.The radiation of this undulator was investigated with a high resolution Ge-detector at an electron beam energy of 180 MeV. First results of the radiation spectra of the doped crystal as well as for undoped crystals will be discussed.

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Th-III-2

Bent Crystals as a Tool for Electron Beams Manipulation

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In the last decades, the effect of channeling of charged particle beams in bent crystals has been investigated for application in hadron accelerator for beam collimation and extraction. Recently, experiments with electron beams have been carried out. The interest in such a case is connected to the fact that the deflection of electrons beams is accompanied by the generation of intense electromagnetic radiation.

Here, we present the last results on beam steering and intense e.m. radiation generation through interaction of high-energy electrons with bent crystals, by exploiting not only channeling but also a coherent effect typical of bent crystals, i.e., the volume reflection. Volume reflection consists in the deflection of over-barrier particles in a bent crystal and occurs in a wider angular acceptance than for channeling, being equal to the crystal bending angle [1]. A wide energy range for electrons has been selected, from sub-GeV at MAMI to hundreds-GeV at the CERN-SPS. A particular attention is given to the combination of beam steering and intense e.m. radiation generation in view of possible applications, such as an intense γ-ray source for the lowest energies to a crystal-based collimation at the highest ones.

The results of an experiment carried out at the CERN SPS-H4 beamline are reported. A 120 GeV/c electron beam was deflected by a 2 mm long been Si crystal in single and multiple volume reflection [2] orientation [3]. The resulting energy-loss spectrum of electrons was very intense over the full energy range up to the nominal energy of the beam and much more intense than for an amorphous medium. The beam deflection and the strong energy lost by electrons under single and multiple volume reflection makes this effect suitable for application in crystal-assisted beam dump and collimation for future linear colliders, such as the ILC or CLIC. Indeed, usually channeling is not efficient to steer negatively charged particles since they oscillate around the plane in the region of high nuclear density, thus being soon dechanneled due to incoherent scattering. For this reason, in a recent experiment, a shorter bent crystal has been used, with a length of 0.5 mm along the beam, demonstrating the possibility to steer hundreds-GeV beam through planar channeling.

We also report the first observation of efficient steering of a 0.855 GeV electron beam by means of planar channeling and volume reflection in a bent silicon crystal [4] carried on at the MAMI facility. Since the dechanneling length decreases with energy, an even shorter bent Si crystal (30.5 μm) was used to steer the electron beam. This experiment opened up the way for the investigation and exploitation of coherent interactions in bent crystals in the Sub-GeV/GeV energy range accessible by many electron accelerators worldwide, and which is interesting for innovative X- or gamma-ray sources. The radiation emitted by the electrons via planar channeling and single volume reflection was also recorded [5], being more intense than for an equivalent amorphous material, and peaked in the gamma range. A recent experiment has been carried out with an even shorter crystal (15 μm), thus increasing the deflection efficiency.

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Th-III-3

Recent Developments in Manufacturing of Crystalline Undulators

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Techniques used at the Sensor and Semiconductor Laboratory of Ferrara for producing self standing deformed crystals were recently enhanced by exploiting ion implantation. A silicon sample 0.2 mm thick was bent to a radius of curvature of 10.5 m. The sample curvature was characterized by interferometric measurements; the crystalline quality of the bulk was tested by X-ray diffraction in transmission geometry through synchrotron light at ESRF (Grenoble, France). Lattice damage induced by ion implantation affect only a very superficial layer of the sample, namely, the damaged region is confined in a layer 1 μm thick. Finally, an elective application of a deformed crystal through ion implantation is proposed, i.e., the realization of a crystalline undulator to produce X-ray beams.

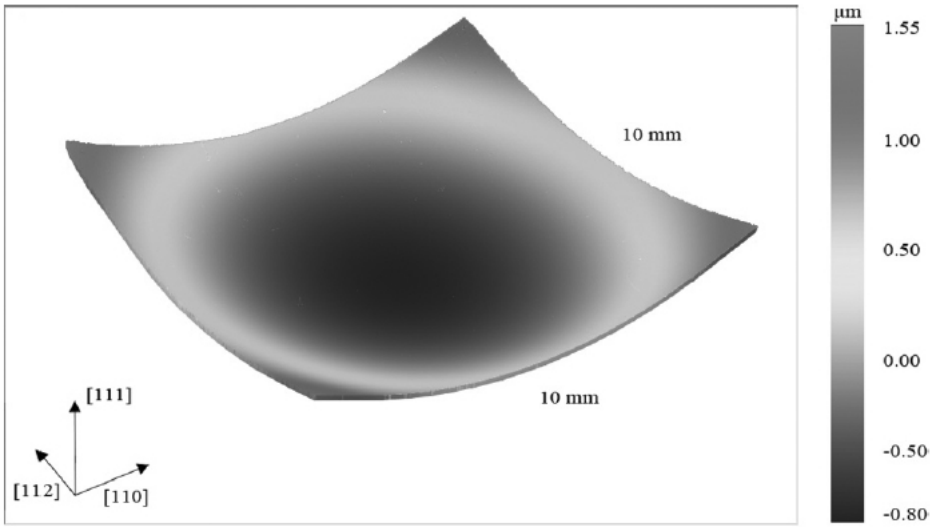

Figure 1: Morphological surface of the sample measured through interferometric profilometry.

Th-IV-1

The DYNECHARM++ Toolkit for the Simulation of the Particle Interaction with Crystals

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Charged particle impinging onto a crystal with small angle with respect to an atomic plane or axis can undergo planar or axial channeling regime with high probability. Trajectory of a ultra-relativistic particle under channeling regime can be studied through the usage of continuous potential approximation [1] and approximation of relativistic equations of motion [2]. Averaged electric field experienced by particles in their motion can be calculated through classical physical equations and the expansion of periodic functions as a Fourier series [3]. Based the on these calculation methods we have developed the DYNECHARM++ code [4,5], which allows to integrate the particle equations of motion under channeling regime inside a complex atomic structures. The code has been written in C++ programming language to simplify the integration within other software.

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Dynamical Coupling of Electrons and Ions in X-Ray-Induced Dynamics

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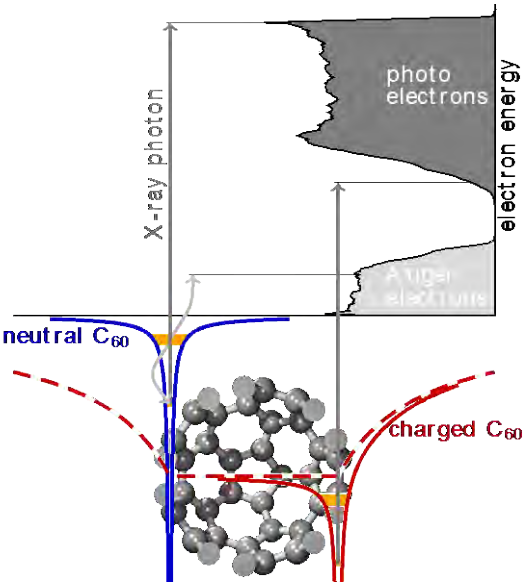
Multiple ionization of a polyatomic system in an intense X-ray pulse lead — in contrast to narrow photo lines observed for atoms — to broad photo-electron spectra [1, 2], since the charge built-up modifies the overall potential, as shown in the figure to the right for a C_{60} molecule. Typically, such spectra are difficult to interpret. Fullerenes offers a way to separate out the electron dynamics since the cage structure confines spatially the origin of photo and Auger electrons. Together with the sequential nature of the photo processes at intensities available at X-ray free electron lasers, this allows for a remarkably detailed interpretation of the photo-electron spectra [3]. The general features derived can serve as a paradigm for situations where an ion dynamics becomes relevant. For C_{60} this may occur already for pulses as short as 10 fs.



The situation becomes more involved for clusters consisting of small molecules. We study systematically the electronic sequence of methane CH_4, ammonia NH_3, and water H_2O clusters, augmented by the "atomic limit" of neon clusters. Those containing hydrogen do eject fast protons when illuminated by short X-ray pulses. A suitable overall charging of the cluster controlled by the X-ray intensity induces electron migration from the surface to the bulk leading to efficient segregation of the protons. This "dynamical segregation" hinders globally the explosion of the heavy atoms even outside the screened volume. In contrast to core-shell systems where the outer shell is sacrificed to reduce radiation damage, the intricate proton dynamics of hydride clusters allows one to keep the entire backbone of heavy atoms intact [4]. Further studies on large molecules – being neither as homogeneous nor as spherical as the molecular cluster above — confirm this segregation effect.

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Th-IV-3

Stability and Fragmentation of Multiply Charged Van der Waals clusters

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The stability of multiply charged clusters is determined by the balance between the Coulomb energy and the surface energy. Therefore, a multiply charged cluster with charge z is stable if its size n is larger than the appearance size $n_c(z)$. Echt et al. [1] prposed a model to estimate the appearance sizes for many kinds of multiply charged van der Waals clusters. In the model, the two fragment clusters are in contact at the transition point. The energy barrier is calculated using the liquid drop model. It is also assumed that the excess charge distributes uniformly in the volume of the cluster. The model reproduced the appearances sizes of many multiply charged van der Waals clusters measured in experiments. However, the observed appearance sizes for doubly and triply charged neon clusters [2] were found to be much smaller than those expected by the model [1]. There have been some attempts to shed light on this problem. Nakamura [3] calculated the appearance size of rare gas clusters with including the geometrical shell effects. Calvo [4] introduced quantum corrections to explain for the discrepancy. The discrepancy between the model and experiments has been improved. Still the model cannot sufficiently explain the discrepancy. However, making the assumption [5] that the excess charge is distributed over the cluster surface rather than within the volume, the appearance sizes for doubly and triply charged neon clusters can be obtained in a good correspondence with the experiment [2].

We also discuss the stability of multiply charged van der Waals clusters built of carbon atoms, such as clusters of fullerenes [6], and those of PAH (Polycyclic aromatic hydrocarbon) molecules [7]. These clusters are expected to play an important role in the molecular evolution in intersteller clouds [8].

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Th-IV-4

Recent Updates of the RADAM (RAdiation DAMage) Database

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RADAM (RAdiation DAMage) database portal (http://radamdb.mbnresearch.com/) is an interface to the network of RADAM databases that contain data on interactions of ions, electrons, positrons and photons with biomolecular systems, on radiobiological effects as well as on relevant multiscale phenomena occurring at different time, spatial and energy scales in irradiated targets during and after the irradiation. The RADAM database has been created within the framework of the COST Action Nano-IBCT (http://mbnresearch.com/project-nanoibct) and includes five principal areas: (i) Ionic Interactions, (ii) Electron/Positron Interactions, (iii) Photonic Interactions, (iv) Multiscale RADAM phenomena and (v) Radiobiological phenomena. The general structure of the database is described in Ref. [1].

Each of these areas is represented by at least one database node, where the corresponding information is stored. All this data can be accessed through the RADAM database portal, created and maintained by MBN Research Center gGmbH. The portal provides an interface for creating database queries using a unified query language for all the database nodes. The RADAM nodes for ionic, electron/positron and photonic interactions are connected to the VAMDC (Virtual Atomic and Molecular Data Centre) database portal (http://www.vamdc.eu/) in order to provide the possibility for users to search for data in all other VAMDC databases. Multiscale RADAM and Radiobiological phenomena nodes extend VAMDC to the new set of queries, defined specifically for the RADAM database.

The Multiscale RADAM node stores experimental and theoretical data on RADAM related phenomena such as stopping power, electron range, thermo-mechanical damage, diffusion coefficients, yields of radicals and molecular species, as well as reaction rate constants for different chemical reactions. The Radiobiological phenomena node currently stores or will store the data on the effect of radiation on cell survival, nanosensitization effect in cells, toxicity of radiosensitizing agents, their structural properties and localization in cells, bystander effect, single and double strand breaks in plasmids and DNA repair process.

In this presentation, the Early Stage Researchers of the FP7 Initial Training Network Project "ARGENT" (http://www.itn-argent.eu) will report on recent updates of the Multiscale RADAM and Radiobiological phenomena nodes of the database. It will be demonstrated how the results, presented in other talks at DySoN 2016, can be easily accessed by the scientific community.

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Fr-I-1

Effect of Support in Reducing Sintering, Improving Catalytic Activity, and Stabilizing Magnetic Order in Deposited Clusters

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The talk will highlight three distinct aspects of a cluster-support interactions, namely (1) Reduce sintering of catalysts by supporting core shell clusters on supports, (2) Activating catalytic reactions via suitably chosen supports, and (3) Controlling magnetic interactions between absorbed species via support.

Catalyst deactivation from sintering of catalytic surface is a major industrial problem particularly for catalysts that operate at higher temperatures. Controlling the catalyst support interaction can be a key to reduce sintering. I will present results of our recent joint theory/experimental effort on how one can use supported core-shell particles to reduce sintering. In particular, I will focus on the use of density functional calculations to determine the best combination of core shell compositions having the catalyst metal as the shell component and strong core support interaction. The role of support and the choice of metals will be highlighted.

I will then show how a support can activate a reaction. The carbon-carbon cross coupling reactions using palladium catalysts are one of the most important chemical transformations in the preparation of complex organic molecules. The Suzuki coupling reaction is particularly important in pharmaceutical applications due to its mild reaction conditions and broad application across a wide range of functionalized substituents. These reactions are generally carried out under homogeneous conditions that cannot be used in continuous flow processes, and leads to product contamination, and loss of expensive catalyst. Binding the palladium catalyst to a conventional support fails to overcome these limitations because the active sites are adversely affected and the catalytic activity is still homogenous because it is performed by palladium that has leached into solution. We demonstrate that a catalyst consisting of palladium clusters supported on reduced graphene not only minimizes leaching but also offers superior catalytic activity with extremely high turnover frequencies and remarkable recyclability. Theoretical investigations reveal that while the vacancy/void sites strongly bind the clusters thereby reducing leaching, the support also serves as a reservoir of charge that causes the reaction barriers to be even lower than those for homogeneous catalysts, explaining why such catalysts are active enough for continuous flow processes. Through state of art experiments involving a three-phase test, we unambiguously demonstrate that the catalyst operates in a heterogeneous mode.

Finally, I will show how a support can stabilize magnetic order in clusters/nanoparticles and induce coupling between absorbed species. Stability of magnetic order at elevated temperatures is a fundamentally challenging problem. The magnetic anisotropy energy (MAE) that prevents the thermal fluctuations of the magnetization direction can be around 1-10K in free transition metal clusters of around dozen atoms. I will show that a graphene support can lead to an order of magnitude enhancement in the anisotropy of supported species. Our studies show that the MAE of supported Co_5 and Co_{13} clusters on graphene increase by a factor of 2.6 and 33, respectively. The conductive support also enables a magnetic coupling between the deposited species and the nature of the magnetic coupling can be controlled by the separation between supported clusters or by vacancies offering an unprecedented ability to tune characteristics of assemblies.

Fr-I-2

Improving the Photocatalytic Potential of Nanostructured Tin Oxide

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Metal oxide semiconducting nanoparticles show enormous promise in photocatalysis with work on the nanostructuring of tin oxide, SnO_2, having focused on increasing sensitivity and selectivity towards targets and improving activity and reliability [1]. With these aims in mind, we have probed routes by which to modify SnO_2.

The facile production of SnO_2-based nanomaterials for applications in photocatalysis can take multiple forms. Hence, the synthesis of SnO_2-based nanocomposites in which the modulation of structure and composition improves the lifetimes of photogenerated electron-hole pairs has been explored. Highly active and recyclable photocatalysts with potential in dye degradation under simulated solar irradiation have resulted [2]. More recently we have immobilized SnO_2 nanoparticles using a filtering membrane that can potentially deliver substrate separation and which suggests applications in flow chemistry. The doping of a monolithic metal-organic framework [3] has been achieved and data point to the resulting composite demonstrating molecular sieving performance and delivering separated targets to photocatalytic reaction.

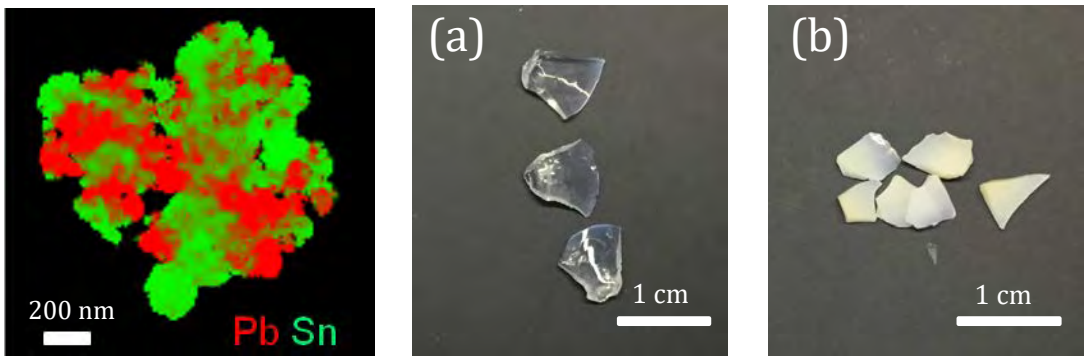

Figure 1: HAADF-STEM map of a SnO_2-PbS nanocomposite (far left) and samples of monolithic MOF before (a) and after (b) the introduction of SnO_2.

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Fr-I-3

Structure, Magnetism, Thermal and Optical Properties of Some Functionalized Iron Oxide Nanoparticles and Clusters of Medical and Industrial Interest

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In this talk we review some of the recent theoretical work [1] performed in our institute in order to better understand the properties of magnetic nanoparticles synthetized [2][3]; functionalized and characterized by other groups (S.Ammar, Paris 7, L.Fontaine, Le Mans)

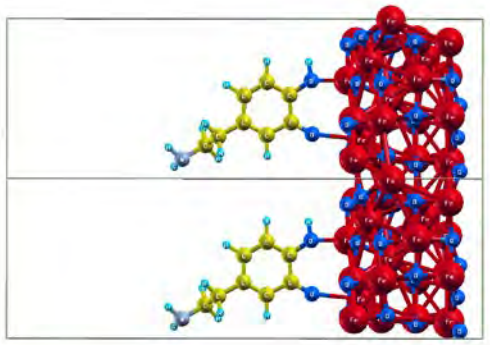

Figure 1: Surface of an iron oxide nanoparticle functionalized by dopamine

We present the effect of functionalization on magnetic properties; discuss some optical properties of hybrid nanoclusters, as well as the heat conduction effects [4] around the nanoparticle and possible drug release by hyperthermia if a polymer is present.

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Fr-I-4

Size Dependence of Catalytic CO-Oxidation Driven by Uni-Sized Pt Clusters Directly Bound to Si Surface Through Steady-State and Transient Measurements

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As tackling with a crucial issue of low-temperature and anti-poisoning catalysis for gas treatment, our experimental studies on the CO oxidation driven by uni-sized Pt clusters directly bound to a Si substrate surface, Pt_N/Si (N=10–71) [1-7], are reviewed [8-14].

Temperature-programed desorption mass-spectroscopy and steady-state and transient measurements of the turnover rate were employed. Figure 1 shows the turnover rate of the CO oxidation driven by Pt_{45}/Si with sudden change in the ^{13}CO pressure along with schemes of the molecular behavior. Analyzing with numerical simulation according to the rate equations, the rate constants of the elemental steps and the transient coverages of the ^{13}CO and O adsorbates on Pt_N/Si were obtained. It appeared that the rate of the reductive promotion of O_2 to an oxidizing agent by electron transfer from the catalyst is 1.5 times higher than that of the Pt(110) surface [15] owing to electrons accumulated at the subnano-interface between Pt_N and the Si surface [3,4,11]. The results were interpreted according to bistability in CO-rich and O-rich adsorption on the clusters.

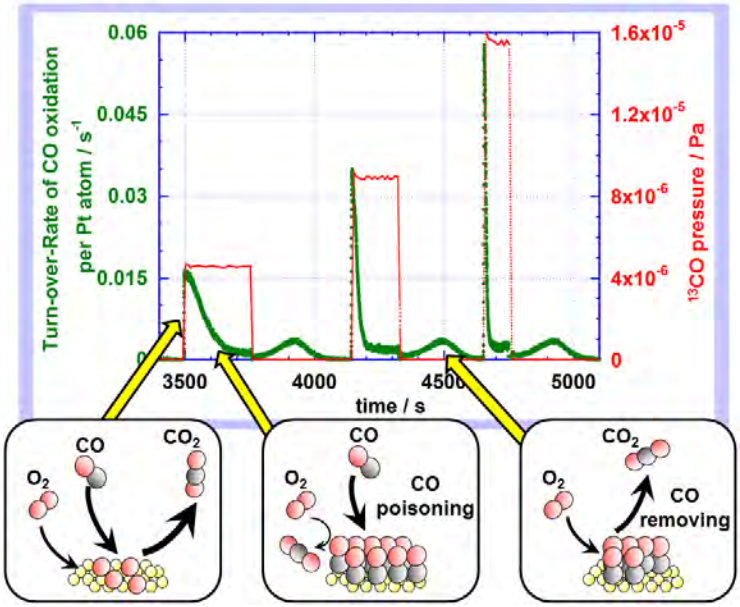

Figure 1: Transient turnover rate (per Pt atom) of CO oxidation driven by Pt_{45}/Si with sudden change in the ^{13}CO pressure in relation to bi-stability at CO-rich and O-rich regimes as illustrated in the insets. The O_2 pressure and catalyst temperature are fixed at 5.5×10^{-6} Pa and of 420 K, respectively.

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Fr-II-1

Recognition of DNA UV-Damage by Repair Enzymes

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Different factors can lead to damage in DNA and if these damages are not repaired in due time, the damaged DNA could lead to mutagenesis and cancer. To avoid this, different enzymes can attack and repair the different types of DNA damage, but the enzymes have first to bind to the damaged DNA sites. We have investigated this binding for a specific enzyme called as (6-4) photolyase, which is capable to repair certain UV-induced damage in DNA.

Photolyases specifically repair the UV-induced photoproducts between two adjacent pyrimidine rings: cyclobutane pyrimidine dimer (CPD) and pyrimidine-pyrimidone (6-4) photoproduct [1]. The repair mechanism is dependent on the cofactor flavin adenine dinucleotide (FAD) which is located inside the enzyme and drives its function. A schematic of the process is shown in Fig. 1.

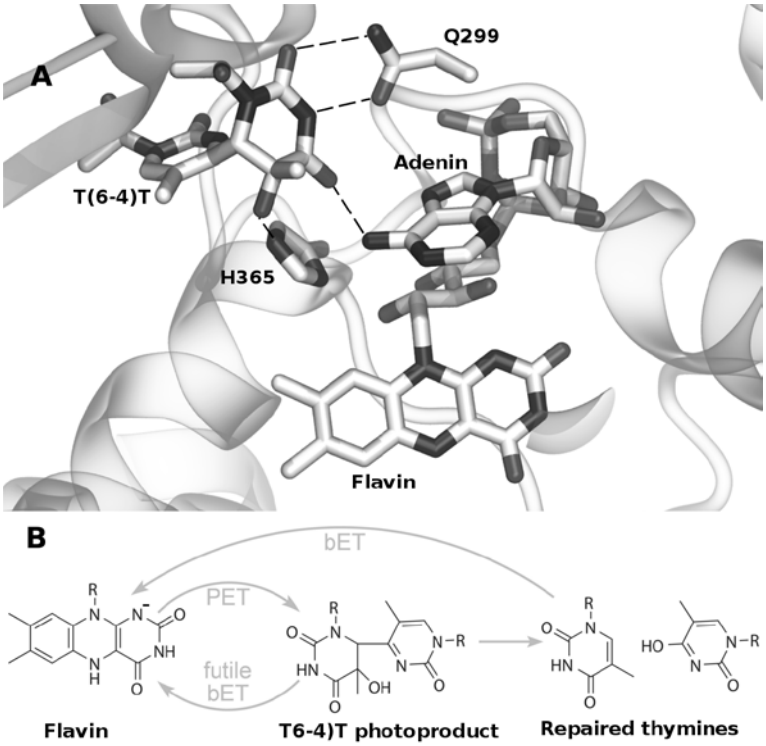

Figure 1: **A**: The important residues for the repair of the (6-4) photoproduct. The dashed lines show hydrogen bonds. **B**: The repair mechanism of the T(6-4)T photoproduct where the fully reduced $FADH^-$ makes an electron transfer to the photoproduct. The electron can be futile back transferred or the photoproduct is repaired.

We have employed molecular dynamics to understand the binding between the (6-4) photolyase and a UV-damaged DNA. Electrostatic interaction gives the largest contribution to the binding energy and several charged amino acids, such as arginines and lysines turn out to be important. Especially

R421 is crucial, as it keeps the DNA strands at the damaged site separated and the photoproduct inside the repair pocket of the enzyme [2].

DNA photolyase is highly homologous to another protein called as the cryptochrome. The two proteins are from the same flavoprotein family, have a high sequence similarity, and poses an overall very similar secondary and tertiary structures [3]. Moreover, both proteins are biological activated in a similar fashion through flavin photoexcitation. It is, however, striking that cryptochrome cannot repair UV-damaged DNA. An in-depth investigation allowed us to understand the small but, apparently critical differences between photolyase and cryptochrome. The performed analysis gives insight to important factors that govern the binding of UV-damaged DNA and reveal why cryptochrome cannot have this functionality.

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Fr-II-2

Molecular Simulation of Interstellar Ice Surfaces

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Nanoscale molecular thin films are nowadays of fundamental importance in a broad range of scientific fields ranging from nanotechnological applications, such as the nanofabrication with focused particle beams, to laboratory astrochemistry. The experimental study of organic thin films under extreme astrochemical conditions, which should mimic the icy mantles on interstellar dust grains, has received much attention recently. Here, the deposition, thermal processing and irradiation of thin films containing diverse mixtures of organic molecules is commonly studied with experimental methods, such as infrared absorption spectroscopy. Computational modeling allows for a complementary understanding of the physics and chemistry of these interstellar ice surfaces. Molecular dynamics simulations are capabale of providing atom-level insights into their structural, thermal, vibrational properties and other dynamical features, including phase transitions. In the present work, we present as well as discuss recent computer simulation results, which have been obtained using the MesoBioNano (MBN) Explorer software package [1].

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Fr-II-3

Transport of Secondary Electrons from Gold Nanoparticles through PEG Coating

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Gold nanoparticles (AuNPs) have been shown to possess radiosensitizing properties promising a better dose localization during radiotherapy treatment of cancerous tumors mainly through an increased production of secondary electrons [1] which promote the production of reactive chemical species in the vicinity of the AuNPs. To increase the blood circulation time, and thereby the concentration in tumors, AuNPs are often coated with the polymer poly(ethylene glycol) [2], however, the influence of the coating on the radiosensitizing properties of the NPs is not fully understood. The ability to correctly account for the effect of the coating is crucial in order to model the radiosensitization potential of coated NPs.

In this study, we present an analytical model based on the random walk approximation [3] of the diffusion of electrons emitted from the AuNP surface through the PEG coating, the density and thickness of which is found by classical molecular dynamics simulations using MBN Explorer [4] with the CHARMM force field [5]. Interaction cross sections between electrons and the coating are determined from the dielectric formalism [6] and the number of electrons emitted is calculated using the plasmon resonance approximation [1].

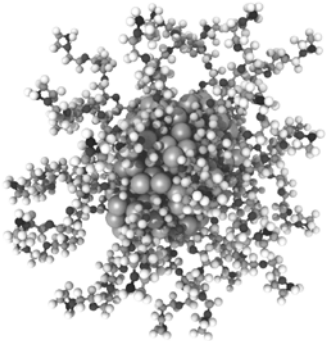

Figure 1: Frame from a molecular dynamics simulation of gold nanoparticle with PEG coating

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Posters

PS-01

Effect of Mutant $A\beta_{1-40}$ on Amyloid Aggregation of $A\beta_{1-40}$WT

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Amyloid fibrils are perspective object for creating new bionanomaterials. Because the fibrils are self-organized protein structure. For creating new materials with requisite properties amyloid aggregation should be operated. The fibrils have two active growth ends [1], so we can operate their formation by 'closing' or initiating the ends. In current research we studied an effect of amino acids substitution on fibril ends on amyloid aggregation rate. PDB structures of $A\beta_{1-40}$ were analyzed and two mutant forms were constructed. The mutations should stabilize Aβ amyloid conformation, but destroy some hydrogen bonds between molecules. Amino acids were substituted for Pro in 13, 19, 34 (3Pro) and in 18, 21, 26, 29 (4Pro). The mutant peptides should 'close' fibril from opposite directions. We supposed that each mutant separately would initiate aggregation, but together they would stop amyloid fibrils formation by 'closing' both its ends.

We found that any of analyzed peptides have no constant secondary structure in monomeric form. Neither 3Pro nor 4Pro form amyloid fibrils under the conditions where $A\beta_{1-40}$ wild type (WT) does. Adding mutant peptide to WT before incubation decreases amyloid fibrils formation rate. A few proportion concentrations were used (mutant peptide/WT: 1/1, 1/2)

This work was supported by Russian Scientific Foundation (project 14-24-00157).

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PS-02

A Radiation Dose-Response Curves and Analytical Model of Ion Tracks

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Chromosome aberrations (CA) arising from the interaction of ionizing radiation with living cells are regarded as the most sensitive indicator of genetic alterations since they represent the misrepair of DNA damages. The corresponding dose-response curves are usually described by a linear-quadratic model using the tissue specific α and β parameters [1]. The ab initio Monte Carlo calculations based on the ion track formation by irradiating heavy charged particles cannot yet explain the experimentally obtained data [2]. Thus, phenomenological models are still necessary to include the biological effects, such as dependence of the repair mechanisms on dose and radiation quality. Especially, the low relative biological effectiveness (RBE) of fast protons remains one of the most important questions which is also important for practical application of the proton radiotherapy [3].

In the present work, we investigated induction of CA in human lymphocytes exposed to 150 MeV and spread out Bragg peak (SOBP) proton beams, 199 MeV/u ^{12}C and 22 MeV/u ^{11}B ions and for comparison to ^{60}Co γ rays. Distributions of aberration frequency and the dose-response curves were studied for several doses.

The experimental data were compared with the statistical Neuman A distribution [4] and predictions of a new analytical model which explicitly takes into account overlapping of ion tracks at high particle fluencies. From the dose-response curves, it was possible to extract values of a biological effective track radius and to compare them with physical expectations. Both values were in a good agreement for used radiations with exception of fast protons for which a much smaller biological radius was obtained. The latter was interpreted in terms of more effective repair mechanisms in the irradiated regions of low ionization density and supported by observation of a nearly independence of the dose-response β parameter of the beam quality.

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PS-03

Auger Electron Spectroscopy of Liquid Water: The Role of Intermolecular Electronic Relaxation and Proton Transfer

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Electronic relaxation of core-ionized water molecules in liquid is far more diverse and complex than anticipated, and extremely different from that in an isolated water molecule. This was revealed by simulating Auger electron spectra of normal and heavy liquid water using *ab initio* and quantum dynamical methods and comparing the theoretical results with the available experimental data [1]. A core-ionized water molecule in the liquid phase, in addition to a local Auger process, relaxes through non-local energy- and charge-transfer processes, such as Intermolecular Coulombic Decay (ICD) [2] and Electron Transfer Mediated Decay (ETMD) [3]. These intermolecular decay processes play a surprisingly important role, especially ETMD which was considered for the first time in the core-level regime. Electronic relaxation is accompanied by ultrafast proton transfer [4] that enhances considerably the efficiency of the non-local processes [1]. As a consequence, the double charge forming at the end of electronic and nuclear relaxations tends to be distributed between different water monomers rather than be localized on a single molecular unit. Due to charge delocalization, various reactive oxygen species are created. Our study provides insight into the types and yields of these species.

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PS-04

Fast Heavy Ion Induced Biological Radiation Damage Using DNA Origami as a Probe

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One of the pillars of cancer therapy is tumor treatment by means of ionizing radiation. In the last decades, radiation therapy has matured into a powerful and sophisticated medical technique, however fundamentals of physical mechanisms are not yet fully understood. It is well established however, that DNA damage is initiating many biological pathways following irradiation of biological tissue. In this context, proton therapy and heavy ion therapy have proven to be particularly efficient for the treatment of solid tumors. The reason for this efficiency lies on distribution of unique dose of fast ions, as a function of penetration depth, which can be tuned to be maximum at the tumor location, dropping almost to zero right behind the tumor. The exact mechanisms of energy deposition, however are still under debate. Recently a new model based on the action of thermal shockwaves along the particle tracks has been proposed [1].

The molecular radiation damage in aqueous solution has mostly been investigated using plasmid DNA (pBR322) as a target and probe [2]. Damage is then typically quantified by means of agarose gel-electrophoresis technique, where the migration of charged DNA complexes through the polymer network of the gel is induced by an external electric field. Conformational changes of the plasmids due to radiation damage are directly manifest in changes in migration speed and can be quantified. However, the 3-D conformation of plasmid DNA is notoriously ill defined, rendering direct comparison between experiments and simulations difficult.

We have chosen to systematically investigate fast heavy ion induced damage using DNA origami as molecular probe. In addition, a comparison of radiation effect has been made for γ-ray irradiation at different doses. A proper choice of the DNA sequence allows for “construction “of almost arbitrary two and three dimensional shapes. We used this approach to prepare triangular shaped DNA structures and present our preliminary irradiation results. As mentioned, the radiation induced damage effect has shown to be difficult to quantify by means of gel-electrophoresis technique. Therefore, an extent was made to acquiring AFM images of the DNA origami triangle on an Si surface.

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PS-05

Selective Cancer Cell Toxicity and Radiosensitization Using Coated High Atomic Number Nanoparticles

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Radiotherapy is currently used in around 50% of all cancer treatments. Although it is generally effective, it is damaging to surrounding healthy tissues. This damage can be reduced by better targeting to cancer cells. Improved radiotherapy outcomes can be also achieved by using radiosentitising agents [1]. The most recent advances in combined radio and chemotherapy are based on introducing heavy elements to cancer cells, since these produce low energy electrons, due to the photo-emission effect when illuminated with incident high energy photons, and free radicals that further increase the effectiveness of radiotherapy [2,3]. Because of their biocompatibility and amenability to surface modification, gold nanoparticles (AuNPs) show significant promise in this area [4].

In our work we focus on the variation of the coating of the AuNPs and their effect with radiation treatment of skin cancer and normal skin cells. In addition, we investigate the uptake and localization of these different NPs in cells and their possible intrinsic toxicity levels.

Here, we would like to present our preliminary results obtained for NPs bearing various surface charges.

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PS-06

Modeling Secondary Particle Tracks Generated by Intermediate- and Low-Energy Protons in Water

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An important feature of interaction of ionizing radiation with biological systems is the complexity of biodamage [1]. A thorough understanding of radiation therapy requires evaluation of molecular-level effects related to dose deposition on the nanoscale [2]. One of the commonly used methods to study these effects in detail is based on Monte Carlo simulations performed by the track structure codes. By sampling a sufficiently large number of tracks, a Monte Carlo simulation can provide, to a high level of accuracy, insights into the mechanisms of the interaction of radiation with matter [1].

By means of the Low-Energy Particle Track Simulation (LEPTS) code (see [2] and references therein), it has become possible to model dynamics of secondary species down to the sub-eV scale. This Monte Carlo-based tool has been developed to address the molecular-level mechanisms of biological damage and to describe radiation effects in nanoscale volumes of the medium in terms of induced molecular dissociations [3]. LEPTS is based on reliable and self-consistent databases of interaction cross sections and energy-loss distributions for electrons and positrons, compiled from experimental data and complemented with theoretical calculations.

Here, we present a recent extension of the LEPTS methodology which allows one to model the slowdown of heavy charged particles propagating in water, combined with an explicit molecular-level description of radiation effects due to the formation of secondary electrons, their propagation through the medium, and electron-induced molecular dissociations [4]. As a case study, we consider traverse of protons with the initial energy of 1 MeV until their thermalization, so that we cover the energy range that contributes mainly to the energy deposition in the Bragg peak region. In order to include protons into the simulation procedure, a comprehensive dataset of integral and differential cross sections of elastic and inelastic scattering of intermediate- and low-energy protons from water molecules is created [4]. Development of a new database that include adequate data for biologically relevant material provides an opportunity for a more realistic, physically meaningful description of radiation damage in living tissue. Hence, the utilized approach allows one to study radiation effects on the nanoscale in terms of the number and the type of induced molecular processes.

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PS-07

Quantitatively Correct Description of Metallic Systems Melting with a New Interatomic Potential

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The investigation of phase transitions is an important general problem which spans across different fields of physics. Temperature-driven mechanisms of phase transitions as well as thermo-mechanical properties of a wide range of materials can be efficiently explored on the atomistic scale by means of classical molecular dynamics (MD) simulations [1]. The proper quantitative numerical modeling of these phenomena calls for accurate interatomic potentials which are used to describe interactions in the system. Most classical many-body potentials which are commonly utilized in MD simulations of metal systems are capable of describing their geometrical, mechanical, and energetic properties but can rarely reproduce the experimentally measured melting temperature, sometime yielding the discrepancy of several hundred degrees.

We present a recently proposed modification [2] of the widely utilized embedded-atom method (EAM)-type potential [3] and demonstrate its applicability to different monatomic metal systems, namely titanium, magnesium, gold, and platinum, as well as to bimetallic nickel-titanium nanoalloys [2,4]. Simulations performed with the modified force field describe quantitatively correctly both the melting temperature and the properties of metal systems at the normal conditions by means of classical MD simulations.

We found that the proper accounting for the long-distance interatomic interactions is crucial for a quantitatively correct simulation of melting and other excited vibrational state properties of the system being sensitive to the behavior of the interaction interatomic potentials far from their potential energy minima [2]. The presented force field keeps its behavior in the vicinity of the potential energy surface minima and weakens the interatomic interactions at distances beyond the atomic equilibrium regions, as these interactions are typically overestimated by the conventional EAM. The presented modification of the many-body potential has a general nature and can be applicable to metals with different characteristics of the electron structure and alloys.

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PS-08

MBN Explorer and MBN Studio: Universal Tools for studying Complex Molecular Structure and Dynamics

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MBN Explorer [1] is a powerful 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 MBN Explorer allows to simulate the structure and dynamics of different molecular systems, such as atomic clusters and nanoparticles [2-4], fullerenes [5], nanotubes [6,7], metallic nanomaterials [8-10], proteins and DNA [11,12], crystals [13-15] composite bio-nano systems and nanofractals [16,17]. 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 a broad range of problems involving complex molecular systems. More information on MBN Explorer can be found on the dedicated website, http://www.mbnexplorer.com/.

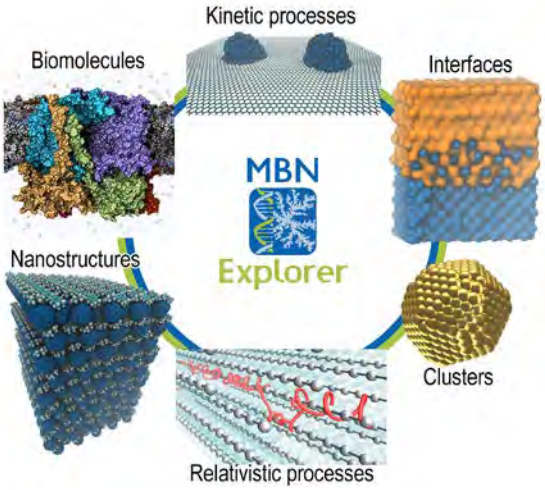

Figure 1: Illustration of different application areas of MBN Explorer [1].

MBN Studio is a graphical user interface for MBN Explorer that has been developed to facilitate setting up and starting the calculations, monitoring their progress, examining and visualising the results. MBN Studio can be utilized for any type of calculations that are supported by MBN Explorer, i.e. single-point energy calculations, structure optimization, molecular dynamics (nonrelativisic, relativistic, Euler), and kinetic Monte Carlo simulations. Apart from that, MBN Studio has a number of built-in tools allowing the calculation and analysis of specific characteristics that are determined by the output of MD simulations.

The poster will give an overview of the main capabilities of the two software tools, which are under permanent development conducted by MBN Research Center in Frankfurt am Main, Germany [18]. The poster will also highlight a number of recent case studies carried out with the use of MBN Explorer, some of which are illustrated in Figure 1.

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PS-09

Influence of Secondary Electron Energy and Angular Distributions on Swift Proton Radial Doses in PMMA

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The high energy deposition rates characteristic of accelerated ion beams find plenty of applications in industry and medicine, such as in ion beam nanolithography [1] and ion beam cancer therapy [2]. Such applications exploit the pattern of energy distribution at the nanoscale, where intense radial doses arise around ion tracks, being exhausted in just a few nanometres. This allows, on the one hand, the production of nanometric structures with high precision (for nanofabrication) and, on the other hand, the clustering of damage in biomolecules such as DNA (which justifies the increased biological efficiency of ion beams over conventional radiotherapy). It is, then, important to know precisely how these radial doses build up in materials of interest, such as the polymer polymethyl methacrylate (PMMA). This material is widely used as a resist in nanolithography and as a water equivalent material in dosimetric studies.

The way in which the energy lost by an ion is distributed around its path is mainly determined by the number of ejected secondary electrons, and by their energy and angular spectra. All these characteristics can be accurately determined for organic materials within a semiempirical method based on the dielectric formalism [3, 4]. This formalism also permits to obtain the energy loss characteristics of both ion and electron beams in condensed materials, accounting for all the electronic excitations and ionisations [5]. Once all these data are known, they can be used as input in Monte Carlo track structure codes to follow the complete slowdown of the secondary electron cascade. In this work, the cross sections calculated within the dielectric formalism are used within the Monte Carlo code SEED (Secondary Electron Energy Deposition) [6], which also includes other relevant interaction phenomena between the electrons and the condensed target, namely multiple elastic scattering and excitation of phonons and polarons. The radial doses for proton beams at several energies of interest are calculated having into account the realistic energy and angular distributions of electrons, and the results are compared with other simpler approaches, such as considering isotropic distributions or the binary encounter approximation. The influence of the different levels of approximation in the radial doses is analysed.

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PS-10

Electronic Structure and Radiation Stability of the Reference DNA pUC18/19

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The method of electron spectroscopy has been used more than one to study of the electronic structure of the DNA converted from solution into the solid state and put in high vacuum [e.g., 1-2]. However, the problem of influence of the DNA preparation ways, vacuum conditions and DNA tolerance to diagnostics beams has been remained insufficiently studied. In this work, the density of occupied electronic states for the reference DNA pCU18/19 reproducibly prepared by standard procedure [3] has been obtained. Exceptionally low radiation stability has been revealed.

DNA pCU18/19 was separated from the laboratory strain E.coli DH5α with using reagent of the Thermo Fisher Scientific Inc. according to the producer's instructions. Three DNA plasmid vectors with the nucleotide pare lengths of 420, 500 and 1766 in the proportion 1:1:1 were obtained. The drop of the DNA water solution was deposited, dried and put into the high vacuum chamber of the photoelectron spectrometer at the German-Russian beamline of the Electron Storage Ring BESSY-II.

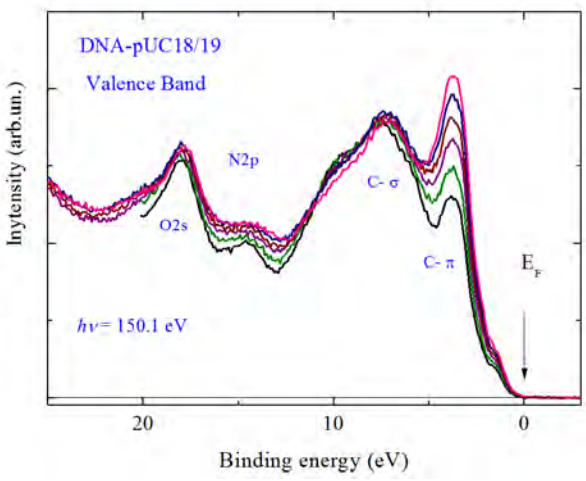

Figure 1: Photoemission spectrum of DNA in the course of its irradiation by photons with energy $h\nu$ = 150 eV.

Figure 1 presents a set of the valence band photoelectron spectra of the plasmid DNA fragments, characterizing its density of occupied electronic states (DOS). Symbols point the density pecks with dominating electronic states derived from different elements. The spectra were obtained in the course of one-hour irradiation by the low-intense diagnostic flux of photons with energy $h\nu$ = 150 eV. The DNA spectrum shows an essential transformation already in first several minutes of the measurements, thus demonstrating a drastic redistribution of the DOS towards the π-states, including those near the Fermi level. The last one evidences occurrence of an essential electrical conductivity of the film. Despite the extremely low radiation stability, the spectrum of the undamaged DNA has been obtained.

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PS-11

Electron-Beam-Induced Graphite Oxide Reduction

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A possibility of a lithographic image formation by electron beam on a few-layer graphene oxide (GO) film has been recently demonstrated [1]. The image was created due to partial thermal reduction of GO induced by local heating of the film with the dense 20 keV electron nanoprobe. A disadvantage of thermal GO reduction is the formation of numerous defects because of the probable detachment of a GO carbon atom together with a departing oxygen group [2]. Therefore, searching for new nonthermal and nondestructive reduction processes is a topical task. In this work, we demonstrate the possibility of the efficient nonthermal reduction of GO by a weak electron beam which does not heat the irradiated area.

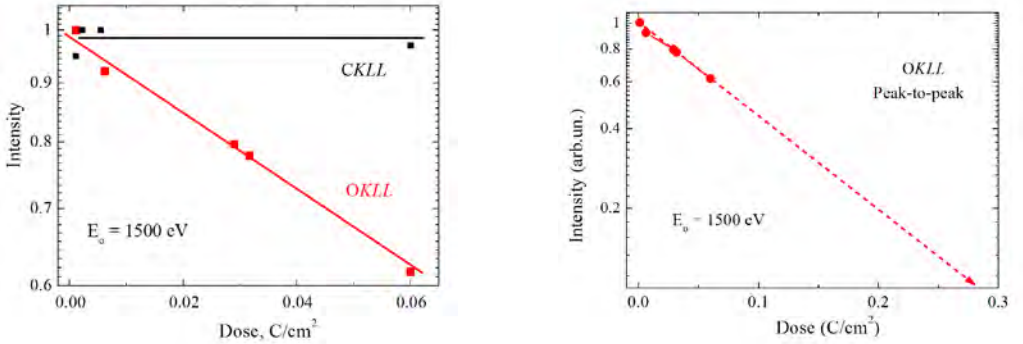

Figure 1: Dependences of the O*KLL* and C*KLL* Auger line intensities of the graphite oxide film on the electron irradiation dose density in different scales.

A multilayer GO film prepared in Ioffe Institute on the surface of a silicon wafer [3] and tested previously [4] has been studied. The film was irradiated in high vacuum by a low-intense (15–250 nA) electron beam with the energy E_0 =1500 eV. Extremely low released power (2–40 mW/cm^2) excluded heating the irradiated area. Fig.1 shows decrease of the O*KVV* oxygen peak intensity almost by a factor of 2 in the range of very low irradiation doses. The intensity of the C*KVV* carbon line remains unchanged in the first approximation in the process of the film irradiation. This means that the atoms of the carbon layer do not form free complexes with oxygen groups and that the carbon layer remains mainly undamaged. The oxygen dose dependence proved to be possible to be described by one exponent. Its extrapolation shows the possibility of complete GO reduction at low doses. The effective cross section of the oxygen group detachment was estimated to be $\sigma_{in} \approx 1.2 \times 10^{-18}$ cm^2 [5]. The mechanism of the GO reduction involves the local excitation of the valence electrons of an oxygen group and carbon atoms bonded to it, subsequent transition of such a quasimolecular group to a repulsive state, and the removal of an oxygen group.

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For notes

Monday, October 03

$12^{00} – 16^{00}$	Participants registration
$14^{00} – 14^{45}$	**DySoN 2016 Opening** **Andrey V. Solov'yov**
14^{45} - 16^{15}	*Afternoon session I: Structure and dynamics of clusters, nanoparticles and biomolecules* **Eric Suraud / Julius Jellinek / Kit Bowen**
$16^{15} – 16^{45}$	**Coffee break**
$16^{45} – 18^{45}$	*Afternoon session II: Nanoscale phase and morphological transitions* **Nigel Mason / Michael Moseler /** **Florent Calvo / Thomas Schlathölter**
$19^{00} – 21^{00}$	**Conference reception**

Tuesday, October 04

$9^{30} – 11^{00}$	*Morning session I: Multiscale physics of radiation damage processes* **Eugene Surdutovich / Pablo de Vera /** **Alexey Verkhovtsev**
$11^{00} – 11^{20}$	**Coffee break**
$11^{20} – 13^{00}$	*Morning session II: Biomedical applications of radiation* **Steffen Greilich / Martin Falk /** **Malgorzata Smialek / Ilko Bald**
$13^{00} – 14^{30}$	**Lunch**
$14^{30} – 16^{00}$	*Afternoon Session I: Nanostructured materials* **Richard Palmer / Simon Connell /** **Victor Balykin / David Field**
$16^{30} – 17^{00}$	**Coffee break**
$17^{00} – 18^{30}$	*Poster session &* *H2020-RISE-PEARL management board meeting*

Wednesday, October 05

$9^{15} – 10^{45}$	*Morning session I: Surfaces and interfaces* **Wolfgang Ernst / Yuri Vainer /** **Nouari Kebaili**
$10^{45} – 11^{10}$	**Coffee break**
$11^{10} – 12^{50}$	*Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules* **Rodolphe Antoine / Michael Beuve /** **Elette Engels / Vadim Ivanov**
$12^{50} – 13^{00}$	**Conference photo**
$13^{00} – 14^{30}$	**Lunch**
$14^{30} – 16^{00}$	*Afternoon Session I: Electron transport in molecular systems* **Kurt Stokbro / Vincenzo Guidi /** **Jean-Patrick Connerade** (conference discussion)
$16^{30} – 18^{30}$	**Conference tour**

Thursday, October 06

$9^{30} – 11^{00}$	*Morning session I: Propagation of particles through medium: H2020 RISE-PEARL Project* **Andrei Korol / Hartmut Backe /** **Ulrik Uggerhøj**
$11^{00} – 11^{30}$	**Coffee break**
$11^{30} – 13^{00}$	*Morning session II: Collision processes, fusion, fission, fragmentation* **Franco Gianturco / Bernd Huber /** **Jorge Kohanoff**
$13^{00} – 14^{30}$	**Lunch**
$14^{30} – 16^{00}$	*Afternoon session I: Propagation of particles through medium: H2020 RISE-PEARL Project* **Werner Lauth / Laura Bandiera /** **Andrea Mazzolari**
$16^{00} – 16^{30}$	**Coffee break**
$16^{30} – 18^{15}$	*Afternoon session II: Modelling of nano- and biomolecular systems* **Enrico Bagli / Ulf Saalmann /** **Masato Nakamura / Alexey Verkhovtsev,** **Kaspar Haume, Pablo de Vera**
$19^{00} – 22^{30}$	**Conference dinner**

Friday, October 07

$9^{15} – 11^{00}$	*Morning session I: Clusters and nanoparticles: structure, reactivity and catalysis* **Shiv Khanna / Andrew Wheatley /** **Florent Calvayrac / Hisato Yasumatsu**
$11^{00} – 11^{30}$	**Coffee break**
$11^{40} – 12^{50}$	*Morning session II: Irradiation driven transformations of complex molecular systems* **Katrine Jepsen / Christian Kexel /** **Kaspar Haume**
$12^{50} – 13^{00}$	**DySoN 2016 Closing**
$13^{00} – 14^{30}$	**Lunch and departure**