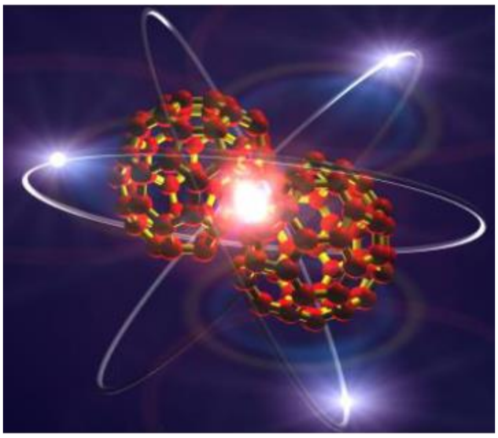
The Ninth International Symposium “Atomic Cluster Collisions”



ISACC 2019

Canterbury Cathedral Lodge & University of Kent
Canterbury, United Kingdom
July 31 - August 03, 2019

Book of Abstracts

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Preface

The ninth International Symposium “Atomic Cluster Collisions” (ISACC 2019) will take place on July 31 - August 03, 2019 at Canterbury Cathedral Lodge and the University of Kent (Canterbury, United Kingdom). The ISACC 2019 is co-organized by the University of Kent and MBN Research Center, Frankfurt am Main, Germany.

ISACC started as an international symposium on atomic cluster collisions in St. Petersburg, Russia in 2003. The second ISACC was held at the GSI, Darmstadt, Germany in 2007. Both symposia were satellites of the International Conferences on Photonic Electronic and Atomic Collisions (ICPEAC). The third ISACC returned to St. Petersburg in 2008 and was organized as a separate conference. The fourth ISACC took place in Ann Arbor, Michigan, USA in 2009; the fifth ISACC - in Berlin, Germany in 2011; the sixth - in Wuhan, China in 2013; the seventh - in Madrid, Spain in 2015. All four conferences were ICPEAC satellites. The eighth symposium was held in Varadero, Cuba in 2017. The ninth ISACC symposium will be held just after the ICPEAC 2019 (Normandy, France, July 23-30, 2019).

The ISACC 2019 will promote the growth and exchange of scientific information on the structure, properties and dynamics of complex atomic, molecular, biological and cluster systems studied primarily by means of photonic, electronic and atomic collisions. Particular attention will be devoted to dynamical phenomena, many-body effects taking place in clusters, nanostructures, molecular and biological systems, which include problems of fusion and fission, fragmentation, collective electron excitations, phase transitions, radiation damage, and many more. Both experimental and theoretical aspects of cluster physics uniquely placed between nuclear physics on one hand and atomic, molecular and solid state physics on the other will be subject of the symposium. Particular attention will be devoted to the utilization of advanced computational techniques and high performance computing in studies of collisions involving complex molecular systems. Links of the ISACC topics to novel and emerging technologies will be an important focus of ISACC 2019.

Finally, ISACC 2019 will provide a platform to host discussions about current research, technological challenges and related initiatives within the ISACC 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!

Topical Areas of ISACC:

- Structure and dynamics of atomic and molecular clusters, and nanoparticles
- Structure and dynamics of biomolecules
- Cluster structure and dynamics on a surface
- Cluster-molecule interactions, reactivity and nanocatalysis
- Clustering in systems of various degrees of complexity
- Clusters and biomolecules in external fields: electric, magnetic, laser etc.
- Electron and photon cluster collisions
- Ion-cluster collisions
- Collision processes with biomolecules
- Cluster and biomolecular research with Free Electron Lasers

Conference Venue

The Conference will be hosted by the Canterbury Cathedral Lodge (on July 31 - August 02) and Darwin College of the University of Kent (on August 03), Canterbury, United Kingdom.

Canterbury is one of the UK's oldest cities (predating Roman arrival) befitting its role as capital of Kent, the Gateway to the United Kingdom from Europe. Canterbury and its cathedral is also the ecclesiastical centre of the Church of England.

Conference Reception

The conference reception will take place on Wednesday, July 31, from 19^{00} to 22^{00} and will be located at the Canterbury Cathedral Lodge.

Conference Dinner and Tour

The conference dinner will take place on Friday, August 2, from 19^{00} to 22^{00}. The dinner will be preceded by a guided conference tour around the historical centre of Canterbury. The tour will take place from 16^{15} to 18^{00}.

ISACC2019 Topical Issue of EPJD

A Topical Issue **"Atomic Cluster Collisions 2019"** will be launched in **the European Physical Journal D**: Atomic, Molecular, Optical and Plasma Physics, https://epjd.epj.org/. All conference participants are encouraged to submit their novel results to this Topical Issue. The deadline for submission is **December 30, 2019**. Guest Editors are Dr. Alexey Verkhovtsev, Dr. Pablo de Vera, Prof. Nigel Mason, and Prof. Andrey Solov'yov.

International Advisory Committee

- Andrey Solov'yov (MBN Research Center, Germany) **Chair**
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- Jean-Patrick Connerade (Imperial College London, United Kingdom)
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- Irina Solovyeva (MBN Research Center, Germany)
- Alexey Verkhovtsev (MBN Research Center, Germany)

Sponsors

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

- University of Kent, Canterbury, United Kingdom
- MBN Research Center, Frankfurt am Main, Germany
- Springer

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ISACC Conference Series Web Portal

Updated information on the conference series is available at www.isacc-portal.org

Conference Program

Wednesday, July 31 (Canterbury Cathedral Lodge)

12^{00} – 16^{00}	Participants registration
14^{00} – 14^{15}	**ISACC 2019 Opening** **Nigel J. Mason and Andrey V. Solov'yov**
	(1) Afternoon session I: Structure and dynamics of atomic clusters and nanoparticles (Chair: Andrey Solov'yov)
14^{15} – 14^{45}	**Henrik Cederquist**, Stockholm University, Stockholm, Sweden *Slow electron emission from excited dimer anions*
14^{45} – 15^{15}	**Manfred Kappes**, Karlsruhe Institute of Technology, Karlsruhe, Germany *Experiments with carbon containing clusters*
15^{15} – 15^{45}	**Eleanor Campbell**, University of Edinburgh, Edinburgh, Scotland *Molecular Maracas: a multi-state molecular switch based on* $Li@C_{60}$
15^{45} – 16^{15}	**Mathias Rapacioli**, Université Paul Sabatier, Toulouse, France *Charge and excitation resonance in ionized aromatic molecular clusters*
16^{15} –16^{45}	Coffee break
	(2) Afternoon session II: Clustering in systems of various degrees of complexity (Chair: Eleanor Campbell)
16^{45} – 17^{15}	**Andrey V. Solov'yov**, MBN Research Center, Frankfurt am Main, Germany *Irradiation driven multiscale dynamics of MesoBioNano systems*
17^{15} – 17^{45}	**Jean-Patrick Connerade**, Imperial College London, London, United Kingdom *The value of K-matrix theory for all systems held together by coulombic forces*
17^{45} – 18^{15}	**Eric Suraud**, Université Paul Sabatier, Toulouse, France *On the inclusion of dissipative effects in clusters and molecules*
19^{00}– 22^{00}	Welcome reception

Thursday, August 01 (Canterbury Cathedral Lodge)

	(3) Morning session I: Collisions with atomic clusters and biomolecules (Chair: Eugene Surdutovich)
9^{00} – 9^{30}	**Thomas Schlathölter**, University of Groningen, Groningen, the Netherlands *Interactions of gas-phase biomolecular ions with fast ions and with soft X-ray photons*
9^{30} – 10^{00}	**Jefferson Shinpaugh**, East Carolina University, Greenville, North Carolina, USA *Gold nanoparticles as a radiosensitiser for proton and carbon ion irradiation*
10^{00} – 10^{30}	**Rodolphe Antoine**, Université Claude Bernard Lyon1, Villeurbanne, France *Collision induced dissociation and collision cross sections of gold nanoclusters: new tools for structural characterization?*
10^{30} – 11^{00}	**Alexey Verkhovtsev**, MBN Research Center, Frankfurt am Main, Germany *Computational studies of collision-induced fragmentation of molecular systems*
11^{00} – 11^{30}	Coffee break
	(4) Morning session II: Clusters and biomolecules in external fields: electric, magnetic, laser, etc. (Chair: Jean-Patrick Connerade)
11^{30} – 12^{00}	**Brendan Dromey**, Queen's University Belfast, Belfast, United Kingdom *Studying nascent proton-driven radiation chemistry in* H_2O *in real time using laser-*

	based sources
12^{00} – 12^{30}	**Andrew Ellis**, University of Leicester, Leicester, United Kingdom *Accessing elusive molecular species by combining helium droplets with IR spectroscopy*
12^{30} – 13^{00}	**Eugene Surdutovich**, Oakland University, Rochester, Michigan, USA *Multifragmentation of Ar clusters by protons and heavier ions as a way to observe ion-induced shock waves*
13^{00} – 14^{30}	Lunch
	(5) <u>Afternoon session I: Cluster structure and dynamics on a surface</u> (Chair: Shiv Khanna)
14^{30} – 15^{00}	**Nigel J. Mason**, University of Kent, Canterbury, United Kingdom *Electron and photon induced chemistry in molecular clusters*
15^{00} – 15^{30}	**Richard Palmer**, Swansea University, Swansea, United Kingdom *Nanoparticle beam deposition: A novel route to the solvent-free creation of heterogeneous catalysts*
15^{30} – 16^{00}	**Armin Gölzhäuser**, University of Bielefeld, Bielefeld, Germany *Functional 2D nanomaterials and devices made by electron, ion and EUV induced processes*
16^{00} – 16^{30}	**Pablo de Vera**, MBN Research Center, Frankfurt am Main, Germany *Joint Monte Carlo and molecular dynamics simulation of electron beam-induced chemistry on surfaces*
16^{30} – 17^{00}	Coffee break
17^{00} – 18^{00}	**<u>Poster session</u>**

Friday, August 02 (Canterbury Cathedral Lodge)

	(6) <u>Morning session I: Ion-cluster collisions</u> (Chair: Henrik Cederquist)
9^{00} – 9^{30}	**Michael Dingfelder**, East Carolina University, Greenville, North Carolina, USA *Track-structure simulations in nanometer geometries*
9^{30} – 9^{55}	**Himadri Chakraborty**, Northwest Missouri State University, Maryville, Missouri, USA *Matter (ion) and antimatter (positron) collisions with fullerene nanomolecules*
9^{55} – 10^{20}	**Mark Stockett**, Stockholm University, Stockholm, Sweden *Non-statistical fragmentation of* C_{60} *and the formation of endohedral defect fullerenes*
10^{20} – 10^{40}	**Suvasthika Indrajith**, Normandy University, CEA-CIMAP, Caen, France *Energetic processing of hydrocarbons molecular species by ionizing radiation: towards the formation of cyclic species*
10^{40} – 11^{00}	**Andreas Alberg-Fløjborg**, University of Southern Denmark, Odense, Denmark *Ion collisions with biological targets. The early stages of ion beam cancer therapy*
11^{00} – 11^{30}	Coffee break
	(7) <u>Morning session II: Cluster-molecule interactions, reactivity and nanocatalysis</u> (Chair: Ilya Fabrikant)
11^{30} – 12^{00}	**Shiv N. Khanna**, Virginia Commonwealth University, Richmond, USA *Transforming redox properties of clusters using ligands to create super dopants for two-dimensional semiconductors and to synthesize nano p- n- junctions*
12^{00} – 12^{30}	**Sam Eden**, The Open University, Milton Keynes, United Kingdom *Tracing radiation-induced reaction products to specific neutral isomer and cluster precursors*

12^{30} – 13^{00}	**Jon Golding**, The Open University, Milton Keynes, United Kingdom *Element choice for nanoparticle radiosensitisers*
13^{00} –13^{15}	Conference photo
13^{15} – 14^{30}	Lunch
	(8) <u>Afternoon session I: Cluster and biomolecular research with Free Electron Lasers</u> (Chair: Thomas Schlathölter)
14^{30} – 15^{00}	**Kiyoshi Ueda**, Tohoku University, Sendai, Japan *Atomic cluster experiments at SACLA, an XFEL in Japan*
15^{00} – 15^{30}	**Jan-Michael Rost**, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany *Purification of XFEL spectra*
15^{30} – 16^{00}	**Sadia Bari**, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany *Gas-phase proteins studied at advanced light sources*
16^{00} –16^{15}	Coffee break
16^{15} - 18^{00}	Conference tour
19^{00} - 22^{00}	Conference dinner

Saturday, August 03 (Darwin Conference Suite, Darwin College, the University of Kent)

	(9) <u>Morning session I: Electron and photon cluster collisions</u> (Chair: Nigel Mason)
9^{00} – 9^{30}	**Ilya Fabrikant**, University of Nebraska-Lincoln, Nebraska, USA *Recent advances in the theory of electron attachment to molecules and clusters*
9^{30} – 9^{55}	**Andreas Mauracher,** Leopold-Franzens-University, Innsbruck, Austria *Size-selected charged helium droplets*
9^{55} – 10^{20}	**Jozef Lengyel**, Technische Universität München, Garching, Germany *Effect of cluster environment on electron- and ion-mediated chemistry: from atmospheric chemistry to nanocatalysis*
10^{20} – 10^{40}	**Xin Wang**, University of Groningen, Groningen, the Netherlands *Soft X-ray photofragmentation of gas phase oligonucleotides*
10^{40} – 11^{00}	**Alfred Msezane**, Clark Atlanta University, Atlanta, United States *New manifestations in low-energy electron scattering from the actinide atoms Pu, Cm, Bk and Lr*
11^{00} –11^{30}	Coffee break
	(10) <u>Morning session II: Collisions with biomolecules</u> (Chair: Sam Eden)
11^{30} –12^{00}	**Linda Feketeová**, Université Claude Bernard Lyon 1, Villeurbanne, France *Evaporation of water molecules from excited water nanodroplets*
12^{00} –12^{30}	**Roland Wester**, Leopold-Franzens-University, Innsbruck, Austria *Reactions dynamics of small ionic clusters*
12^{30} –13^{00}	**Hidetsugu Tsuchida**, Kyoto University, Kyoto, Japan *Influence of secondary electrons on biomolecular damage in water by fast heavy-ion irradiation*
13^{00} –13^{15}	**ISACC 2019 Closing**

Overview of Abstracts

Talks

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Talks

We-I-1

Slow Electron Emission from Excited Dimer Anions

E.K. Anderson[1], A.F. Schmidt-May[2], P.K. Najeeb[1], G. Eklund[1], K.C. Chartkunchand[3], S. Rosén[1], K. Hansen[4,5], H. Zettergren[1], H.T. Schmidt[1], and H. Cederquist[1]

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We report on the decay of hot copper dimer anions injected and stored in one of the cryogenic ion-beam storage rings of the DESIREE infrastructure at Stockholm University. The DESIREE storage rings are purely electrostatic, they are operated at a temperature of 13 Kelvin and a pressure of 10^{-14} mbar [1,2] allowing for ion beam storage for up to hours [3]. Most molecular ions will relax their internal excitations considerably by emitting (and absorbing) photons in the black-body radiation field in the cryogenic ring on these and much shorter time scales [4,5]. However, this does not apply to homonuclear dimers, or homonuclear dimer anions, which lack permanent electric dipole moments and therefore do not emit photons on the present experimental time scale. Instead, such dimer anions may only decay by fragmentation or by electron emission provided that they are suffiently excited in order to make such processes energetically possible. Here, we report separate measurements of the fragmentation and electron emission rates of internally hot (excited) copper dimer anions as functions of time after they have been extracted from a Cesium sputter ion source (and accelerated to keV energies and stored in the ring). Such an ion source is known to produce rotationally and vibrationally hot ions with a broad internal energy distribution [6]. Shortly after injection, the decay is dominated by fragmentation (as suggested already by an earlier study by Fedor *et al.* [7] in which, however, contributions from fragmentation and electron emission were not separated). For Cu_2^- storage times exceeding 100 ms, we find that electron emission dominates. The electron emission mechanism is vibrational autodetachment through very weak couplings between nuclear and electronic degrees of freedom in absence of avoided crossing between the potential energy curves of Cu_2^- and Cu_2. The observation of electron emission is evidence for a dramatic breakdown of the Born-Oppenheimer approximation, where a large amount of vibrational energy in Cu_2^- is converted to electronic energy as the electron is emitted. This means that the kinetic energy of the heavy nuclei changes abruptly in the $Cu_2^- \rightarrow Cu_2 + e^-$ process. As electron emission is very slow, the cross section of the reverse process, $Cu_2 + e^- \rightarrow Cu_2^-$ is very small. These aspects will be discussed along with results for the decays of other metal cluster anions including ones that are larger than the dimers [8,9]. The extreme ultra-high vacuum in DESIREE, 10^{-14} mbar, is a prerequisite for the present new findings.

We-I-1

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We-I-2

Experiments with Carbon Containing Clusters

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The talk will provide a summary of recent work on size-selected, carbon-containing clusters which comprise in particular polyaromatic hydrocarbons (PAH), fullerenes and derivatives thereof. Starting with experiments in which we have probed the oligomerization of partially dehydrogenated PAH´s on inert graphitic surfaces, I will discuss related studies of (halogenated) PAH derivatives which selectively decompose into fullerene cages upon energization. Then, I will touch upon the structure of the giant fullerenes present in bulk scale fullerene preparations - which we have probed by electrospray coupled with high resolution ion mobility spectrometry. After a discussion of the thermal conversion of dumb-bell fullerene oligomers into larger closed shell fullerene species, I will finish by presenting experiments in which fullerenes and hydrogenated fullerenes are fragmented by electron impact to form smaller fullerene cages, carbon chains and (for hydrogenated fullerenes) PAHs. These experimental observations and their rationalization by theory are of possible relevance to both nanoscience and astronomy.

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We-I-3

Molecular Maracas: A Multi-State Molecular Switch Based on Li@C_{60}

Eleanor E.B. Campbell[1], Renald Schaub[2], Henry J. Chandler[2], Minas Stefanou[1]

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By combining gas phase Rydberg Fingerprint photoelectron spectroscopy measurements with low temperature UHV scanning tunneling spectroscopy studies, we probe the properties of the low-lying Rydberg (SuperAtom Molecular Orbital, SAMO) states of Li@C_{60} [1]. We show that the off-centre presence of the Li inside the fullerene cage strongly distorts the electron density of the S and P_z SAMOs. This is most apparent in the STM studies where the energies of these states are strongly shifted compared to the gas phase and show a strong interaction with the underlying Au substrate. By applying a relatively high current pulse at a bias voltage of ca. 5V from the STM tip we can move the Li from its equilibrium position towards the top of the cage to 14 different stable cage positions [2]. All of these positions can be distinguished from the STM topology and the measured tunnel current. The switching mechanism and potential use of such a unique single molecule device will be discussed.

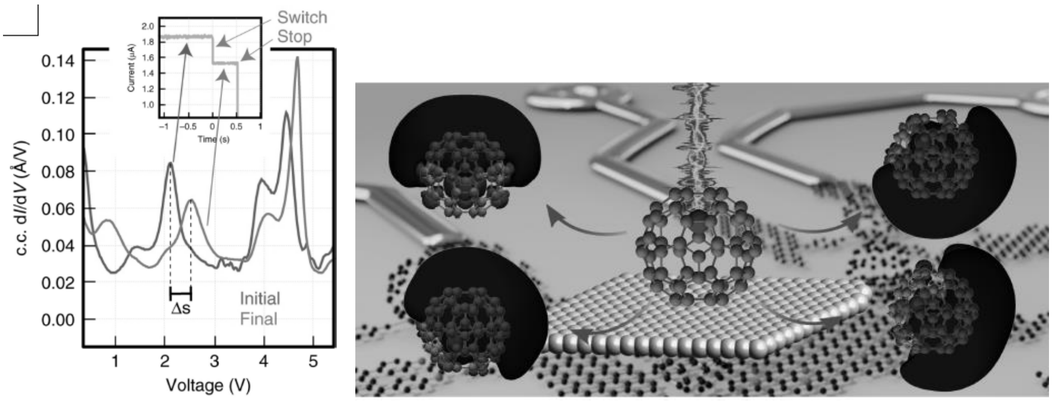

Figure 1: Left: STS measurement of tunnel current through initial and final (switched) state of Li@C_{60} [2]. Right: Schematic cartoon of the switching process.

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Mo-I-4

Charge and Excitation Resonance in Ionized Aromatic Molecular Clusters

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Experimental and theoretical investigations of Polycyclic Aromatic Hydrocarbon clusters properties are performed to probe their stability in the interstellar medium. These clusters are stabilized by van der Waals and electrostatics interactions and, in the case of cations, by charge resonance between the PAH units. Containing tens to hundreds of atoms, such systems can hardly be approached via traditional ab initio schemes at the moment. Density functional based tight binding method (DFTB, an approximate DFT scheme) allows to deal with systems of this size range. Unfortunately, it inherits from DFT the difficulties to describe the typical interactions met in molecular clusters, in particular charge resonance in ions. This presentation will give an overview of how DFTB can be modified to become a realistic and efficient tool to investigate the structural, electronic and energetic properties of PAH clusters [1]. We will compare the computed observables with recent experimental results and will use the theoretical electronically excited potential energy surfaces to propose mechanisms involved in photo-dissociation experiments [2].

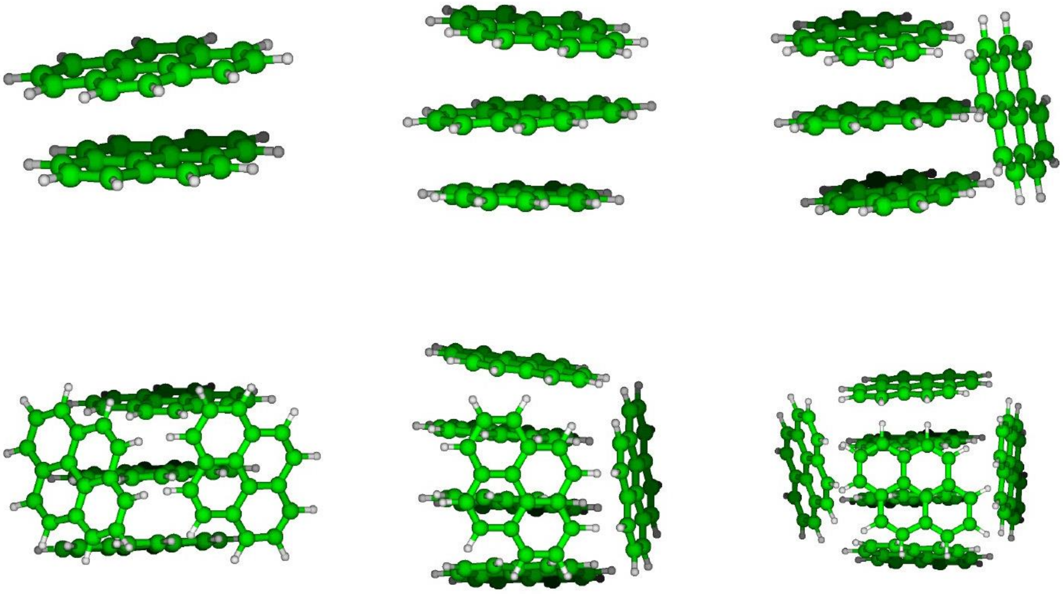

Figure 1: Most stable structures obtained for cationic pyrene clusters

Acknowledgments: NanoCosmos ERC, ANR GASPARIM

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We-II-1

Irradiation Driven Multiscale Dynamics of MesoBioNano Systems

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MesoBioNano (MBN) Explorer [1] is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics developed by MBN Research Center. It has many unique features and a wide range of applications in Physics, Chemistry, Biology, Materials Science, and Industries. A broad variety of algorithms and interatomic potentials implemented in the program allows simulations of structure and dynamics of a very broad range of Meso-Bio-Nano systems with the sizes from the atomic up to the mesoscopic scales, see [2] and references therein. MesoBioNano (MBN) Studio is a special multi-task software toolkit with graphical user interface developed for MBN Explorer [3] to facilitate setting up and starting MBN Explorer calculations, monitoring their progress, examining and analysing the calculation results.

The talk will give an overview of the main features of the packages, will highlight a number of current challenging research areas and recent case studies based on the utilisation of irradiation driven molecular dynamics (IDMD) [3-6]. IDMD is a powerful novel multiscale computational technique implemented uniquely in MBN Explorer enabling efficient computational studies of a broad range of collision and irradiation driven processes involving numerous MesoBioNano systems.

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We-II-2

The Value of K-matrix Theory for All Systems Held Together by Coulombic Forces

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Wigner's theory of scattering is of course well-known to all physicists. It is extremely general and describes scattering as well as half-scattering phenomena for a very wide range of targets. It is not even necessary, as Wigner himself stressed, to solve the Schrödinger equation in order to establish the validity of his scattering theory. The only requirement is the existence of a Schrödinger type equation with the boundary conditions usually applied in Quantum Mechanics. Wigner's theory originated in Nuclear Physics, but can be applied to any system and any type of force. It is even used in solid state physics. In particular, it is applicable to clusters and to large molecules. In Atomic Physics, use is often made of Multichannel Quantum Defect Theory (MQDT) which seems superficially to be a different and specific theory because it is usually derived by solving the Schrödinger equation asymptotically and phase shifting the regular from the irregular solutions. However, it can be proved that MQDT is in fact only a special application derived much more directly by a replacement in Wigner's theory. It is important to recognise this in the interest of the unity of physics. MQDT only seems different because of a specific property of the coulomb field which also allows the K scattering matrix (directly related to Wigner's S matrix) to be inverted analytically. The conceptual framework of the K matrix has the advantage that it allows the meromorphic pole structure of scattering resonances to be analysed exactly. This leads to a variety of new phenomena (now observed for atoms) which cannot be typefied numerically but also emerge in numerical calculations. These effects of scattering poles are not limited to atoms. They apply to any system held together by coulombic forces and can of course be followed through for clusters and perhaps even larger systems. Wigner's theory provides a unifying framework which extends to all scattering problems. The only issue which, in practice, arises differently for calculations involving long range forces is the manner of definition of the Wigner sphere since a typical scattering length only occurs for short range forces.

On the Inclusion of Dissipative Effects 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 mean 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. An 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 archetypal Time Dependent LDA or Time Dependent Hartree Fock (TDHF) approaches. We have explored a set of dissipative theories starting from the most sophisticated Stochastic TDHF approach which describes dynamics via an ensemble of mean fields [4,5,6]. We have also developed an averaged version thereof (Average STDHF, ASTDHF) which opens the door to applications in realistic systems [7]. Finally, the latter, which corresponds to solving a quantum Boltzmann equation, can be simplified to a quantum Relaxation Time Ansatz (RTA) providing an approximate quantum kinetic treatment [8]. 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 because of the computational cost. We have explored it in simple molecular systems and been able to analyse its capabilities in detail [9]. Finally, ASTDHF is currently being implemented in a realistic full 3D package (already including RTA) open to the scientific community [10].

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Th-I-1

Interactions of Gas-phase Biomolecular Ions with Fast Ions and with Soft X-ray Photons

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By combining mass spectrometric techniques such as electrospray ionization and radiofrequency ion manipulation with beamlines for high energy photons or fast ions, it is now possible to study radiation action on a virtually unlimited range of biologically relevant molecular ions in the gas phase. In living organisms, DNA occurs in de-protonated form which is why our studies focus on ionization and fragmentation of oligonucleotide anions. Such studies are experimentally challenging, because fragmentation competes with electron detachment. Furthermore, not only negatively charged product ions are formed, but also cations and neutrals.

As an example, we have focused on deprotonated telomeric DNA, i.e. oligonucleotides based on the sequence dTTAGGG. Telomeric DNA is particularly relevant in the context of radiation action, because of the important role telomers play in carcinogenesis. In agreement with theoretical predictions [1], we find strong indications that soft X-ray induced holes migrate towards the GGG part of telomer-containing oligos where they eventually induce strand breakage.

Besides its particular sequence causing the hole-trapping features, telomeric DNA is known for its ability to fold into non-canonical secondary structures known as G-quadruplexes (G4s) formed due to Hoogsteen hydrogen bonding between G moieties within a single strand. G4s play an important role in regulation of transcription and in genome stability and are of great potential relevance for cancer therapy [2,3]. We have studied unimolecular G4s formed from the $d(TTAGGG)_4$ oligonucleotides but also tetramolecular model systems, self-assembled e.g. from dTGGGGT strands. Interaction of XUV photons, soft X-rays and MeV ions (at Bragg peak energies) are all subject to single or multiple electron detachment as a dominant channel. For soft X-ray absorption, positive fragments (mostly from glycosidic bond cleavage) are only observed for the case of relatively small oligonucleotides such as dTTAGGG. In G4s, fragmentation is almost entirely quenched.

MeV carbon ions on the other hand, also lead to formation of small positive fragments when colliding G4s and also with duplex DNA. This is in line with the notion that ions can induce complex DNA damage, such as clustered lesions.

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Th-I-2

Gold Nanoparticles as a Radiosensitiser for Proton and Carbon Ion Irradiation

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The use of nanoparticles as radiosensitizers has been studied widely for enhancing tumor cell killing in radiation therapy. While most studies have focused on sensitization for irradiation by photons, there are opportunities for additional applications to charged particle radiation as hadron therapy continues to expand. At East Carolina University, we are conducting experimental and computational studies of gold nanoparticles as a radiosensitizer for charged particle radiation. Results are presented for cell survival and radiation damage for *in-vitro* irradiation by protons of malignant prostate and breast epithelial cells treated with gold nanoparticles in an energy range approaching the Bragg peak. These results are intended to serve as benchmark data as interest expands for using a wide range of materials as radiosensitizers in hadron therapy; comparison to our previous results for proton irradiation of nonmalignant and cancer cells treated with cerium oxide nanoparticles will be presented.

In addition, we are expanding current Monte Carlo track structure simulation models to include secondary electron production from gold surfaces. To help guide the models, we have measured absolute doubly differential electron emission yields from gold surfaces induced by fast proton and carbon ion impact; these measurements include electron emission from both clean and hydrated gold surfaces, as well as from nanostructured gold. These recent data are compared to our previous measurements of electron emission from amorphous solid water [1], and the experimental results are compared to electron transport simulations using the PARTRAC track structure simulation code.

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Th-I-3

Collision Induced Dissociation and Collision Cross Sections of Gold Nanoclusters: New Tools for Structural Characterization?

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Thiolate-protected metal nanoclusters have highly size- and structure-dependent physicochemical properties and are a promising class of nanomaterials [1]. As a consequence, for the rationalization of their synthesis and for the design of new clusters with tailored properties, a precise characterization of their composition and structure at the atomic level is required.

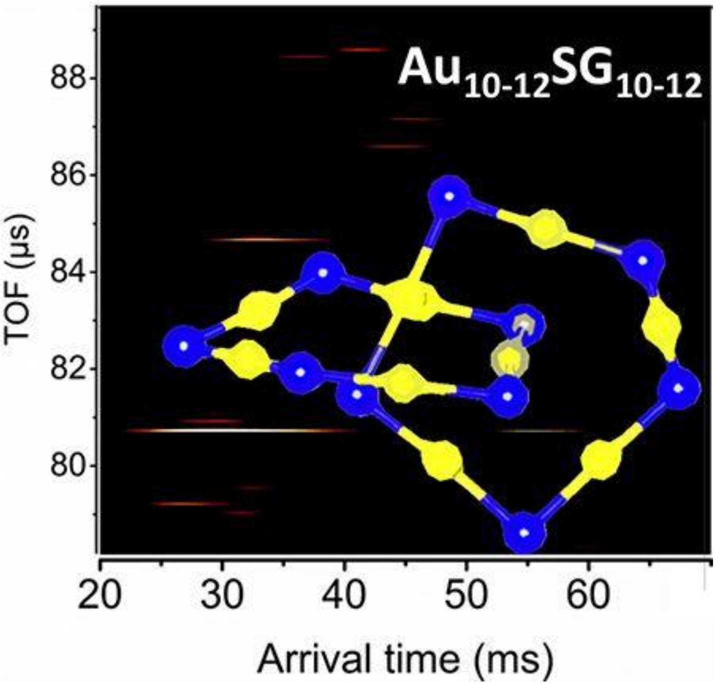

Figure 1: IM-MS map showing time of flight (y axis) versus arrival drift time (x axis) for the analysis of Au10-12(SG)10-12. Inset: catenane structure of Au10SG10.

In this lecture, I will compare liquid and gas phase size characterization methods for selected glutathione- (SG-) protected gold clusters (namely $Au_{15}(SG)_{13}$, $Au_{18}(SG)_{14}$, and $Au_{25}(SG)_{18}$). I will also investigate the relative stability of the gas-phase multiply deprotonated $Au_{25}(MBA)_{18}$ nanoclusters by collision-induced dissociation (with three isomers of mercaptobenzoic acids (*p*/*m*/*o*-MBA) as capping ligands) [2]. This allows to evaluate the possible isomeric effect on the Au–S interfacial bond stress. Finally, I will report recent tandem-ion-mobility-spectrometry (IMS) and mass spectrometry (MS) studies to monitor the diversity of the clusters in terms of composition and structure, as well as their stability [3-5]. Also IMS-resolved high-resolution MS measurements will be used to determine how the charge on the cluster is shared by the metal core and the ligands.

Th-I-3

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Th-I-4

Computational Studies of Collision-induced Fragmentation of Molecular Systems

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Irradiation- and collision-induced fragmentation studies provide information about geometry, electronic properties and interactions between structural units of various molecular systems. Such knowledge brings insights into irradiation-driven chemistry (IDC) of molecular systems which is exploited in different technological applications. For instance, IDC plays an important role in modern radiotherapies such as ion-beam cancer therapy [1] or in the formation and controllable growth of metal nanostructures under the exposure to focused electron or ion beams [2]. An accurate atomistic-level simulation of IDC requires reliable models of molecular fragmentation which can be verified against mass spectrometry experiments.

In this talk we will present a recently developed model for molecular fragmentation after energy deposition [3] which can be used in Irradiation-Driven Molecular Dynamics (IDMD) [4] simulations for studying IDC in complex molecular systems. This approach is a unique feature of the MBN Explorer package [5], which allows for modeling covalent bond dissociation events and further reactivity on the time and spatial scales exceeding by far those accessible by rigorous quantum-mechanical methods.

As an illustrative case study we have analyzed fragmentation of a tungsten hexacarbonyl, $W(CO)_6$, molecule, which belongs to a popular class of precursors for focused electron beam induced deposition (FEBID) as well as other nanofabrication techniques. We demonstrate that the quantitatively correct fragmentation picture including different fragmentation channels is reproduced well by means of classical MD simulations with reactive force fields [6].

The fragmentation model developed has a clear physical explanation and describes the different stages of electron-induced fragmentation of a molecular target, namely a localized energy deposition into a specific covalent bond and the redistribution of deposited energy among all bonds of the molecule. These situations represent limiting cases of the possible pathways for energy redistribution in a molecule, which involve the excitation to specific antibonding electronic orbitals or the energy transfer to vibrational modes of the molecule. Being a general physical model, this approach can be utilized to study radiation-induced fragmentation of other FEBID precursors as well as biomolecular systems whose fragmentation pathways are of great relevance for radiotherapy applications.

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Th-II-1

Studying Nascent Proton-Driven Radiation Chemistry in H_2O in Real Time Using Laser-based Sources

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Beams of energetic ions are finding application in multiple cutting edge technologies ranging from hadrontherapy to semiconductor device manufacture/metrology. To date, however, ion interactions in matter have been dealt with in a manner similar to those of electrons/photons, with attention primarily being paid to the energy, E, lost over path length, dx, giving the stopping power $S(E) = -dE/dx$. The obvious distinction is of course that ion stopping in matter exhibits a Bragg peak. In both scenarios the expected cell death or material damage are then generally extrapolated from empirical studies of dose deposition.

For ions, however, it is not immediately clear that this is the correct approach as it masks a critical phase of the interaction. When ions are incident on matter they generate dense tracks of ionisation that rapidly evolve. Exactly how this evolution, which occurs on femtosecond and picosecond timescales, determines the nascent radiation chemistry is still largely unknown.

Recently we have demonstrated that laser driven ion accelerators can provide an ultrafast tool for studying this inherently multiscale regime with temporal resolution < 0.5 ps [1,2]. Here we present novel results that show a) that this ultrafast evolution indeed plays a dominant role by extending our earlier results in SiO_2 and b) leads to a marked difference in the solvation dynamics for electrons generated due to the passage of fast electrons/X-rays and protons (>10 MeV) in water. We discuss the potential role of nano-cavitation during ion radiolysis in H_2O and how this may play a significant role in the physical-chemical stage emerging in the immediate aftermath of the interaction.

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Th-II-2

Accessing Elusive Molecular Species by Combining Helium Droplets with IR Spectroscopy

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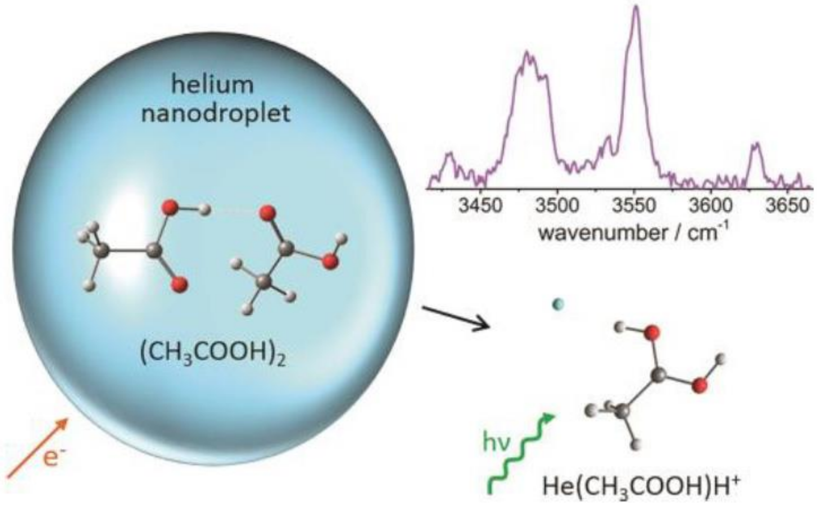
This presentation will describe recent work on the infrared spectroscopy of molecules and clusters in helium nanodroplets. It will combine an overview of the capabilities of the technique with some specific examples from recent work in our lab, including (1) the investigation of metastable structures of neutral hydrogen-bonded clusters1,2 and (2) the use of helium nanodroplets to create helium-tagged ions for IR photodissociation spectroscopy.

As well as their intrinsic interest as local minima on complex potential energy surfaces, the neutral dimers can act as precursors for the production of helium-tagged molecular ions and we will show how this technique is starting to be applied in our laboratory. One important example is protonated acetic acid, whose IR spectrum has been recorded for the first time via this technique (see below).



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Th-II-3

Multifragmentation of Ar Clusters by Protons and Heavier Ions as a Way to Observe Ion-Induced Shock Waves

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The possibility of multifragmentation of Ar clusters by incident protons is assessed [1] using the multiscale approach to radiation damage with ions [2-3]. First, the characteristics of proton propagation in liquid Ar, such as linear energy transfer, secondary electron energy spectrum, and the radial range of energy deposition by secondary electrons, are calculated and the shock wave prediction is tested theoretically. It is shown that liquid Ar only quantitatively different from liquid water, and all predictions of [4] regarding ion-induced shock waves remain valid.

Second, the shock wave pressure is compared to the surface tension pressure at the surface of Ar clusters and the condition for cluster multifragmentation as in [5] are explored. Then, the multifragmentation of Ar droplets is studied using classical molecular dynamics simulations. The dynamics of irradiated droplets is observed as well as their survival or fragmentation. The studies are done at different values of impact parameter of ions with respect to spherical droplets. The mass distribution of Ar droplets after irradiation is obtained. This distribution is deemed to be observable experimentally.

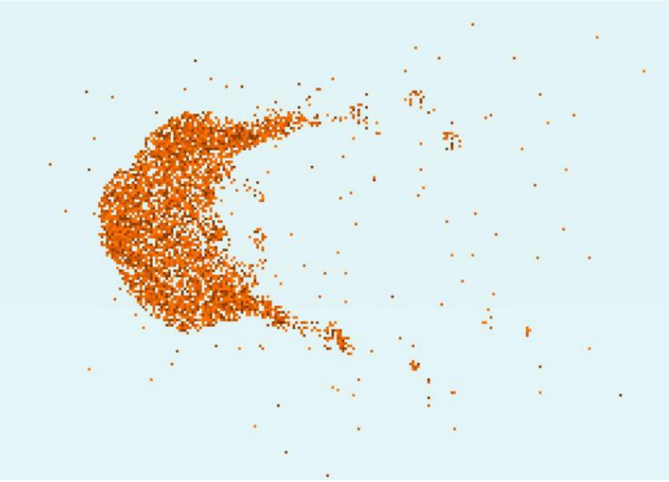

Figure 1: A snapshot of simulation of fragmentation of a 10-nm-radius Ar cluster hit by a 100-keV proton with impact parameter of 7 nm 80 ps after the traverse. The proton's path is perpendicular to the page plane.

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Th-III-1

Electron and Photon Induced Chemistry in Molecular Clusters

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Molecular clusters are prevalent in many natural and industrial environments both terrestrially and in the atmosphere of other (exo)planets and their moons (e.g. in the haze of Titan Saturn’s largest moon). Clusters may be in the gas phase accreting to form liquid drops or aerosols or may be formed in the condensed phase as part of amorphous ices. When such clusters are irradiated for example by UV light in the atmosphere or by electrons in industrial plasmas they may initiate a new type of chemistry between that of simple gas phase unimolecular chemistry and condensed phase (bulk) chemistry leading to new molecular dissociation pathways and chemical reactions that may be intra or inter cluster in nature. In this talk I will provide some examples of such cluster chemistry and provide an overview of our knowledge of the dynamics and reactions that may be induced by UV and electron irradiation of clusters in gaseous and condensed phase and how it influences the local environment.

Examples will be given in the Earth’s tropo- and stratospheres, Titan’s rich organic haze and in several industrial processes including plasma processing and the new nanofabrication method of Focused Electron Beam Induced Processing (FEBIP). The important role of water in creating ‘solvated’ clusters will be emphasized and the creation of OH radicals and their subsequent chemical reactivity discussed.

The talk will highlight the need for more experimental and theoretical work to determine the structure, dissociation dynamics and chemistry induced in such clusters and discuss progress in developing new methodologies for advancing such studies. The need for a coordinated research programme will be emphasized.

Th-III-2

Nanoparticle Beam Deposition: A Novel Route to the Solvent-Free Creation of Heterogeneous Catalysts

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Size-selected nanoparticles (atomic clusters), deposited onto supports from the beam in the absence of solvents, represent a new class of model systems for catalysis research and possibly small-scale manufacturing of selective catalysts. To translate these novel and well-controlled systems into practical use, two major challenges have to be addressed.

(1) Very rarely have the actual structures of clusters been obtained from direct experimental measurements, so the metrology of these new material systems has to improve. The availability of aberration-corrected HAADF STEM is transforming our approach to this structure challenge [1,2]. I will address the atomic structures of size-selected Au clusters, deposited onto standard carbon TEM supports from a mass-selected cluster beam source. Specific examples considered are the “magic number clusters” Au_{20}, Au_{55}, Au_{309}, Au_{561}, and Au_{923}. The results expose, for example, the metastability of frequently observed structures, the nature of equilibrium amongst competing isomers, and the cluster surface and core melting points as a function of size. The cluster beam approach is applicable to more complex nanoparticles too, such as oxides and sulphides [3].

(2) A second major challenge is scale-up, needed to enable the beautiful physics and chemistry of clusters to be exploited in applications, notably catalysis [4]. Compared with the (powerful) colloidal route, the nanocluster beam approach [5] involves no solvents and no ligands, while particles can be size selected by a mass filter, and alloys with challenging combinations of metals can readily be produced. However, the cluster approach has been held back by extremely low rates of particle production, only 1 microgram per hour, sufficient for surface science studies but well below what is desirable even for research-level realistic reaction studies. In an effort to address this scale-up challenge, I will discuss the development of a new kind of nanoparticle source, the “Matrix Assembly Cluster Source” (MACS) [4-6]. The results suggest cluster beam yields of grams per hour may ultimately be feasible; 10 mg scale has been demonstrated. Some practical applications [5,7,8] in heterogeneous catalysis (both gas and liquid phases), as well as electrocatalysis, will be presented, showing attractive activities and especially selectivities.

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Th-III-3

Functional 2D Nanomaterials and Devices Made by Electron, Ion and EUV Induced Processes

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Carbon Nanomembranes (CNMs) are extremely thin (~1nm), functional two-dimensional (2D) layers or sheets with tailored physical, chemical or biological function [1]. Their fabrication scheme utilizes a sequence of molecular monolayer assembly on a solid surface and radiation (electron, ion or EUV) induced cross-linking in two dimensions. The cross-linked monolayer is then released from the surface, forming a self-supporting nanomembrane with properties that are determined by properties of the precursor molecules and its monolayer.

CNMs can be engineered with a controlled thickness, elasticity and surface functionalization. Helium ion lithography can be used for the fabrication of well-defined nanopores in CNMs [2]. Here, I will present two recent applications of functional CNMs: (i) All Carbon Capacitors [3] and (ii) water purification membranes [4]. I will present functional tests that determine the dielectric properties of and the water permeation through CNMs. Electron spectroscopy, atomic force and helium ion microscopies are utilized to investigate the structure and composition of CNMs.

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Th-III-4

Joint Monte Carlo and Molecular Dynamics Simulation of Electron Beam-Induced Chemistry on Surfaces

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Irradiation-driven chemistry (IDC) on surfaces plays an important role in electron beam-based techniques for the fabrication of nanostructures such as Focused Electron Beam Induced Deposition (FEBID) [1]. In FEBID, organometallic molecules are deposited on a substrate and fragmented by radiation to release their metallic atoms and form nanostructures. IDC on surfaces is a complex problem involving many interlinked phenomena, including the interaction of the beam with the substrate (production of secondary electrons and their multiple scattering and ejection), and the adsorption, desorption and diffusion of the molecules on the substrate. Primary and secondary electrons interact with the molecules, producing their fragmentation and chemical reactions.

The complexity of the problem has limited so far the amount of detail which can be achieved by theoretical models, hindering their predictive power. For the first time the atomistic simulation of the entire FEBID process has been performed in [2]. This was achieved by means of the newly developed simulation technique of irradiation driven molecular dynamics (IDMD) [2]. This methodology makes use of a reactive force field [3] embedding random, local, fast quantum transformations (e.g. rupture of chemical bonds induced in a molecular system by its irradiation and subsequent formation of new bonds) into the classical molecular dynamics (MD) framework. The IDMD was implemented in the software package MBN Explorer [4]. The visualization and analysis of the entire set of simulated processes behind FEBID were performed by means of a special multi-task software toolkit with graphical user interface called MBN Studio [5]. In this contribution we report on accounting for the realistic irradiation conditions in IDMD simulations of FEBID. This was achieved through Monte Carlo (MC) simulations of the propagation and interaction of primary and secondary electrons in the substrate and with the precursor molecules performed with the SEED code [6, 7]. The MC simulations employ the realistic cross sections for the interaction of electrons with condensed-phase targets [6, 8]. Illustrative examples of the capabilities of the MC/IDMD approach will be given in the context of the FEBID process.

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Fr-I-1

Track-Structure Simulations in Nanometer Geometries

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Track structure simulations are used to characterize spatial distributions of energy depositions in the early physical and chemical stages of radiation action with matter. These Monte Carlo (MC) simulations are designed for a 3-dimensional infinite transport in a homogeneous medium (*bulk* material) and follow all primary particles as well as all produced secondary particles from starting or ejection energy down to total stopping. Radiation transport through interfaces, i.e., between two different materials require radiation equilibrium. Single events within the tracks are considered independent. Therefore, if the sampled mean free path to the next interaction would cross a border, the transport will be stopped at the border, and continued with a new, independently sampled mean free path in the new material.

Nano particles and other nanometer sized geometries appear more frequently in a variety of biomedical applications and need to be considered appropriately in radiation transport simulations. New materials like gold or gadolinium are used, and density scaling may not work. Nano sized structures may differ from *bulk* material, surfaces may have to be considered. This project investigates proton and electron transport within micro- and nanometer geometries using the track structure code PARTRAC. New interaction cross sections and a transport model for gold are under development. Radiation transport is analyzed with respect to geometry and (non-) equilibrium effects. Radiation transport is simulated in standard geometries with different length scales, including interfaces and surfaces and other non-equilibrium scenarios. Simulation results are analyzed using micro-dosimetry and nano-dosimetry concepts like electron emission spectra, radial energy distributions and ionization cluster size distributions. Results are compared with theoretical expectations and experimental results.

Fr-I-2

Matter (Ion) and Antimatter (Positron) Collisions with Fullerene Nanomolecules

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Response of fullerenes to matter/antimatter-type charged particles can probe processes not accessible by photons. For instances, while bare ion collisions can trigger plasmonic ionizations, positron impacts can transiently form exotic electron-positron binaries, the positroniums (Ps). In this presentation, I will discuss our recent theoretical studies based on these spectroscopic processes applied to fullerene molecules.

The structure of C_{60} is described by the local-density approximation (LDA) with the core of C^{4+} ions modeled as a spherical jellium [1]. For the ion collision, a time dependent LDA variant, TDLDA, [1] is utilized to capture multipolar plasmon modes while describing the collision itself by the plane-wave Born approximation. The positron impact, leading to the Ps formation, is treated by the continuum distorted-wave-final-state approximation [2].

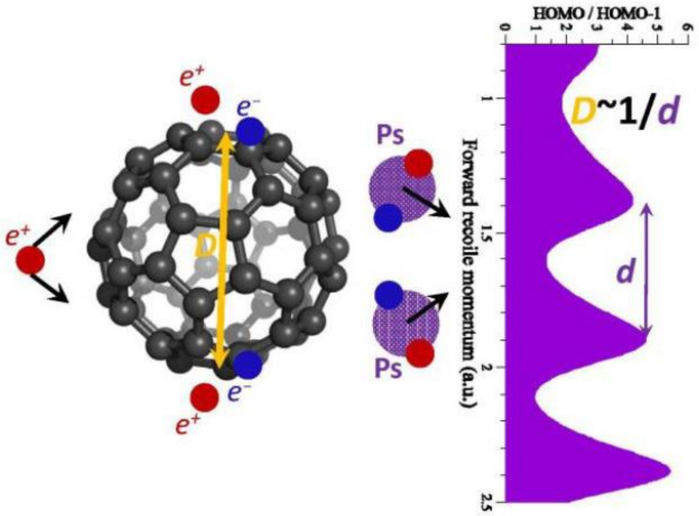

Figure 1: Schematic of a C_{60} diffractor in Ps formation. Resonances in the ratio of cross sections of HOMO and HOMO-1 captures are presented.

Results access various multipole, including even the monopole, plasmon resonances in the ion-impact emissions and reveal diffractions as a function of the recoil momentum in the Ps formation spectra (Figure 1). The findings spotlight on novel impact-spectroscopies with gas phase nanoparticles. The research is supported by the US National Science Foundation.

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Fr-I-3

Non-statistical Fragmentation of C_{60} and the Formation of Endohedral Defect Fullerenes

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Non-statistical fragmentation (i.e. prompt single-atom knockout) of fullerenes following collisions with energetic H and He atoms in supernova shocks is considered a key destruction mechanism for these and other large molecules in space [1]. We have investigated this process through laboratory experiments and classical Molecular Dynamics (MD) simulations of C_{60}-+He collisions at center-of-mass energies of 20-80 eV. As the electron affinity of C_{60} is much lower than any of its dissociation energies, collisions depositing enough energy to induce statistical unimolecular dissociation most likely lead to electron loss and thus do not contribute to the measured negative ion product mass spectrum, eliminating the major source of background.

Non-statistical fragmentation is observed directly by detecting C_{59}^-, see Figure 1. We observe for the first time the endohedral defect fullerene complex with an odd number of carbon atoms: $He@C_{59}^-$. Secondary decay products of these ions, C_{58}^- and $He@C_{58}^-$, are also observed. We measure the threshold center-of-mass energy for knocking out a single carbon atom from C_{60} in collisions with He. Combining this with our MD simulations, we determine a semi-empirical value for the (projectile-independent) threshold displacement energy, the minimum energy needed to remove a single carbon atom from the C_{60} cage [2]. Our value, 24.1(5) eV, is much higher than generally assumed previously for fullerenes (around 15 eV), and is similar to that determined for graphene and Polycyclic Aromatic Hydrocarbons [3].

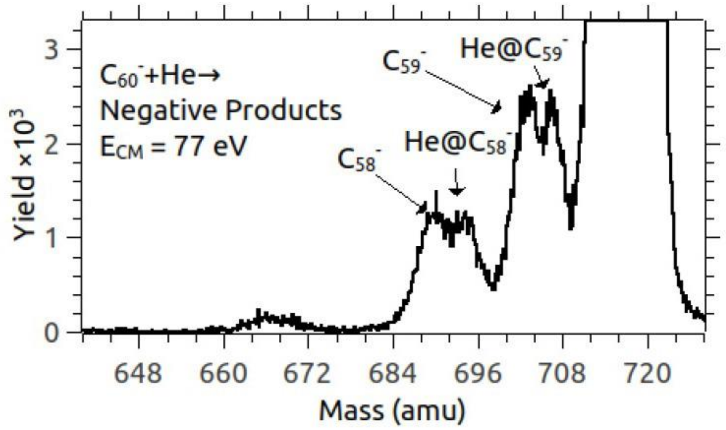

Figure 1: Negatively charged products of C_{60}^-+He/D_2 collisions.

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Fr-I-4

Energetic Processing of Hydrocarbons Molecular Species by Ionizing Radiation: Towards the Formation of Cyclic Species

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Recently, Cassini-Huygens mission brought interesting results concerning one of Saturn's biggest satellites, Titan. In fact, it has been shown that this moon's typical orange-brownish haze layers could be due to the presence of aerosols. These aerosols are essential for Titan's climate, radiation balance and atmosphere chemistry. The formation of such aerosols is a complex process ranging from the molecular scale to large particle scale. Polycyclic Aromatic Hydrocarbons (PAHs) have been identified by Cassini's spectrometers. PAH and their clusters are important components in terrestrial soot formation and their presence in Titan's atmosphere can be considered as a nucleation agent, which triggers aerosol formation in the low temperature atmosphere. However, since it is mainly composed of nitrogen, methane and a small amount of more complex hydrocarbons, understanding the way such PAHs are formed is mandatory [1].

In order to understand the formation process of larger particles, we have studied collisions of low energy ions with loosely bound clusters of molecules. We aim to analyze either the fragmentation processes - which occur due to the transfer of energy and charge - and on the other hand, the complementary processes which lead to molecular growth and the formation of new, larger, covalently bound molecules. These processes are based on the energy transfer into the heavy particle system (nuclei). In the case of ion collisions, this can take place either by electronic excitation or by the direct knockout of an atom from the molecule. In the first case, the process ends up in longer time scale via coupling into vibrational motion degrees of freedom, while in the latter we obtain a prompt (fs) removal of atoms during the ion-molecule collision. By the knockout of an atom, highly reactive radicals and molecular species are formed which on very short time scales (≤ ps) react with their neighbor molecules in the cluster. When several atoms are kicked out along the ion trajectory in the cluster, large covalently bound systems can be formed.

We present results on cluster systems containing linear chain molecules like butane, butadiene and acetylene (non-aromatic molecules). We will discuss the formation of ring structures and the path to aromatic molecules. The irradiation of hydrocarbons clusters using different radiation sources (electrons, ions and UV photons) allows to determine the balance between ionization induced reactivity and collision induced one. The latter is the typical collision occurring in Titan's atmosphere involving slow and heavy ions (few keV O cations). It has been shown that this triggers reactivity, as observed in C_{60} clusters [2] or PAH ones [3].

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Fr-I-5

Ion Collisions with Biological Targets. The Early Stages of Ion Beam Cancer Therapy

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Ion beam cancer therapy (IBCT) has gained popularity as a non-invasive and precise alternative compared to the more commonly used photon therapy [1,2]. The understanding of IBCT today mainly relies on quantitatively obtained results from medicinal research, but more and more theoretical models such as the Multi Scale Approach [3-6] are being developed to increase the understanding of the treatment method. Due to the characteristic dose deposition of charged ions, most studies have focused on the effects arising around the Bragg peak where most of the energy is deposited.

This work aims to investigate the first events occurring upon collision of a highly charged ion with several biological targets by employing time-dependent density functional theory (TDDFT). The simulations specifically allow estimating collision cross sections, velocity distributions of the target atoms and stopping powers for a charged ion. Results for the collisions of C^{4+} / single H_2O, C^{4+} / H_2O cluster, C^{4+} / CYT+GUA pair and C^{4+} / phospholipid will be discussed. Comparison of the TDDDFT simulations with theoretical estimates will be presented and it will be revealed that the obtained results agree well with the results obtained using the PASS code [7] within the limitations of the modified Bohr theory.

We will argue that the acquired statistics for secondary electron production and velocity distributions of the atomic species emerging from the C^{4+} / H_2O cluster collision and the C^{4+} / phospholipid collision close to the Bragg peak suggests that a significant amount of energy is transferred to the cell membrane through atomic and electronic collisions. The predicted perturbation of the cellular membrane is likely sufficient to induce a well-known shock wave behavior, which is expected for highly charged ions passing through a medium close to the Bragg peak [4].

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Fr-II-1

Transforming Redox Properties of Clusters Using Ligands to Create Super Dopants for Two-dimensional Semiconductors and to Synthesize Nano p- n-Junctions

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A promising direction in the research on clusters is to design nanomaterials with size selected clusters or the nanoparticles as the building blocks. Since the properties of clusters/nanoparticles change with size and composition, nano-assemblies offer the unique prospect of designing nanoscale materials with controlled properties. The presentation will focus on using ligands to transform the redox properties of a variety of clusters and their use as dopants to design novel semiconductors where the location of Fermi energy and n- and p- characteristics can be controlled. I will end my talk with a recent discovery where we have used ligands to induce intense electric fields and dipole moments in molecules of homo-atomic clusters. Such units have the characteristics of nano p- n- junctions.

Organic ligands that protect the surfaces of clusters and nanoparticles against reactions and control the rate of growth are generally considered to be inert passive coatings. I will demonstrate that the ligands can also strongly affect the redox properties of clusters. I will present our results of the effect of ligation on the ionization energy (I.E). of a variety of clusters including simple and noble metal clusters, Au_7, Au_{11}, $Au_{13}Cl_2$, Ag_{11}, and Al_7; an Al_4O_6 cluster corresponding to an insulator; $Ga_{12}N_{12}$, and $Zn_{12}O_{12}$ as representative of semiconductor clusters; Co_6, Pd_6, and Pd_7 as representative of transition metal clusters; and Mo_6Te_8 corresponding to the important metal-chalcogenide clusters recently synthesized by Roy and co-workers. For all cases, the ionization energy is reduced. In many cases, ligated clusters are transformed into super donors with ionization energies nearly half that of cesium atoms, and extremely low second and third ionization energies creating super donors that can donate multiple electrons. I will show that the reduction in ionization energy can be split into initial and final state effects. The initial state effect derives in part from the surface dipole, but primarily through the formation of bonding/antibonding orbitals that shifts the HOMO. The final state effect derives from the enhanced binding of the donor ligand to the charged cluster.

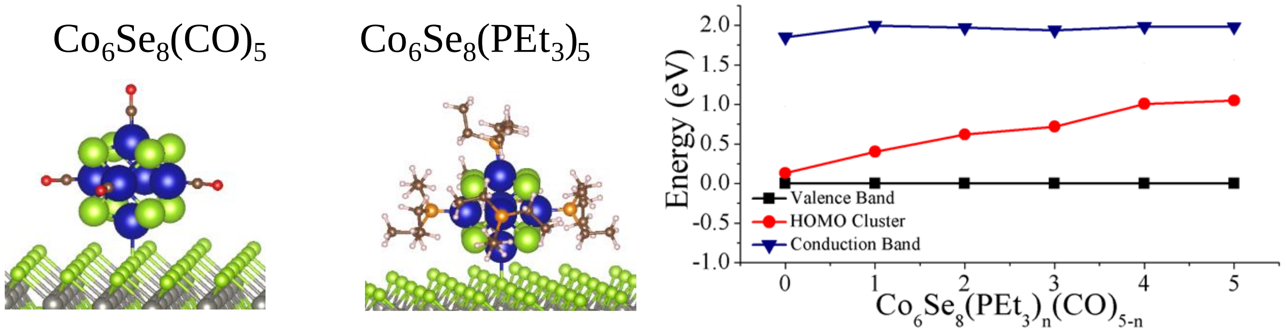

Figure 1. (Left) Structure of Co_6Se_8 clusters supported on WSe_2 with different ligands. (Right) Effect of ligand exchange on electronic structure

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The new donor and acceptor superatoms can be used to create doped semiconductors by using superatoms, as effective super-dopants for two-dimensional semiconducting films. Unlike conventional dopants that are embedded in the semiconductor, the superatom dopants act by using the two dimensional semiconductor as a solid state ligand. I will demonstrate this intriguing possibility by considering WSe_2 films that are transformed from a p-type to an n-type semiconductor when $Co_6Se_8(PEt_3)_6$ (PEt_3-tri-ethylphosphene) superatoms are supported on the surface. The theoretical findings complement recent experiments by Yu et. al. where WSe_2 films doped with $Co_6Se_8(PEt_3)_6$ indeed showed a change in behavior from p- to n-type. We further show that by continually replacing the PEt_3 ligands by CO ligands, one can control the chemical potential of the semiconductor and even introduce magnetic carriers by controlling the number of ligands, opening a pathway to superatom doped magnetic semiconductors.

The talk will highlight the properties of the new semiconductors and how one can use the binding energy of clusters to support as a tool to identify p- or n- type semiconductors.

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Fr-II-2

Tracing Radiation-Induced Reaction Products to Specific Neutral Isomer and Cluster Precursors

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Radiation induced processes in biomolecules have been investigated intensively recently, notably to better understand the fundamental processes that can initiate lesions in key macromolecules [1]. Our experiments apply UV multi-photon ionization (MPI) and electron collision methods to investigate unimolecular and intermolecular reactivity in the neutral and ionic excited states of gas-phase biomolecules and clusters. While studies of relatively small isolated biomolecules generally provide the clearest mechanistic interpretations, equivalent measurements on larger molecules and on clusters enable closer analogies to be drawn with macromolecules in biologically-realistic environments. However, increasing the size of a biomolecule generally increases the number of different structures in a gas phase experimental target, complicating interpretations. Similarly, distributions of different clusters within neutral beams can present a major challenge in analysing experimental results and drawing comparisons with theory.

Having previously studied molecules up to the scale of nucleobases and their clusters [e.g. 2-4], we have recently built a *laser-induced thermal desorption* system at the OU (based on Greenwood and co-workers' design [5]) in order to carry out experiments on gas-phase nucleoside targets without thermal decomposition. Our MPI results on uridine have provided new evidence for isomer-dependent neutral excited state dynamics, highlighting the importance of applying experimental methods to trace specific reaction products to specific neutral structures. This links to our on-going development of experiments at the OU to analyze electron interactions with molecules and clusters in Stark-deflected beams. As part of a wider update on this project, this talk will present results showing that Stark deflection can be used to trace protonated nitromethane and (nitromethane)CH_3^+ products to specific electron-irradiated neutral dimer configurations of nitromethane.

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Fr-II-3

Element Choice for Nanoparticle Radiosensitisers

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We have performed the first comparative survey of the radiosensitisation ability of solutions of 22 different element metal oxide nanoparticles, irradiated with 6 MV clinical X-rays.

We find large differences in the production of reactive oxygen species. Thus, V_2O_5 produces high levels of hydroxyl radicals, while Lanthanides are radioprotective with respect to hydroxyl radicals.

Differences are also seen in superoxide and singlet oxygen production. Finally, we examine the ability of these nanoparticles to produce DNA damage. Some nanoparticles produce single-strand DNA damage in the absence of X-rays, while the greatest radiation-specific damage is seen using CuO nanoparticles.

We propose that many of these metal oxides take part in catalytic reactions with metastable species in irradiated water to either promote or quench radical production.

These data will be of interest to researchers designing and optimising novel radiosensitisers and radioprotectants.

Fr-III-1

Atomic Cluster Experiments at SACLA, an XFEL in Japan

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The advent of x-ray free-electron laser has opened new pathways in the investigations of electronic and structural dynamics in any form of matter. One of the expected studies using XFEL is single-shot X-ray imaging based on “before destroy” concept. However, the target samples may be affected by ultrafast reactions occurring during XFEL pulse duration. In order to utilize XFEL for “before destroy” imaging, it is indispensable to understand what happens in the matter during irradiation of the XFEL pulse. The ultrafast reaction dynamics in an isolated atomic cluster of the nanometer size are not only fundamentally interesting but also important for this purpose.

In March 2012, SPring-8 Angstrom Compact free electron LAser (SACLA) started user operation in Japan [1]. We have investigated reaction dynamics in atomic clusters induced by intense (~50 $\mu J/\mu m^2$), ultrashort (~10 fs) XFEL pulses generated by SACLA. The results for electron spectroscopy on argon and xenon clusters, with help of theoretical calculations, illustrate that nanoplasma are formed by the XFEL pulse, in tens of fs, and continuous thermal emission from the plasma occurs in ps [2]. The experiment also confirmed x-ray induced origomer formation from rare-gas clusters [3]. XFEL pump-NIR probe experiments for xenon clusters at time resolution down to a few tens of femtoseconds revealed the birth of nanoplasma [4].

We have also studied morphology of Xe nanoclusters using single-shot X-ray imaging of based on “before destroy” concept, using both small-angle and wide-angle diffractions [5], and ultrafast reaction induced in a single nanocluster irradiated by the intense near-infrared laser pulse using the wide-angle diffraction as a probe [6]. The latest results will be shown and discussed.

I am grateful to coauthors of Refs. [2-6] for their invaluable contributions and to the support by XFEL strategy program by MEXT. five-star alliance and IMRAM program.

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Fr-III-2

Purification of XFEL Spectra

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Photo electron spectra taken by SASE X-ray free electron lasers are necessarily noisy and vary from shot to shot due to the fluctuating pulses generated by the SASE process. We have simulated such spectra by the partial coherence method. Using a fully connected feedforward artificial neural network we purify the spectra as if they were generated with a Fourier limited light pulse.

The underlying physical system is modeled by a class of random hamiltonians and therefore in principle applicable to a wide variety of problems.

We discuss first results for a system which is dominated for given parameters by non-linear two-photon absorption in the XUV, where we demonstrate that indeed, the noise free spectrum can be uncovered with good accuracy.

Fr-III-3

Gas-phase Proteins Studied at Advanced Light Sources

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Investigating the interaction of light with biologically relevant molecules has gained interest for a wide variety of research fields including photochemical reactions such as light harvesting as well as radiation damage in proteins and DNA related to cutting-edge cancer treatment techniques. However, in the condensed phase, disentangling direct and indirect radiation effects is often difficult. Electrospray ionization introduces biomolecular ions from solution into the gas phase, allowing for studies of molecular systems in a well-defined state.

The coupling of electrospray ionization sources with synchrotrons [1,2] and free-electron lasers [3] opens the way to the investigation of the electronic structure of biomolecular systems and of a fine description of their relaxation mechanisms in the VUV and soft X-ray energy range. The wide-ranging photon energy available at the synchrotrons enables systematic studies of ionization and dissociation as a function of the photon energy. Inner-shell excitations provide a localized site of energy deposition. The extremely high photon flux and fs pulse duration offered by free-electron lasers allow studying the molecular properties in intense fields. Furthermore, using the assets of free-electron lasers in a pump-probe scheme enables the study of the dynamics of charge migration and charge transfer within gas-phase biomolecules.

Results will be presented of mass-spectrometric experiments at advanced light sources with different gas-phase peptides, proteins [4] and related molecules.

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Sa-I-1

Recent Advances in the Theory of Electron Attachment to Molecules and Clusters

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Dissociative electron attachment (DEA) to polyatomic molecules is a complicated process involving couplings between electron and nuclear motion. Completely ab initio calculations are presently possible only for diatomics, and model approaches should be developed for more complex targets, particularly if nonlocal effects, leading to vibrational Feshbach resonances (VFR) and threshold cusps, are important [1-3]. In the last few years we have been working on several problems related to DEA to polyatomic molecules:

Extension of the nonlocal theory to two and more degrees of freedom. The properties of the Green’s operator describing the evolution of the resonant state play the crucial role in the nonlocal effects. Quantum-mechanical and semiclassical methods of its calculation have been developed. They can be incorporated in the equivalent resonant R-matrix theory which is more convenient for model calculations. The general theory, has been applied to the CF_3Cl compound.

Application of the effective range theory to description of VFRs and threshold cusps in polyatomics. This theory was applied recently to description of cusp structure in DEA to $Fe(CO)_5$ [4], the molecule important for the development of the Free-Electron-Beam Induced Deposition technique, and to a series of 5-membered heterocyclic rings [5].

Investigation of the role of the water cluster environment in DEA to polyatomics, particularly to biological-relevant molecules. We have found two effects in the N-H bond breaking in thymine due to electron impact, one leading to the enhancement of the DEA cross section due to the increased lifetime of the intermediate negative-ion state [6], and the other leading to the decrease of the yield of the anionic fragments due to the hydrogen bonding between the nucleobase and the solvent [7]. The hydrogen bond rapidly channels the kinetic energy away from the N−H, into the surrounding water molecules, and back into the nucleobase.

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Sa-I-2

Size-Selected Charged Helium Droplets

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Since the early 1990s, helium droplets have been utilized to study atoms, molecules and clusters at very low temperatures [1]. The most common way to produce helium droplets is by means of a supersonic expansion of pressurized and precooled helium through a small nozzle into vacuum [2]. The resulting, broad size distribution can be described well with a log-normal distribution. Doping neutral helium droplets with atoms or molecules is a statistical process which depends on the cross section of the interacting helium droplets and thus leads also to a considerable broad distribution depending on the experimental conditions.

In this contribution we introduce our experimental setup to investigate size distribution of positively and negatively charged helium droplets. In brief, helium droplets formed in a cluster source are ionized by an electron beam of defined energy and current. The formed positively and negatively charged helium droplets are analyzed according to their mass-to-charge ratio by means of an electrostatic analyzer. The selected helium droplets pass a second ionization chamber, where again an electron beam of defined energy and current can interact with the charged helium droplets. The resulting ions are analyzed by a second electrostatic analyzer before they are detected by a channeltron multiplier. We report our results on the size distribution of helium droplets in the range of 10^5 to 10^{10} helium atoms. We were able to assign high charge states both for positively and negatively charged helium droplets. Due to the second ionization chamber we could increase the charge state of helium droplets as well as neutralize them. We also find that fragmentation occurs via rather asymmetric Coulomb explosion and evaporation of helium atoms. We discuss our findings in the light of possible experimental investigations utilizing size selected, charged helium droplets.

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Sa-I-3

Effect of Cluster Environment on Electron- and Ion-Mediated Chemistry: From Atmospheric Chemistry to Nanocatalysis

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Clusters as flying nanoreactors enable investigation of reactions in aqueous environment and on active sites of a catalyst at a detailed molecular level. In the present talk, I will discuss two distinct topics. The first part focuses on the effect of hydration on the reaction between an electron and nitric acid. We probe the negative ion formation upon the interaction of free electrons with gas-phase HNO_3 and its clusters mixed with water [1-3]. The electron attachment to gaseous HNO_3 leads almost exclusively to NO_2 (>96%), which is the most exothermic channel. The addition of water to HNO_3 changes the DEA outcome dramatically, yielding predominantly NO_3^- containing clusters (57%). A series containing NO_2^- is observed with lower intensities (32%). Only traces of OH^- products are found (2%). In the cluster case, the initial driving force is the proton transfer to form the H_3O^+/NO_3^- ion pair where the attached electron recombines with the proton, yielding the hydrogen atom and NO_3^- [1-2]. In addition, the electron-induced chemistry exhibits strong electron energy dependence [3]. A different order of hydration, done by the preceding solvation of electrons via the formation of anionic water clusters prior to the reaction with HNO_3, changes the reaction to an exclusive formation of OH^- containing cluster products [2,4].

The second part is focused on the C–H bond activation of methane mediated by tantalum clusters. Small Ta cluster cations and their oxides mediate the dehydrogenation of methane and a concomitant elimination of hydrogen molecules [5]. The clusters exhibit a rich size- and composition-dependent chemistry in the activation of methane, which ranges from their complete inertness to the observation of potential catalytic cycles. In this talk, these peculiar reaction properties will be illustrated on selected examples.

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Sa-I-4

Soft X-ray Photofragmentation of Gas Phase Oligonucleotides

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In many cancer treatments, 5-halouracil (such as FU, BrU) is used to reduce radiation dose and accordingly ease side effects to patients. The reason is that, halouracils act as radiosensitizers which enhance the efficacy of ionizing radiation on tumor cells. The molecular mechanism of their action has been intensively studied [1,2] but is not yet fully understood.

Here we explore the potential of FU/BrU incorporated in gas-phase oligonucleotides for the investigation of X-ray induced charge and energy migration in these systems. In oligonucleotides of the type-d(FU/BrU-A_nG) (n=1-5), the F/Br atom acts as a soft X-ray chromophore whose K/L-shell can be selectively excited, leaving the 5'terminal of the molecule positively charged. Short A_n sequences are known to facility charge transport. G has the lowest oxidation potential of the nucleobases and is most likely carrying the photoinduced positive charge when migration is finished.

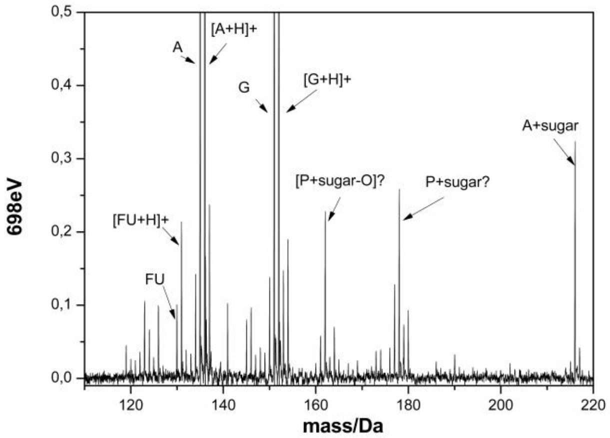

Figure 1: Photofragmentation patter of FUAG cations for the photon energy 698eV. P represents the phosphate group and O represents the oxygen atom.

In a first series of experiments, conducted at the 3rd generation synchrotron BESSY II (Berlin) and PETRA III (Hamburg), we have studied the ionization and fragmentation of FU/BrU containing oligonucleotides for photon energies around the C,N,O K-edges, P L-edge and F K-edges/Br L-edges.

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Sa-I-5

New Manifestations in Low-Energy Electron Scattering from the Actinide Atoms Pu, Cm, Bk and Lr

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In this investigation we have found the Regge-pole calculated electron elastic total cross sections (TCSs) for the Pu, Cm, Bk and Lr actinide atoms to be characterized generally by ground, metastable and excited negative ion formation; they also exhibit fullerene molecular behavior near threshold [1]. Additionally, a polarization-induced metastable TCS with a deep Ramsauer-Townsend (R-T) minimum at around 0.12 eV is identified in the Pu TCSs (see FIG. 1) as well as in those for Cm and Bk; it is absent in the TCSs of U and Np. However, in the TCSs for Lr this R-T minimum has flipped over to a shape resonance with the energy position of 0.025 eV close to threshold and the ground state binding energy (BE) of the formed during the collision Lr^- negative ion is large, viz. 3.88 eV compared to the ground state BEs of the Pu^-, Cm^- and Bk^- anions. These peculiar behaviors in the TCSs of these large actinide atoms are attributed to the size effects and orbital collapse, impacting significantly the polarization interaction in these atoms. Indeed, the rich resonance structure in the TCSs of Pu has led to the ambiguous determination of the electron affinity of Pu and the other actinide atoms as well.

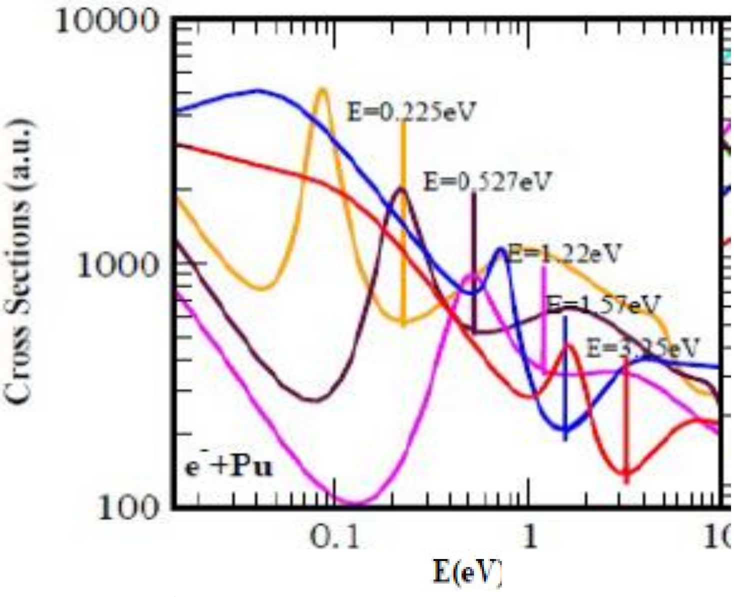

Figure 1: TCSs (a.u) for atomic Pu. The red, blue and pink curves represent TCSs for the ground and metastable states, respectively; the brown and the orange curves are for the excited states TCSs.

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Sa-II-1

Evaporation of Water Molecules from Excited Water Nanodroplets

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The evaporation of a water molecule occurs through the breaking of one or several hydrogen bonds. These hydrogen bonds are responsible for many remarkable features of water. At the macroscopic scale, water is known for its exceptional ability to thermalize a system, while at the microscopic level, a high-speed transfer of vibrational energy via hydrogen bonds is observed. What happens for only a small number of water molecules?

In the experiment carried out with the device DIAM at IPN Lyon, the relaxation of protonated water nanodroplets is observed after electronic excitation of one of its molecules [1-6]. The implementation of a velocity map-imaging (VMI) method associated with the Correlated Ion and Neutral Time-Of-Flight (COINTOF) technique allowed us to measure the velocity distribution [5] of molecules evaporated from mass- and energy-selected protonated water clusters [3,4]. The behavior of the measured velocity distributions shows that even for extremely small water nanodroplets, a complete energy redistribution before evaporation prevails and the velocity distributions of these events are close to those expected for macroscopic droplets from around ten water molecules. However, these measurements of the velocity distributions also feature a distinct high-velocity contribution corresponding to the evaporation of a molecule before complete redistribution of energy [1,5]. The measured velocity distributions for heavy water nanodroplets show a proportion of these non-ergodic events more important than for normal water. The measurements carried out with different target atoms show that the proportion of non-ergodic events decreases with decreasing the energy deposited in the droplet.

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Sa-II-2

Reactions Dynamics of Small Ionic Clusters

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A major focus of our research group is to obtain detailed insight into the atomistic dynamics of ion-molecule reactions [1,2]. An example are reactions of small anions reacting with alkyl halides, which may proceed along two competing reaction channels, nucleophilic substitution (S_N2) or base-induced elimination (E2). When adding solvent molecules to the reacting anion, effects of a microsolvation environment may be tested. Using crossed-beam velocity map imaging, we found that the addition of water to OH^- reactants strongly influences the reaction dynamics of S_N2 reactions [3,4]. Recently we have studied the differential scattering cross section for the isoelectronic anion F^- bound to water molecules and have compared the observed dynamical features [5].

A second research focus of our group is on understanding the properties and reactivity of interstellar molecular ions. Unsaturated carbon chain anions have been discovered in interstellar molecular clouds as the first negative molecular ions [6]. Crossed beam imaging experiments have allowed us to study different ion-molecule reactions that can form the interstellar negative ions C_nH^- by step-wise chain growth [7].

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Sa-II-3

Influence of Secondary Electrons on Biomolecular Damage in Water by Fast Heavy-ion Irradiation

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Study of the biomolecular damage induced by ionizing radiation has been of longstanding interest in radiation physics, chemistry, and biology. In this talk, we present our recent investigations on the effects of water environment on fast heavy-ion radiation damage of biomolecules in aqueous solution [1,2]. A fast heavy-ion penetrating through matter releases an electronic energy in a biomolecular system along its trajectory and then generates secondary electrons by ionization of the water medium. Based on this situation, we discuss the biomolecular damage induced by secondary electrons ejected from water molecules surrounding biomolecules.

The experiments were performed using a 2.0-MV tandem Pelletron accelerator at the Quantum Science and Engineering Center, Kyoto University. We used liquid microdroplet techniques developed by Majima et al. [3,4] to prepare liquid targets under high vacuum. Microdroplet targets of the amino acid glycine (Gly) solution with a concentration of 0.1 M were irradiated by carbon projectiles with energies of 0.4–8.0 MeV, which correspond to energies in the Bragg peak region in heavy-ion radiotherapy. Ion-induced reaction products emitted from the droplets were measured by time-of-flight secondary-ion mass spectrometry. This enables identification of dissociated ion species at the atomic level.

We investigated the formation of positive and negative Gly fragments, and the dependence of the yields of these fragments on the projectile energy. Observed Gly fragments are $CH_2NH_2^+$, $[Gly–H]^−$, $CN^−$, and $HCO_2^−$. The yield of each fragment exhibits different projectile-energy dependence for positive and negative fragments. Considering that biomolecular fragmentation may be caused by secondary electrons from water molecules, we compared the experiments with dependence of the calculated cross section for secondary electrons from liquid water on the projectile energy investigated here. We found that the formation process of positive fragment $CH_2NH_2^+$ originating from the C–C_α bond cleavage of Gly is related to molecular dissociation by high-energy electrons. In addition, the formation of negative Gly fragments may be caused by attachment of electrons from the low-energy part of the secondary electron distribution.

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Posters

PS-01

Gold nanoparticles: Interaction with DNA Molecules through Visible Light

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A long-standing goal in the development of cancer treatments is to use visible light in photodynamic therapy. Although in recent years, techniques and therapies have undergone many changes and enormous evolution, the development of new and more efficient cancer treatments remains one of the major challenges to the scientific community [1]. One of the emergent treatments is photothermal therapy in conjunction with nanoparticles [1]. Gold nanoparticles (AuNPs) have been brought to the forefront of medical research due to their optical characteristics (e.g. tunable surface plasmon resonance in the visible region) as well as their excellent biocompatibility [2,3]. The integration of AuNPs in cancer cells increases cell death by radiation and this has been attributed to two major processes local to the AuNPs: 1) sharp increases of the temperature and 2) enhanced production of water-derived free radicals [4]. These radicals react with nearby molecules in a very short time (half-life 17 s to 10^{-10} s), resulting in breakage of chemical bonds or oxidation of the affected molecules [5,6]. Though, the critical effect in the cells results from the formation of strand breaks in DNA [2,3]. However, the specific mechanisms responsible for AuNP-enhanced radiation damage to DNA and their relative importance are still not fully understood.

In this work, plasmid DNA in aqueous solutions were irradiated with 532 nm pulsed laser light for different periods of time (up to 150 minutes) in the presence and absence of AuNPs. The irradiation setup and method were developed by I. Bald and co-workers and are described in reference [3]. A selection of different techniques was applied to characterize DNA damage effects of AuNPs in the irradiated samples, most notably agarose gel electrophoresis (AGE), UV-Vis spectroscopy and fluorescence spectroscopy. AGE and fluorescence measurements following irradiation with and without free-radical inhibitors confirm that water-derived free radicals produced during the laser exposure are responsible for extensive cleavage of the DNA strands. Moreover, the free-radical driven damage is strongly enhanced in the presence of AuNPs. These findings support the hypothesis of the size dependency of AuNPs on laser-induced DNA damage. Further experiments are in progress to better understand the effect of the size distribution of AuNPs on DNA-radiosensitization and to assess the response of different types of DNA.

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PS-01

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PS-02

Dynamic Effects in the Dissociative Electron Attachment of Isolated Molecules and Clusters

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When a molecule absorbs an electron, a transient negative ion is formed, and one of several outcomes is possible. The electron can be simply ejected to leave the molecule in its ground or excited state (resonant electron scattering), the ion can be stabilised to give a long-lived anion (associative electron attachment), or the ion can dissociate by the cleavage of a covalent bond (dissociative electron attachment, DEA).

DEA is an important process, which occurs across a range of chemical systems, including plasmas, interstellar space and the Earth's atmosphere. Of particular interest in recent years has been the role of DEA in radiotherapy, where ionising radiation produces a cascade of low-energy electrons, which damage both cancerous and non-cancerous tissue.

I will present some of the recent findings from our lab, including measurements of the DEA of halopyrimidines, both as isolated molecules, and in small water clusters. For these experiments, a molecular beam of the target molecule was crossed with a beam of low-energy electrons and the product anions were recorded with a mass spectrometer. The identity of the product anions, their relative intensities and the electron energies which lead to their formation all provide important clues, which are used to understand the dynamics of the DEA process.

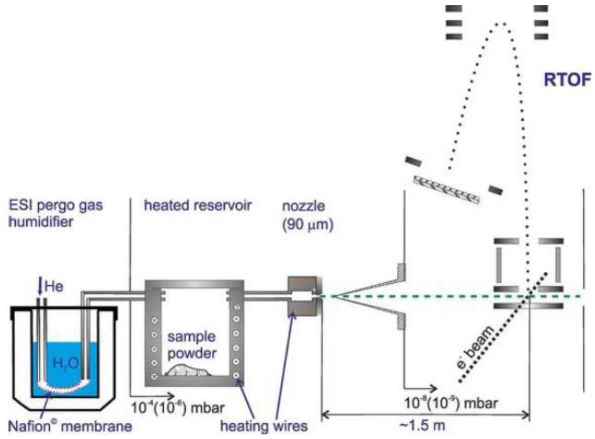

Figure 1: Schema of the experimental setup.

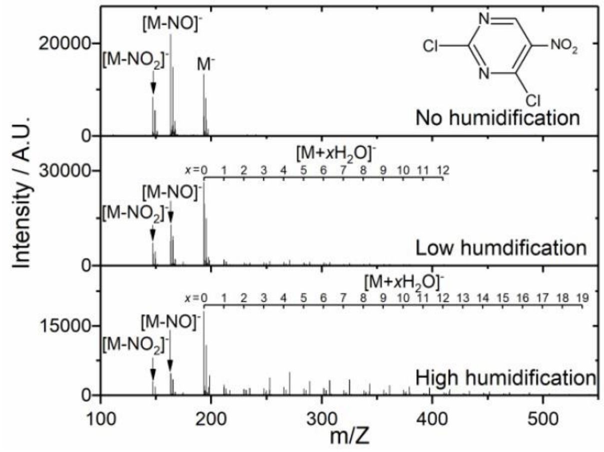

Figure 2: Cumulative negative ion mass spectra in the energy range from 0 to 14 eV for 2,4-dichloro-5-nitropyrimidine with: (top) no humidification; (middle) low humidification of; (bottom) high humidification of the molecular beam.

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PS-03

Electron Scattering Cross Section of Biomolecules

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The biological effectiveness of ionizing radiation is closely related to its track structure at the DNA level. The calculation of this track structure requires the knowledge of the interaction cross sections of DNA constituents for secondary electrons which are to a great extent responsible for radiation induced damages.

Total, differential elastic and doubly differential inelastic electron scattering cross sections of the building blocks of the DNA such as pyrimidine, tetrahydrofuran and trimethylphosphate were absolutely measured for primary electron energies *T* from 30 eV to 1.0 keV, at scattering angles from 15° to 135°. The energy of secondary electrons ranges from 4 eV to $(T\text{-}I)/2$, where *I* is the ionization potential of the respective molecule. As an example, Fig. 1 shows the doubly differential ionization cross sections of trimethylphosphate as function of the secondary electron energy *W* for different emission angles.

In addition to the measurement, electron scattering cross sections of several biomolecules pyrimidine were calculated by means of semiempirical and theoretical methods and compared to the experimental results.

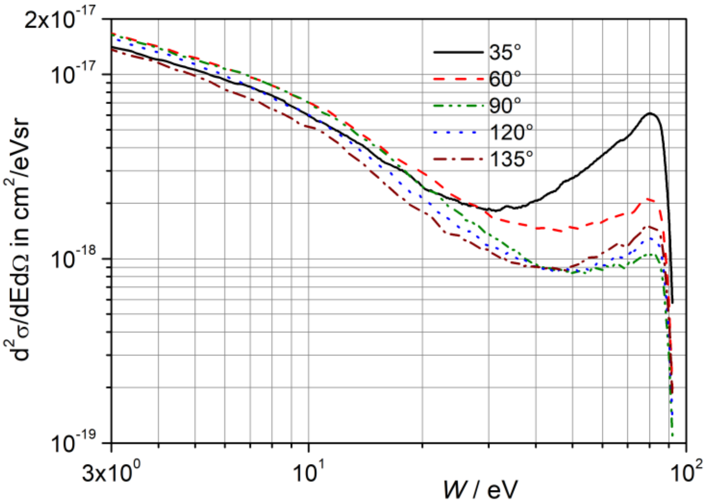

Figure 1: Doubly differential ionization cross sections of trimethylphosphate as function of the energy W of secondary electrons for different emission angles.

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Sodium Deposition on Magnesium Oxide Surfaces: Comparison of Quantum and Classical Molecular Dynamics Simulations

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For several decades, the interest of the scientific community on clusters has not stopped to increase. Their variable and finite sizes allow us to understand the transition between atom/molecule and a bulk material. Due to peculiar electronic and optical properties of clusters there is a great variety of their important applications in nanoelectronics [1], astrophysics [2], medicine [3-5] and other fields.

The purpose of this work is to study theoretically the physical mechanisms behind the deposition of metal clusters on a substrate of MgO (001). The dynamics of a deposited cluster, substrate and their interaction represent a complex many-body problem. Even though this problem can be treated by quantum mechanical methods, these become unpractical with increasing of the system size. However, the classical molecular dynamics (MD) remains an efficient tool for the investigation of structure and dynamics of the aforementioned system up to significantly larger system sizes (~10^7-10^8 atoms), in a wide range of kinetic energies and directions of deposited clusters, as well as temperatures of clusters and the substrate. Such classical MD simulations involve the validation of the utilized force fields which can be performed through the detailed comparison of classical MD results with those obtained from quantum mechanical simulations for the computationally affordable system sizes.

In this study we perform analysis of the results for deposition of a single Na atom on the MgO (001) substrate derived by the quantum-mechanical approach in [6,7]. The classical MD simulations of the very same system and their analysis are performed by means of the MesoBioNano (MBN) Explorer [8,9] and MBN Studio software [10]. Although, for the validation and benchmarking purposes we focus on the deposition of a single atom, the MD methodology used can be directly applied for simulations of much more complex systems (larger clusters and nanoparticles deposited on the substrate at different angles and kinetic energies, different substrate temperatures, etc) and at much larger time scales which are inaccessible for quantum simulations.

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For notes

Wednesday, July 31 (Canterbury Cathedral Lodge)

12^{00} – 16^{00}	Participants registration
14^{00} – 14^{15}	**ISACC 2019 Opening** **Nigel J. Mason & Andrey V. Solov'yov**
14^{15} - 16^{15}	*Afternoon session I: Structure and dynamics of atomic clusters and nanoparticles* ***(Chair: Andrey Solov'yov)*** **Henrik Cederquist / Manfred Kappes / Eleanor Campbell / Mathias Rapacioli**
16^{15} – 16^{45}	**Coffee break**
16^{45} – 18^{15}	*Afternoon session II: Clustering in systems of various degrees of complexity* ***(Chair: Eleanor Campbell)*** **Andrey Solov'yov / Jean-Patrick Connerade / Eric Suraud**
19^{00} – 22^{00}	**Welcome reception**

Thursday, August 01 (Canterbury Cathedral Lodge)

9^{00} – 11^{00}	*Morning session I: Collisions with atomic clusters and biomolecules* ***(Chair: Eugene Surdutovich)*** **Thomas Schlathölter / Jefferson Shinpaugh / Rodolphe Antoine / Alexey Verkhovtsev**
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	*Morning session II: Clusters and biomolecules in external fields: electric, magnetic, laser, etc.* ***(Chair: Jean-Patrick Connerade)*** **Brendan Dromey / Andrew Ellis / Eugene Surdutovich**
13^{00} – 14^{30}	**Lunch**
14^{30} – 16^{30}	*Afternoon Session I: Cluster structure and dynamics on a surface* ***(Chair: Shiv Khanna)*** **Nigel Mason / Richard Palmer / Armin Gölzhäuser / Pablo de Vera**
16^{30} – 17^{00}	**Coffee break**
17^{00} – 18^{00}	*Poster session*

Friday, August 02 (Canterbury Cathedral Lodge)

9^{00} – 11^{00}	*Morning session I: Ion-cluster collisions* ***(Chair: Henrik Cederquist)*** **Michael Dingfelder / Himadri Chakraborty / Mark Stockett / Suvasthika Indrajith / Andreas Alberg-Fløjborg**
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	*Morning session II: Cluster-molecule interactions, reactivity and nanocatalysis* ***(Chair: Ilya Fabrikant)*** **Shiv N. Khanna / Sam Eden / Jon Golding**
13^{00} – 13^{15}	**Conference photo**
13^{15} – 14^{30}	**Lunch**
14^{30} – 16^{00}	*Afternoon session I: Cluster and biomolecular research with Free Electron Lasers* ***(Chair: Thomas Schlathölter)*** **Kiyoshi Ueda / Jan-Michael Rost / Sadia Bari**
16^{00} – 16^{15}	**Coffee break**
16^{15} – 18^{00}	**Conference tour**
19^{00} – 22^{00}	**Conference dinner**

Saturday, August 03 (Darwin Conference Suite, Darwin College, the University of Kent)

9^{00} – 11^{00}	*Morning session I: Electron and photon cluster collisions* ***(Chair: Nigel Mason)*** **Ilya Fabrikant / Andreas Mauracher / Jozef Lengyel / Xin Wang / Alfred Msezane**
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	*Morning session II: Collisions with biomolecules* ***(Chair: Sam Eden)*** **Linda Feketeová / Roland Wester / Hidetsugu Tsuchida**
13^{00} – 13^{15}	**ISACC 2019 Closing**