International Conference
"Dynamics of Systems on the Nanoscale"

DySoN Conference 2010

National Research Council, Rome, Italy
November 16 - 19, 2010

Book of Abstracts

Editors:
Lorenzo Avaldi, Franco A. Gianturco,
Andrey V. Solov'yov

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Preface

The International Conference "Dynamics of Systems on the Nanoscale" (DySoN 2010) will take place in Rome, Italy during November 16 – 19, 2010. The meeting venue will be the National Research Council. The DysoN 2010 conference is organized by the Department of Chemistry, the University of Rome "La Sapienza", CNR-Istituto di Metodologie Inorganiche e dei Plasmi and the Frankfurt Institute for Advanced Studies, Goethe University.

This conference will build upon a series of International Symposia entitled "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" (ISACC 2003, ISACC 2007, ISACC 2008 and ISACC 2009). ISACC started as an international symposium on atomic cluster collisions in St. Petersburg, Russia in 2003 devoted to the physics of atomic cluster collisions. The second ISACC was held at the GSI, Darmstadt, Germany in 2007. Both first and second symposia were satellites of the International Conferences on Photonic Electronic and Atomic Collisions (ICPEAC). The third ISACC returned to St. Petersburg, Russia in 2008. The fourth symposium was held in Ann Arbor, USA in 2009 and was again a satellite of the ICPEAC 2009. The fifth ISACC satellite of the ICPEAC 2011 will be held at the Fritz Haber Institute in Berlin and will be mainly devoted to collision processes involving atomic clusters. However during these meetings it has become increasingly clear that there is a need for an interdisciplinary conference covering a broad range of topics related to the Dynamics of Systems on the Nanoscale. Therefore in 2010 it was decided to expand upon this series of meetings with a new conference organized under the new title "Dynamics of Systems on the Nanoscale", the DySoN Conference, since this title better reflects the interdisciplinary character of the earlier ISACC meetings embracing all the topics of interest under a common theme.

The DySoN 2010 Conference will promote the growth and exchange of scientific information on the structure-formation and dynamics of animate and inanimate matter at the nanometric scale. There are many examples of complex many-body systems of micro- and nanometric size exhibiting unique features, properties and functions. These systems may have very different natures and origins, e.g. atomic and molecular clusters, ensembles of nanoparticles, nanostructures, biomolecules, biomolecular and mesoscopic systems. A detailed understanding of the structure and dynamics of these systems at that scale is a difficult and fundamental task, the solution of which is necessary in numerous applications of nano- and bio-technology, material science and medicine.

Although mesoscopic, nano- and biomolecular systems differ in their nature and properties, a number of fundamental problems are common to all of them: What are the underlying principles of self-organization and self-assembly of matter at the

micro- and nano-scale? Are these principles classical or quantum? How does function emerge at the nano-and the meso-scale in systems with different origin? What criteria govern the stability of such systems? How do their properties change as a function of size and composition? How are their properties altered by their environment? Seeking answers to these questions is at the core of a new interdisciplinary field that lies at the intersection of physics, chemistry and biology, a field now called Meso-Bio-Nano (MBN) Science.

All of these problems, both experimental and theoretical, will be discussed in the DySoN 2010 Conference. Particular attention will be devoted to dynamical phenomena and many-body effects taking place in various MBN systems on the nanoscale, which include problems of structure formation, fusion and fission, collision and fragmentation, collective electron excitations, reactivity, nanoscale phase transitions, nanoscale insights into biodamage, channeling phenomena and many more. The hope is that all participants will be enriched and further motivated by the session topics and the ensuing general discussions. Have a memorable Meeting!

The Scientific and Organizing Committees

Conference Venue

The Conference will be hosted in the National Research Council (CNR) main building, Piazzale Aldo Moro 7, 00185 Rome, Italy

The photo (right) shows the entrance to the main building of the CNR.

The map below shows the route from Termini train station (green circle) to the conference site (the distance is just over 1km).
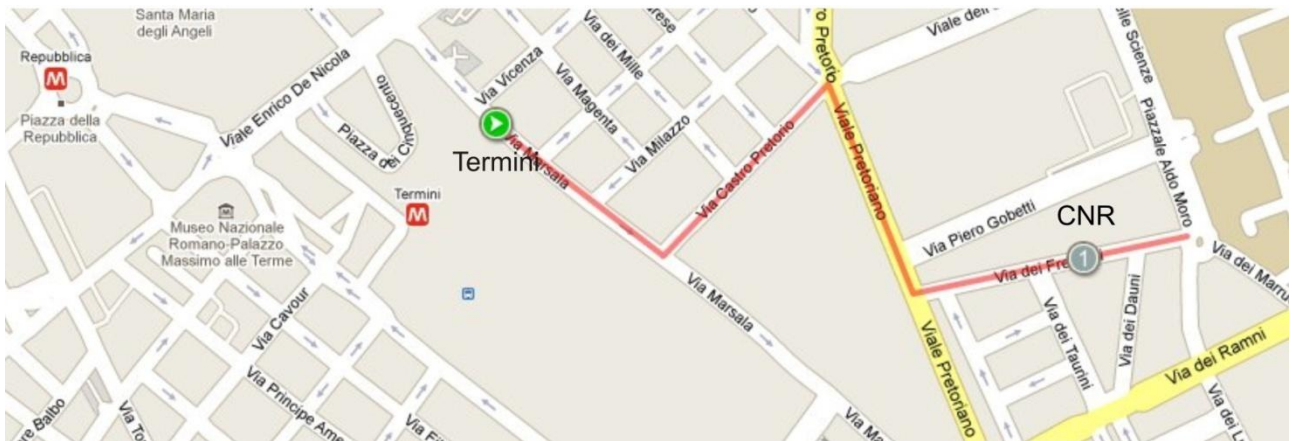
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Buffet Lunches and Conference Banquet

The Buffet lunches on the 17th, 18th and 19th November and the Conference Dinner will take place in Casa dell'Aviatore

(http://www.casaviatore.it/index. php?la=en)

Circolo Ufficiali dell'Aeronautica Militare, Viale dell'Università 20.

The map shows the route from the Casa dell'Aviatore to the CNR main Building.

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DySoN Conference web page

Updated information on the conference is available at the following Internet address:
http://fias.uni-frankfurt.de/dyson2010

Conference e-mail

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Acknowledgements

The organizing committee gratefully acknowledges support by

Conference Program

Tuesday, 16 November 2010

$16^{00} - 18^{00}$	Participants registration
$18^{00} - 21^{00}$	Conference reception

Wednesday, 17 November 2010

$9^{15} - 9^{30}$	**DySoN2010 Opening** **Lorenzo Avaldi, Franco A. Gianturco, Andrey V. Solov'yov**

$9^{30} - 11^{00}$	**Morning session I**
	Chair: Jean-Patrick Connerade
	
	Bernd Huber, CEA-CIMAP, France
	  Energy driven processes in nanosized complex systems
	Nigel J. Mason, The Open University, United Kingdom
	  Electron controlled (nano) chemistry
	Julius Jellinek, Argonne National Laboratory, USA
	  Pt, Mo, and Pt/Mo Clusters: Structural, Electronic, and Chemical
	  Reactivity Properties - Effects of Size and Composition

$11^{00} - 11^{30}$	**Coffee break**

$11^{30} - 13^{00}$	**Morning session II**
	Chair: Jean-Patrick Connerade
	
	Shiv N. Khanna, Virginia Commonwealth University, USA
	  Atomic control over properties via super-orbitals: towards cluster-
	  assembled nanoscale materials
	Yurii Lozovik, Institute of Spectroscopy, Russia
	  Unusual electron properties of graphene and modeling of
	  nanodevices
	Michel Broyer, Université de Lyon, France
	  Size selected metal clusters quasi isolated in transparent matrix or
	  in interaction with biomolecules

$13^{00} - 14^{30}$	**Lunch**
$14^{30} - 16^{00}$	**Afternoon Session I** Chair: Gerardo Delgado-Barrio **Reinhard Dörner**, University of Frankfurt, Germany *Experimental studies of interatomic coulombic decay*

	Ersin Yurtsever, Koc University, Turkey *Dynamical signatures of phase transitions in Coulomb clusters* **Eric Suraud**, Universite Paul Sabatier, France *Dynamics of irradiated clusters and molecules*
$16^{00} - 16^{30}$	**Coffee break**
$16^{30} - 18^{00}$	**Afternoon Session II** Chair: Gerardo Delgado-Barrio **Pablo Villarreal**, Instituto de Fisica Fundamental, Spain *Structure and spectroscopy of doped helium clusters: dependence on the nature of the He-dopant interaction* **Manfred Faubel**, Max-Plank-Institute for Dynamics and Self-Organization, Germany *Photoelectron spectroscopy of liquid chemical solutions* **Stephan Denifl**, Institut für Ionenphysik und Angewandte Physik, Austria *Fragmentation of amino acids and dipeptides upon electron attachment*

Thursday, 18 November 2010

$9^{30} - 11^{00}$	**Morning session I** Chair: Franco A. Gianturco **Marcelo Coreno**, CNR-IMIP, Monterotondo Scalo, Roma, Italy *Photoionization studies with synchrotron radiation: from molecules to clusters* **Francesco Sebastianelli**, University of Rome "Sapienza", Italy *Dynamical role of metastable anions from carbon-rich molecules in planetary atmospheres* **Paola Bolognesi**, CNR-IMIP, Italy *Excitation and fragmentation of biomolecules*
$11^{00} - 11^{30}$	**Coffee break**
$11^{30} - 13^{00}$	**Morning session II** Chair: Franco A. Gianturco **Leon Sanche**, Université de Sherbrooke, Canada *Nanoscale dynamics of radiosensitivity: role of low energy electrons* **Isabella Baccarelli**, CASPUR Supercomputing Consortium, Italy *Dissociative electron attachment in radiation damage and radiosensitisation*

	Ilya I. Fabrikant, University of Nebraska-Lincoln, USA *Recent progress in the theory of dissociative electron attachment: from diatomics to biomolecules*
$13^{00} – 14^{30}$	**Lunch**
$14^{30} – 16^{30}$	**Afternoon session I** Chair: Nigel J. Mason **Eugene Surdutovich**, Oakland University, USA *Nanoscale transport phenomena and radiation damage induced by ions* **Emanuele Scifoni**, GSI, Germany *Radial dose distribution around an ion beam track on the nanoscale* **Alexander Yakubovich**, Frankfurt Institute for Advanced Studies, Germany *Temperature driven nanoscale conformational transitions in biomolecular systems* **Igor Mishustin**, Frankfurt Institute for Advanced Studies, Germany *Role of nuclear fragmentation reactions in ion-beam energy deposition in extended media*
$16^{30} – 18^{00}$	**Poster session and Coffee**

Friday, 19 November 2010

$9^{30} – 11^{00}$	**Morning session I** Chair: Lorenzo Avaldi **Catherine Bréchignac**, CNRS, France *Fragmentation dynamics of nanostructures* **Manfred Kappes**, Karlsruhe Institute of Technology, Germany *From fractals to nanofilms by deposition of non-IPR fullerenes* **Ilia A. Solov'yov**, Frankfurt Institute for Advanced Studies, Germany *Nanoparticles dynamics on a surface: fractal pattern formation and fragmentation*
$11^{00} – 11^{30}$	**Coffee break**
$11^{30} – 13^{00}$	**Morning session II** Chair: Lorenzo Avaldi **Vadim Ivanov**, St. Petersburg State Polytechnic University, Russia *Metal cluster anions: photoionization cross section and photoelectron angular distribution*

	Andrei Korol, Frankfurt Institute for Advanced Studies, Germany *Photo-induced processes in fullerenes* **Alfred Müller**, Institut für Atom- und Molekülphysik, Germany *Response of endohedreal fullerenes to photoabsorption by the encapsulated atom*
13^{00} –13^{15}	**Conference photo**
13^{15} –14^{30}	**Lunch**
14^{30} –16^{00}	**<u>Afternoon session I</u>** Chair: Andrey V. Solov'yov **Joachim Ullrich**, Max-Planck-Institute für Kernphysik, Heidelberg, Germany *Free electron lasers: dynamics and structure towards femtosecond time and nanometer spatial resolution* **Hartmut Backe**, Institute of Nuclear Physics, Germany *Experiments on channeling in crystalline undulators* **Andriy Kostyuk**, Frankfurt Institute for Advanced Studies, Germany *Crystalline undulator as a source of coherent radiation*
16^{00} –16^{30}	**Coffee break**
16^{30} –17^{30}	**<u>Afternoon session II</u>** Chair: Andrey V. Solov'yov **Walter Greiner**, Frankfurt Institute for Advanced Studies, Germany *Exotic nuclear clusters: superheavy, neutron-rich, superstrange, antimatter* **Jean-Patrick Connerade**, Imperial College, UK *The importance of Nanoscience for reversible energy storage and urban vehicles in megacities*
17^{30} – 17^{45}	**Symposium closing**
19^{00} - 22^{30}	**Conference banquet**

Overview of Abstracts

Talks

Posters

Talks

ENERGY DRIVEN PROCESSES IN NANO-SIZED COMPLEX SYSTEMS

B. A. Huber

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The study of finite-size systems allows for a better understanding of fundamental processes occurring in complex systems. These studies can be performed in great detail and on the molecular level. Due to the large but limited number of degrees of freedom, once the system is excited, it can de-excite or decay via a large variety of different processes. Depending on the amount of internal energy and the number of involved charges, the time scale may vary over many orders of magnitudes (fs to ms). On the one hand, the excess energy may lead to a total destruction of the system; however, it may also create subsystems which are more stable. On the other hand, if the amount of energy is relatively low, chemical reactions may be induced which change the type of bonding and may create new molecules. In the present contribution we will describe some of these processes for specific cluster systems:

-       Ion-induced coalescence and cluster formation in clusters of fullerenes,
-       Bond cleavage and formation in clusters of amino acids,
-       Charge- and energy-induced fragmentation of clusters of PAH molecules.

In the experiment we collide multiply charged ions at low velocities with different clusters (projectiles ranging from He^+ to Xe^{30+} in the collision energy range from 10 keV up to 600 keV, depending on the charge state). In general, these collisions will be accompanied by the transfer of energy and charge which may provoke heating and evaporation, delayed fragmentation and electron emission, dissociation and multifragmentation as well as coalescence and the initiation of chemical processes inside the cluster system. The analysis of the charged fragments is made by mass spectrometric methods.

In particular, we will discuss a possible fragment deformation in the case of charge-driven decay processes and the influence of an additional chemical environment.

ELECTRON CONTROLLED (NANO) CHEMESTRY

Nigel J. Mason

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The ability to manipulate and control chemical reactions remains one of the major goals and challenges of modern physical and chemical research but, should (when) we gain such control, it will open unprecedented opportunities for both understanding processes in our natural world and the development of new technologies that will underpin the economic (and social) advances of the 21st century in a similar way to the manner by which control of light (e.g. through the development of lasers) and the control of electronics (through the design of transistors and the 'computer chip') fashioned the 20th Century.

Consequently there has been a major research effort to explore different methodologies that may provide such chemical control. One of the most exciting developments in recent molecular physics has been the discovery that *Low Energy Electrons (LEE)* may not only dissociate the molecular target but may do so at well defined reaction sites often leading to almost 100% bond selectivity thence initiating controlled chemical processing in the local environment. The process by which LEE can induce such bond selective molecular fragmentation is known as Dissociative Electron Attachment (DEA) Figure 1a. An incident electron may be captured by the molecular target (XY) to form an excited state of the molecular negative ion XY$^{\#}$. This state, commonly called a *Temporary Negative Ion (TNI)*, generally decays by ejecting the excess electron within a finite time depending on its lifetime (a process called autodetachment) but the molecular negative ion may also decay through dissociation leading to the formation of a stable negative ion X^{-} and a neutral (often radical) fragment (Y) a 'reaction' summarized as $\mathbf{e^{-} + XY \rightarrow XY^{\#-} \rightarrow X^{-} + Y.}$ In contrast to *direct* electron impact, where the incident electron must have an energy of several eV to dissociate a molecule, DEA can dissociate a molecule at energies *below the dissociation energy* of the ground state. In numerous cases DEA effectively occurs at electron impact energies of a few meV, that is at thermal energies (kT) and generally, these low energy processes have very large cross-sections of 100s to 1000s of Å^{2} which are much larger than cross sections for direct electron (or photon) induced dissociation.
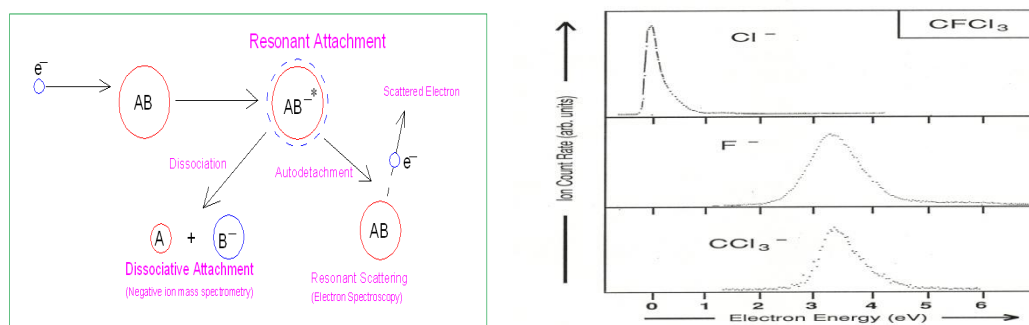
Figure 1 (a) Schematic diagram illustrating the mechanism of Dissociative Electron Attachment (DEA). (b) DEA in CFCl$_3$ Detection of the fragment anion at low energies (sub 1eV, below first excited electronic state) reveals that the C-Cl bond is cleaved whilst at higher energies (2.5 to 5 eV) the C-F bond is cleaved

The formation of such a TNI is a '*resonant*' process, i.e. it occurs only over a limited incident electron energy range (0.1 to 2 eV). Hence in contrast to direct molecular dissociation,

where products are formed continuously above some threshold energy, the products of DEA (X^-, Y) are only formed within a limited energy range (Figure 1 (b)). A remarkable feature of DEA is that it is highly *bond selective,* each TNI often having a single preferred dissociation channel. Consider DEA to $CFCl_3$ (Figure 1 (b)) electrons with meV incident energies cleave the C-Cl bond producing Cl^- and CCl_2F with a very high cross section, whereas at 3.2eV the incident electrons only cleave the C-F bond resulting in F^- and CCl_3^-. Hence by simply varying the energy of the incident electron (tuning) we can open (or close) different dissociation pathways and change the net products of the collision. *This provides us with one of the essential prerequisites of chemical control − control over the production of the reactants*

Should DEA occur in a dense media such as in the condensed phase, within a surface layer or within a cluster the neutral and generally more highly reactive products produced by DEA (Y) may then initiate further chemistry through reactions with neighbouring molecules (AB) i.e. **Y+ AB** $\rightarrow$ **AY+ B**. As an example consider a mixed cluster of NF_3 and CH_3Cl (Figure 2a). The cross section for Cl^- production from CH_3Cl by direct electron impact is negligible $< 10^{-23}$ cm^2. However in the mixed cluster of CH_3Cl and NF_3 F^- ions may be liberated from NF_3 and then react with CH_3Cl by the well known nucleophilic displacement (S_N2) reaction $F^- + CH_3Cl \rightarrow CH_3F + Cl^-$[6]. We thus form CH_3F within the cluster. An identical process may occur on a surface in a mixed multilayer of co-deposited CH_3Cl and NF_3 (Figure 2b). The Cl^- ions can then be liberated/desorbed from the film and the synthesized molecular species CH_3F left on the surface. *Thus DEA may lead to direct chemical transformation of the surface.*
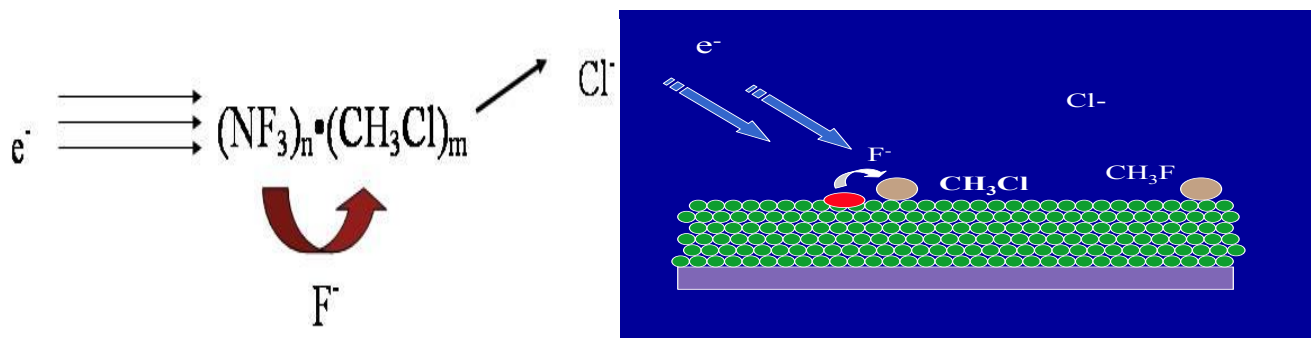
Figure 2: (a) Electron induced S_N2 reaction in a mixed cluster of NF_3 and CH_3Cl molecules [6] and (b) the same process on a surface.

Low energy Dissociative Electron Attachment (DEA) therefore suggests an innovative and highly promising mechanism for chemical control in dense/condensed media that is *universal* (since it occurs in almost all molecular systems), *efficient* (high cross sections) *and deliverable* at a potentially low cost (since it is based on electron beam sources rather than for example high cost high maintenance laser systems). In this talk I will review the field of electron induced (nano)chemistry both in natural phenomena (such as astrochemistry) and as a technological tool (e.g. in nanolithography, plasma processing and radiotherapy). The talk also will seek to provide insight into four key questions:

- Can we exploit electron induced chemistry to build chemical nanostructures thus opening the new field of electron controlled chemical (nano)lithography?
- By tuning the electron temperature in plasma reactors can we use electron controlled chemistry to control physical and chemical processing?
- By exploiting the site selectivity of electron induced reactions in large macromolecules can we control DNA damage and thence develop new radiotherapy techniques?
- Can electron induced chemistry explain the formation of molecules in the interstellar medium?

Pt, Mo, AND Pt/Mo CLUSTERS: STRUCTURAL, ELECTRONIC, AND CHEMICAL REACTIVITY PROPERTIES – EFFECTS OF SIZE AND COMPOSITION

Julius Jellinek and Aslihan Sumer

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Results of DFT studies of structural, electronic, and chemical reactivity properties of Pt_n, Mo_n, and $Pt_{n-m}Mo_m$ clusters with n up to 13 ($m \leq n$) will be presented and discussed. The structural and electronic properties will be analyzed as a function of cluster size and composition. The chemical reactivity will be discussed for the case of CO adsorption on the clusters, and will be characterized as a function of cluster size, structure, and composition, as well as the adsorption site. The analysis will also include structural and electronic consequences of the CO adsorption.

ATOMIC CONTROL OVER PROPERTIES VIA SUPER-ORBITALS: TOWARDS CLUSTER-ASSEMBLED NANOSCALE MATERIALS

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Due to quantum confinement, the electronic states in metal clusters can be grouped into electronic shells, similar to the electron shells in atoms. Unlike atomic orbitals, the super-orbitals are, however, diffuse and delocalized over multiple atoms. This provides unique opportunity to control electronic, magnetic, and chemical behaviors through combinations of geometry and the nature of the individual atomic orbitals contributing to cluster states. The talk will highlight novel chemical, electronic, and magnetic phenomenon associated with these super-orbitals in stable clusters called superatoms.

Starting with a definition of a superatom, I will first illustrate super-shell splitting due to overall deformation ("jellium crystal fields") in metal clusters, and how these can result in stable clusters resistant to etching by strong etchants like oxygen. I will then demonstrate how the localization of different cluster-orbitals on different groups of atoms, allows chemical reaction through cooperative behavior between different pairs of sites that can result in breaking of water and methanol. Finally, I will highlight our development of new Magnetic Superatoms that have a combination of atomic and superatomic orbitals and how these motifs can lead to new molecular electronic devices with applications in spintronics.

An important long standing dream in cluster science has been to design materials with cluster building blocks. I will present our recent successes in synthesizing several such assemblies using Zintl anion (As_7^{3-}) cluster building blocks with counter-cations to illustrate how the cluster assemblies allow control over band gaps through modulations of different parts of the electronic spectrum. I will also report our recent finding of rather unusual effect in cluster solids composed of covalent As_7-Au_2-As_7 species linked via various counter cations. The assemblies offer multiple architectures placing differing number of counter cations in the vicinity of As_7-Au_2-As_7. Optical measurements revealed that the band gaps vary from 1.4-2.0 eV, even though the assemblies are constructed from the identical cluster building block. Theoretical studies explain this variation as being a result of stabilization of the occupied cluster states through large internal electric fields of the cations.

The talk will end with some of the future directions that can lead to "Cluster-Materials by Design" with applications in catalysis and electronics.

UNUSUAL ELECTRON PROPERTIES OF GRAPHENE AND MODELING OF NANODEVICES

Yu. E.Lozovik[1]

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As known graphite consists from coupled through weak, van der Waals forces graphene layers. But inside graphene layers the binding is very high. This gives the possibility to write by graphitic rods by splitting off graphite flakes. But several years ago the wonderful discovery was done by A.Geym team – single graphite monolayer, graphene with only one atom thick was experimentally obtained and its electronic properties were studied rather in detail now. Graphene is essentially harder than steel, its thermoconductivity is much greater than that for copper. But most wonderful are its electronic properties. The energy gap between valence and conductivity bands is identically equal to zero, effective masses both electrons and holes are also equal to zero. In result electrons and holes are described by Dirac equation but with zero mass. In result electrons in graphene penetrate with probability equal to one through any high potential barrier and backscattering for slowly varying potential barriers is impossible. This changes the effect of impurities by cardinal way, particularly weak localization become to be impossible. The last leads to some pecularity in creation of nanodevices based on graphene. From other hand the graphene has great potential for nanoelectronic and nanoelectromechanical system.

We studied the structure from two graphene layers independently gated .We predicted the existence of coherent phase and superfluidity in graphene bilayer originated from pairing of spatially separated electrons and holes. Bose condensation and Kosterlitz-Thouless transition were predicted for bilayer graphene in strong normal magnetic field. The systems considered give the possibility to create nondissipative nanoelements for information transfer operating even at room temperatures. The peculiarities of quantum dots and nanotransistors based on graphene are discussed and new type of nanoelements is considered.

Calculations of nanoelements based on graphene by generalized density functional approach for system with "ultrarelativistic" electronic spectra is developed. Plasma oscillations and polaritons in graphene will be discussed. Possible superconductivity of strongly doped graphene is analyzed. Possible NEMS based on graphene are analyzed.

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SIZE SELECTED METAL CLUSTERS QUASI ISOLATED IN TRANSPARENT MATRIX OR IN INTERACTION WITH BIOMOLECULES

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The low energy deposition of clusters produced in the gas phase is an interesting route for synthesizing nanostructures with specific properties [1]. We have developed a new and versatile apparatus for the deposition of size selected clusters [2]. Firstly, this allows us to explore the auto-organization of size selected metal clusters as a function of the kind of metal and of the surface reactivity. Secondly, the size selected clusters may be also embedded in transparent matrices to study their optical properties as a function of the size. The production and deposition of very small nanoparticles is an issue of fundamental interest to investigate precisely the size evolution of cluster properties from the atom (or molecule) to the bulk phase and especially to highlight the transition from the regime of "quantum size effects" to the regime of the so-called "scalable size effects". For noble metal clusters, this roughly corresponds to particle diameters of the order of 1 to 2 nm (typically 30 to 250 atoms). Results in this size regime will be discussed concerning the electron-lattice energy exchanges and the acoustic response [3].

Finally complexes of small metal clusters and biomolecules can be generated in ESI source and size selected in Ion traps. This allows us to study their optical properties and the influence of the biomolecule on the absorption spectrum [4]. The cluster may also change the conformation of the biomolecule while the biomolecule may stabilize small doubly charged silver clusters. Recent results on $Au_{25}SG_{18}$ will be also presented.

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EXPERIMENTAL STUDIES OF
INTERATOMIC COULOMBIC DECAY

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We will give an overview of recent experimental studies of interatomic coulombic decay (ICD). In ICD an excited ionized atom or molecule which is part of a loosely bound system transfers it excitation energy to a neutral neighbor, where it leads to emission of a low energy electron. The talk will sow experiments in rare gas cluster which illustrate the mechanism of ICD and show the exchange of a virtual photon and discuss most recent results on water clusters and Helium dimers. We will also show that ICD is an efficient mechanism to produce low energy electrons after ion impact on clusters.

DYNAMICAL SIGNATURES OF PHASE TRANSITIONS IN COULOMB CLUSTERS

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Similarly charged particles can form stable structures by employing various potential traps. First proposed by E.Wigner in 1934, such systems have been observed in dust plasmas, colloidal suspensions, Penning and Paul traps. As with all small systems, shapes and physical properties show strong dependence on size. The shapes of such systems can change from two-dimensional disks to three dimensional spherical or cylindrical structures. They could form concentric shells, hexagonal lattices and their mixtures. With Basin Hopping Monte Carlo approach we have collected global (and local) energy minima of these systems. In this study, we present at first the structural variations of clusters with different potential energy expressions; and discuss the stability as a function of the size.

By varying the trap parameters, it is possible to observe the analogs of the sold-liquid phase transitions. We will also present some aspects of the "melting" of these clusters from Molecular Dynamics studies. The examples of the influence of the topological defects, point defects and shell structures on both mechanisms of melting and the melting points are going to be discussed.

DYNAMICS OF IRRADIATED CLUSTERS AND MOLECULES

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

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

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

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STRUCTURE AND SPECTROSCOPY OF DOPED HELIUM CLUSTERS: DEPENDENCE ON THE NATURE OF THE He-DOPANT INTERACTION

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Diffusion and path integral Monte Carlo methods are currently used to describe structures and binding energies of helium clusters doped with some impurity. For diatomic dopants, by considering the He atoms as "electrons" and the dopant as "nuclei", we have developed a complementary tool which in addition to the above mentioned properties provides us with wavefunctions. It allows to perform spectral simulations that can be compared with the experiment. We review the fundamental aspects of such quantum-chemistry-like methodology in which, together with masses, Coulomb interactions are replaced by proper molecular ones. Extensions towards more accurate *ab initio* methodologies are outlined. Also, the challenging scenario arising when the impurity is not immersed but attached to the nanodroplet will be addressed.

PHOTOELECTRON SPECTROSCOPY OF LIQUID CHEMICAL SOLUTIONS

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An emerging photoelectron spectroscopy technique uses micro-focus Synchrotron radiation and liquid water micro-jet probe surfaces in high vacuum for studies of a wide class of liquid aqueous solutions. This allows for complex investigations of electronic energy level structures as well as for nanoscale geometrical surface structure studies of solute and solvent molecules in liquid aqueous solutions.

By core electron spectroscopy, ESCA type, experiments, changes in local environment of a single atom in solvated molecules are accessible to experiment. This is demonstrated in detail for the pH-value dependence of the protonation/deprotonation of NH_2 groups in simple amino acids. Near the liquid surface core electron spectroscopy allows, also, the tracing of surface activities of individual molecular components by exploitation of the energy dependent electron escape depth. In a further example for valence band photoelectron spectroscopy on electrochemical processes in solutions of a transition metal ion, the Marcus –theory solvent reorganization energy for the Mn^{2+}/Mn^{3+} redox process is determined from joint studies of the experimental valence electron spectrum in solution and an advanced molecular dynamics DFT computer study of the electrochemical system.

FRAGMENTATION OF AMINO ACIDS AND DIPEPTIDES UPON ELECTRON ATTACHMENT

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Previous studies of free dissociative electron attachment (DEA) to simple amino acids (e.g. glycine, α-alanine and valine) in the gas phase showed the formation of a variety of fragment anions [1-3]. One motivation for these DEA studies is the fact that the interaction of low energy electrons with biologically relevant molecules is an important issue towards understanding the molecular mechanism in radiation damage by this secondary species [1-3]. In DEA fragmentation can occur via a direct repulsive state of the transient negative ion (TNI) or via substantial redistribution of excess energy or even rearrangement within the TNI. Less attention has been given so far to secondary processes, i.e. the further (metastable) decay of the fragments anions formed upon DEA [4], which can provide additional insight concerning structure and stability of the anions involved.

Here we present a detailed study exploring the decomposition of amino acids and peptides upon electron attachment and the subsequent decomposition of negatively charged fragment anions for the amino acids valine and β-alanine and in addition for the dipeptide dialanine.

In general, like for organic acids (formic acid, etc.) the dehydrogenated parent anion $(M-H)^-$ is one of the most abundant fragment ions formed upon DEA to simple amino acids. In a series of DEA investigations it turned out that at electron energies below 2 eV this main reaction results from the loss of the hydrogen atom from the carboxyl group (COOH). Utilizing a sector field mass spectrometer we are able to measure the subsequent decay of these anions in the microsecond time regime. The energy dependence of the decay reactions of $(M-H)^-$ into smaller fragment anions for initial electron energies from about 0-10 eV provides additional evidence for the site selectivity of hydrogen loss from specific sites from the amino acid molecules. Moreover, the results for β-alanine indicate that at low electron energies the ion yield of $(M-H)^-$ (with features at about 1.2 eV and 1.5eV) strongly depends on the position of the amino group (NH_2).

Recently we have also measured electron attachment to dialanine, where two alanine molecules are linked together via a peptide bond. The ion yield of $(M-H)^-$ for dialanine is considerable modified as compared to the anion yield for simple amino acids. Possible explanations by means of quantum chemical calculations will be discussed.

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PHOTOIONIZATION STUDIES WITH SYNCHROTRON RADIATION: FROM MOLECULES TO CLUSTERS

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Detailed knowledge of the electronic structure of surfaces and solids must be built upon a thorough understanding of spectroscopy and dynamics in isolated systems. To this purpose VUV and Soft-X-Ray radiation is a valuable tool for the investigation of electronic properties of matter. Furthermore many diagnostic and spectroscopic techniques have been developed first in the gas phase and then transferred to other fields such as material and biomedical sciences, energy and sensor technologies.

Flux and energy resolution achievable at third generation facilities, like the Gas Phase beamline of the Elettra storage ring (Trieste, Italy) [1], enable studies of inner-shell electron excitation in experiments that have been so far traditionally characterized by intrinsic low signal level due to the low density of the targets like biomolecules [2] and clusters [3]. Recent examples will be discussed, where photoionization techniques have been used in investigations on gas phase molecular targets of increasing complexity, ranging from molecules of biological interest, to metal containing systems and clusters.

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DYNAMICAL ROLE OF METASTABLE ANIONS FROM CARBON-RICH MOLECULES IN PLANETARY ATMOSPHERES

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It is by now a well established fact that microscopic processes give important information about the bulk properties of the interstellar medium (ISM), and further control several macroscopic features of it such as temperature and density [1]. We know already that every process of radiation-induced photoionization of the atoms and molecules which are present in the ISM yields an electron e^- with energy ($h\blacksquare$-IP), the latter being the ionization potential of the species involved. This excess amount of energy can in turn be shared between the surrounding gas and its constituents and therefore provides an important heat source within the ISM.

The above features suggest quite convincingly that electrons can provide an interesting, and flexible, energy source for driving nanoscopic reactions within the ISM and thus participate in the possible formation of highly reactive anionic intermediates of both the atoms and molecules present in the stellar atmosphere. The formation of polyatomic anions has been predicted in astrophysical environments by earlier model studies [2], where it was suggested that the initial step of the electron-molecule low-energy collisions could produce a metastable species, a transient negative ion (TNI), which then further stabilizes after radiative emission. Recent experimental observations of negatively charged molecular ions like C_4H^-, C_6H^-, C_8H^-, and C_3N^- [3,4] have triggered the search for the possible formation of metastable TNIs in even larger systems [5] and, consequently, for the most likely paths to stable anions which could be proposed to occur in the interstellar environment.

The present study is therefore a computational/theoretical analysis that searches for the existence of TNIs species of the linear carbon chains of the type $NC_{2n}N$ [6] and $HC_{2n+1}N$ molecules that have been recently considered both in laboratory experiments and in computational studies [7]. Our quantum modelling aims at uncovering the most likely pathways to dissociative electron attachment events and thus the characteristics of the negative ions that are more likely to be formed and which could either fragment into smaller, albeit permanent, anionic species or directly into full molecular anions.

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EXCITATION AND FRAGMENTATION OF BIOMOLECULES

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Electromagnetic radiation is known to produce structural and chemical modifications of the DNA bases, which may be either reparable or turn into mutations, single/double-strand breaks of the DNA helix and ultimately to cell death. The use of radiosensitisers incorporated into the DNA of tumour cells enhances these effects and lead to their selective destruction. Several mechanisms based on i) the dissociative electron attachment of low energy electrons [1], ii) the action of Auger electrons emitted following inner shell excitation and iii) Coulomb explosion of the residual ion left after ionisation processes have been proposed. We have undertaken a characterisation of the ejected electron spectra [2] and of the fragmentation patterns of pyrimidine and halogenated pyrimidines. Pyrimidine is the building-block of three nucleobases of the DNA and RNA, while halogenated pyrimidines are used as radiosensitisers.

We selected a few halogenated pyrimidines to investigate both the role of different halogen atoms and of the halogenation site in the functionalisation of the pyrimidine aromatic ring. Excitation and fragmentation spectra were measured at different photon energies across the Br, Cl, C and N inner-shell excitations, showing that different fragmentation patterns exist and the production of specific fragments is enhanced at the various resonant energies (see figure 1).
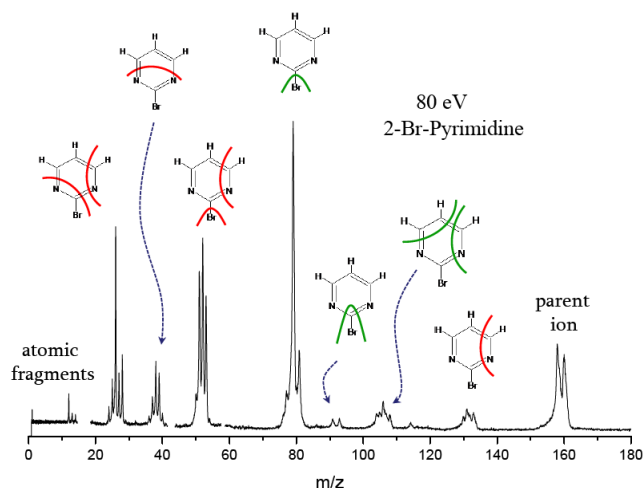
Figure 1: The fragmentation spectrum of 2-Br-pyrimidine measured at 80eV photon energy. The main fragmentation patterns are also reported.

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NANOSCALE DYNAMICS OF RADIOSENSITIVITY: ROLE OF LOW ENERGY ELECTRONS

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When high energy particles pass through a cell, they first produce excited molecules and ionization along their tracks. Most of the energy (~80%) flows into ionization, which yields ions and electrons. Most of the latter are produced with low energies (<30 eV) and hence their number is very large (~30,000 per Mev of deposited energy), but their range is very short (~10 nm). Within the femtosecond time scale, these low energy electrons (LEE) dissociate bonds in biomolecules of cells and, in particular, damage DNA. Thus, the nanoscale dynamics of these electrons cannot be studied in real time but only with direct LEE beam experiments, where the reactions they induced are similar to those occurring within nanometers of the LEE site of formation in cells. From past experimental and theoretical results [1,2], it has become increasingly recognized that LEE are able to induce previously unexpected high levels of single (SSB) and double strand breaks (DSB) in DNA, even at energies below the ionization threshold [3]. Below 15 eV, LEE can break a DNA strand via the formation of a transient anion (i.e., resonant electron capture) of a DNA subunit (e.g., base, deoxyribose, phosphate and structural water); e.g., the sub-unit captures the incoming free electron and the resulting transient anion dissociates. The transient anion can also autoionize leaving a subunit in a dissociative state, a phenomenon which also damages DNA. In this case, the departing electron can transfer to another subunit and cause further damage via DEA (e.g., a DSB). The ballistic fragments produced in such events may thereafter further react within the molecule. The reactions triggered by LEE can be amplified at the nanoscopic level by binding to DNA, species that modify LEE-induced damage or increase the number of LEE. Gold nanoparticles (GNP) belong to this latter category. Their binding to DNA considerably increases DNA damage induced by high energy radiation by increasing near DNA the amount of secondary LEE. The chemotherapeutic agent cisplatin belongs to the other category. This small molecule renders DNA extremely vulnerable to secondary LEE. The added sensitivity is due to a large increase in the magnitude of the electron capture cross section (i.e., the formation of transient anions), which leads to local rupture of single and double DNA strands. Thus, the LEE abundantly produced by high-energy radiation may play a significant role in increasing radiosensitivity. The experiments which led to these findings and the results obtained will be described at the conference. It will be shown that understanding nanoscale mechanisms of the direct effects of radiation in radio- and chemo-sensitized DNA may have implications in the design of new chemotherapeutic and radiosensitizing drugs as well as in the development of more efficient protocols in cancer therapy. In particular, addition of DNA-targeted GNP to clinical protocols using platinum drugs could considerably improve concomitant chemoradiation treatment of cancer.

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DISSOCIATIVE ELECTRON ATTACHMENT IN RADIATION DAMAGE AND RADIOSENSITISATION

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The recent developments in computing capabilities and the last technological advances concerning multi-core architectures mark the start of a new `era' for the computational study of complex phenomena. Among these we can surely place the analysis of the chain of events started by the exposition of living tissues to ionizing radiations and finally resulting in cellular and genetic damages. In such context the role of secondary, low-energy electrons (LEEs), with energy below 20 eV, produced by the initial ionizing radiation, has reached by now a rather broad consensus in the relevant literature[1-3]: through the formation of Transient Negative Ions (TNIs), LEEs can efficiently induce Single-Strand and Double-Strand Breaks of the DNA/RNA. The production of a sufficient amount of LEEs in targeted regions is also among the principal aim of radiotherapic treatments. The most impressive feature of these processes consists in the fact that, due to the quantum mechanical nature of electron-molecule interaction and of the TNIs, LEEs possess the remarkable property of acting on very specific molecular sites and of causing highly selective molecular bond breaks, in most cases at unique values of collision energies. Hence, they offer the unvaluable possibility to control a chemical reaction with `lithographic' precision.

In this context, it is of primary interest to fill the lack of knowledge concerning the final events in the reaction chain started by irradiation on a living tissues. Providing quantitative measurements and a complete characterization of the processes taking place at the nanoscopic level and leading to molecular fragmentation capable to lethally damage DNA and proteing is indeed highly recommended in order to sustain the biomedical community involved in cancer studies and chemo/radio-therapic treatments. However, the quantum mechanical analysis of such processes is a challenging task, due to the size and the generally low symmetry of the system under study and in the perspective of extending the analysis from individual building blocks to larger biological macromolecules.

We will discuss here our computational study of the electron attachment process for selected biosystems [4,5] and the new results obtained by using a multi-core (CPU/GPU) architecture [6,7]. The elastic cross sections and an analysis of the resonance states based on the Delay Matrix formalism are presented for the DNA nucleotides and other macromolecules, together with a first analysis of the radiosensitising properties of a few compounds.

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RECENT PROGRESS IN THE THEORY OF DISSOCIATIVE ELECTRON ATTACHMENT: FROM DIATOMICS TO BIOMOLECULES

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Recent progress in studies of dissociative electron attachment processes was stimulated by development of new experimental techniques involving electron beams with high energy resolution. This allowed detailed investigation of threshold phenomena in low-energy dissociative attachment to diatomic and polyatomic molecules: vibrational Feshbach resonances (VFRs) and threshold cusps.[1]

Theoretical description of DEA process requires solving a challenging nuclear dynamics problem involving motion in a nonlocal complex potential.[2] An alternative approach is the resonance R-matrix theory.[3] In the present talk we review recent experimental and theoretical results for diatomic molecules, simple polyatomic molecules, and some biomolecules: formic acid, glycine and uracil. Several interesting features found in simple molecules, like threshold resonances and cusps, are also observed in biomolecules and can be described by our resonance R-matrix theory. However, many unresolved problems still exist even for diatomics. For example, the observation[4] of low-energy electron attachment to the F_2 molecule is still unexplained. The theory also gives a detailed description of the gas temperature and electron temperature dependencies of the dissociative attachment cross section. In particular, the validity of the Arrhenius law for the dissociative attachment process was analyzed.

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NANOSCALE TRANSPORT PHENOMENA AND RADIATION DAMAGE INDUCED BY IONS

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The multiscale approach to the radiation damage by ions is aimed at studying different physical, chemical, and biological phenomena, leading to the cell death after irradiation with ion beams. One of the key questions is which of the many possible pathways of DNA damage are the most dominant. The answer to this question depends on the specific conditions of projectiles, the medium, and the target DNA molecules. Most of the pathways were studied earlier when photons were used as projectiles. All of these pathways are chemical, i.e., lesions on DNA molecules are caused by chemical reactions brought about by different agents produced as a result of ionization of the medium by projectiles.

Ions lose most of their energy via ionization of the medium in a very small region, called the Bragg peak. This energy is transferred to the adjacent medium by the secondary electrons. As a result, the tissue becomes very hot in a narrow region around the ion's track. This effect has been estimated and then studied by our group in Refs. [1] and [2], respectively. The pressure in this narrow zone increases by several orders of magnitude [2] and this causes an expanding shock wave propagating away from the track on the nanometer scale. We have investigated this shock wave propagating in liquid water [3]. This wave eventually weakens as the front expands further; but before that, it may contribute to DNA damage due to large pressure gradients developed within a few nanometers from the ion's trajectory. We have calculated these gradients and estimated the forces, which can act on DNA molecules.

At the same time, the molecular dynamics simulations of the stability of biomolecules exposed to these conditions are being done [4]. These simulations further analyze the severity of possible damage. Eventually, they will provide the probability of strand breaks caused by the shock wave. It may not only depend on the distance of the DNA from the track, but also from the molecule's orientation with respect to the track. This mechanism of DNA damage may be a very important contribution to the chemical effects of radicals, low-energy electrons, and holes.

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RADIAL DOSE DISTRIBUTION AROUND AN ION BEAM TRACK ON THE NANOSCALE

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Radiation damage induced by ion beams in biological tissues, on a molecular scale, is an expanding topic of research [1], boosted by outstanding possibilities of application for ion beam cancer therapy [2] and assessment of radiation risk in space exploration [3].

A nanoscopic view of the process has a crucial step in the analysis of the secondary electrons.

The key role of secondary electrons produced in the process of ionization, while the energetic ions penetrate the tissue, has been pointed out for a long time, and it is well accepted that a significant part of the resulting damage is related to collisions of these abundant secondary species on the biological target rather than from the direct collision of the primary ion. But several open questions are still debated on the mechanisms and the peculiar efficiency of damage induced by ion projectiles, as compared, e.g., with photons. . Thence, the details of the production and propagation of such electrons in tissue (water, DNA constituents or nuclear cell proteins) and the related radial dose deposition has a great relevance in the assessment of the quantitative entity of the following damage, such as double strand breaks in DNA sub-units which are lying close-by to the ion track and allowing to derive the relative biological effectiveness.
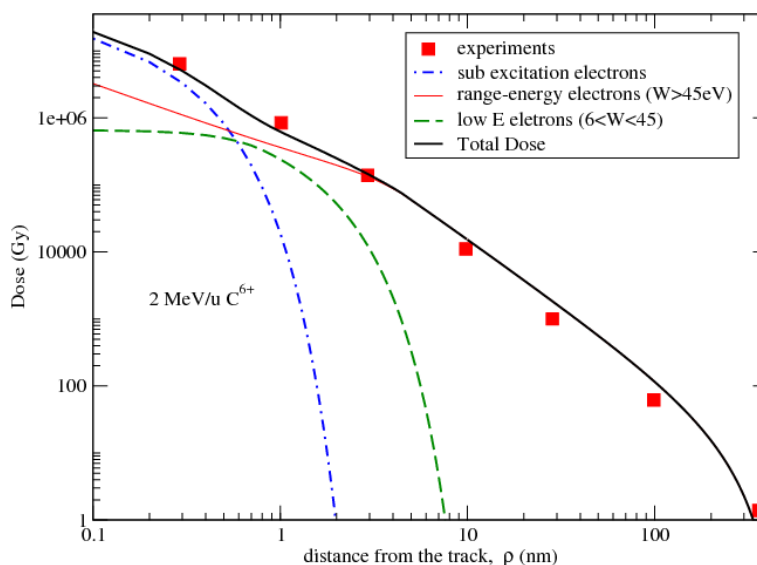
Figure 1: Radial dose from carbon ion irradiation at 2 MeV/u. Present models and different contributions compared to experiments.

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This problem is conventionally tackled with Monte Carlo simulation of tracks, but the latter are limited in handling consistently the large variety of scales in time, distance, and energy involved in the process starting from the ion penetration till the final biomolecular damage.

After reviewing the state of the art in the field, we will present calculations and analysis of radial dose distribution for energetic carbon ions in liquid water. Our method advances further a recently introduced multi-scale approach [4,5], which was suggested to explore the effect of damage by keeping into account the different physical effects and scales in play [6,7,8]. For the electron spectra we introduced a new parametrization based on several effects, including experiments on penetration depth of energetic ions, and also exploited a dielectric response function based approach. For the electron propagation we distinguished between different regions of distance from the track: in the inner region a random walk method is proposed, on its turn with different parameters for the subexcitation region and an intermediate energy one, while in the outer radial distance region another approach based on a energy range formalism is preferred and an overall agreement with experimental results is achieved at all the distances from the track. Preliminary calculations of double strand breaks rates obtainable with the present dose calculation result will be also reported and discussed. as well as comparison with other simulations, such as nanodosimetry based codes.

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TEMPERATURE DRIVEN NANOSCALE CONFORMATIONAL TRANSITIONS IN BIOMOLECULAR SYSTEMS

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The conformational nano-scale transitions in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state and vice versa (also known as (un)folding process) or transitions between liquid and solid phases occur in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes, etc. [1].
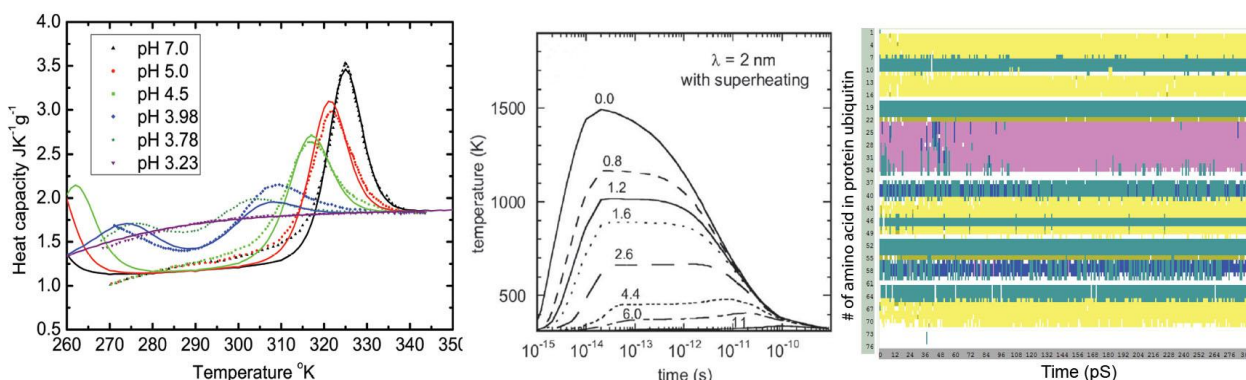
Figure 1. Left: the dependence of the heat capacity on temperature calculated for staphylococcal nuclease at different values of pH. The results obtained using the statistical mechanics model are shown by solid lines, while the results of experimental measurements from Ref [2] are presented by symbols. Center: Energy deposition in eV/atom on the molecular subsystem versus time assuming a superheating scenario. The calculations have been performed for C ions at 0.5 MeV/u with an electronic energy loss of 0.91 keV/nm [3]. Right: The dependence of the secondary structure of protein ubiquitin on time obtained using molecular dynamics simulations. The protein is exposed to the heat spike produced by the propagation of an energetic particle. Prominent disturbance of the secondary structure is observed during first 100 ps after the propagation of a particle.

We suggest a theoretical method based on the statistical mechanics for treating the folding-unfolding transition in proteins. This method describes essential thermodynamical properties of the system such as heat capacity, the phase transition temperature and others from the analysis of the potential energy surfaces of amino acids [4]. We perform thorough comparison of the predictions of the statistical model with the results of experimental measurements of the heat capacity on temperature dependencies for two globular proteins: metmyoglobin and staphylococcal nuclease

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[5]. The comparison with the results of experimental measurements revealed that the developed theoretical formalism is capable to describe with high accuracy various peculiarities of the heat-capacity profiles such as the temperatures of heat and cold denaturations, corresponding maxima and temperature width of the transitions, the dependence of the characteristics of the transition on the properties of external environment, i.e. pH of the solution.

Using the full-atom molecular dynamics simulations we have investigated the influence of the propagation of energetic particles on the conformational structure of proteins. Energetic ions, produced in a therapeutic facility for cancer treatment or proceeding from galactic cosmic rays, while propagating in a biological tissue, generate a large number of electrons through ionization of the medium molecules (mainly water). The interaction of these secondary electrons with water molecules leads to a tremendous short-time local increase of the temperature and pressure in the vicinity of an ion track [3,6]. The molecular dynamics simulations of the temperature spikes caused by energetic particles show that such events result in a distortion of the three dimensional structure of proteins and other biological molecules and their complexes.

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ROLE OF NUCLEAR FRAGMENTATION REACTIONS IN ION-BEAM ENERGY DEPOSITION IN EXTENDED MEDIA

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In this talk I discuss various processes which are responsible for the ion energy deposition in extended media. I demonstrate that in addition to the standard ionization losses one should take into account the nuclear processes, mainly the nuclear fragmentation reactions, leading to disintegration of beam nuclei. These complicated processes can be successfully described by the combination of a dynamical cascade-type model for the initial stage of nuclear reaction and an evaporation/multifragmentation model for de-excitation of residual nuclei. Important requirements to such models is their ability to describe existing experimental data. Recently in FIAS we have developed a Geant4-based Monte Carlo model for Heavy Ion Transport (MCHIT) aimed at simulating propagation of light and heavy ions through different materials. With the MCHIT we are able to calculate not only the 3d distributions of the energy deposition but also the characteristics of secondary fragments which determine the tail beyond the Bragg pick. The model is also used to predict yields of positron-emitting nuclei like 11C and 10C, which are used for PET monitoring of doses. These developments are necessary for accurate dose evaluation in ion-beam cancer therapy and for modeling radiation conditions in interplanetary space missions.

FRAGMENTATION DYNAMICS OF NANOSTRUCTURES

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FROM FRACTALS TO NANOFILMS BY DEPOSITION OF NON-IPR FULLERENES

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Low energy ion beam deposition of mass selected non-IPR (=non isolated pentagon ring) fullerene cations onto clean HOPG has been used to form: (i) fractal aggregates and (ii) at higher coverages mono-dispersed thin film materials /1/. The stability of the films is determined by covalent inter-cage bonds, which can be constituted both by local IPR (=isolated pentagon ring) and by non-IPR sites. Thermal treatment of such cluster aggregates can result in desorption of the original cage building blocks, the formation (and desorption) of fragments and other reaction products as well as in the generation of non-desorbable carbon polymers (which survive the high-temperature regime on the surface). We demonstrate such thermally activated transformations of C_n films using three selected examples: (1) Small non-IPR C_n films ($n \leq 60$, including also non-IPR C_{60} isomers /2/), (2) Cs-doped C_{58} films, (3) C_2 radicals deposited onto C_{58} and C_{60} films. In the first system, desorption of the less coordinated cages competes with the formation of long oligomeric C_n chains. In the second case, Cs addition leads to the cleavage of non-IPR inter-cage bonds (2AP-2AP) as well as to the activation of a disproportionation reaction by which C_{58} bonded partners are converted into C_{60} and $C_{n<58}$. Annealing of the C_2/C_{60} films leads to the formation of "adduct" C_{62}, C_{64} and C_{66} fullerene cages as well as to the formation of stable C_{60}-based polymeric structures. We propose mechanisms to help explain selective cage conversion as well as the observed partition between desorption and irreversible-oligomerization of C_n structures. We also show first surface enhanced Raman (SERS) measurements in support of the proposed mechanisms.

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NANOPARTICLES ON A SURFACE: ATOMISTIC APPROACH FOR STRUCTURE, DYNAMICS AND PATTERN FORMATION

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Nanotechnology is an exploding research domain. This generic word refers to physical and chemical research performed on systems having a characteristic length scale of the order of the nanometer. At that particular length scale, new specific physical and chemical properties emerge. One of the main targets of nanophysics and nanochemistry is the development of controlled, reproducible and industrially transposable, nanostructured materials. An issue of fundamental interest is the precise control of the systems' architecture. All technological developments based on nanostructured materials (potential industrial applications are numerous: micro-electronics, heterogeneous catalysis, magnetic storage, etc) require the understanding of the underlying factors controlling the structuring of the systems.

We present an overview of recent advances in a systematic theoretical description of physical properties of free and supported nanoparticles (atomic clusters) such as their stability, atomic and thermal properties. A special attention is paid to the process of deposition of nanoparticles on a substrate at various energies and to the analysis of dynamics of nanoparticles on a surface. It is demonstrated that the pattern formation on a surface depends crucially on the ratio between the flux of nanoparticles to the surface and their mobility over the surface. We demonstrate that stability of the structures on surface depends strongly on several factors, such as the concentration of impurities and temperature.
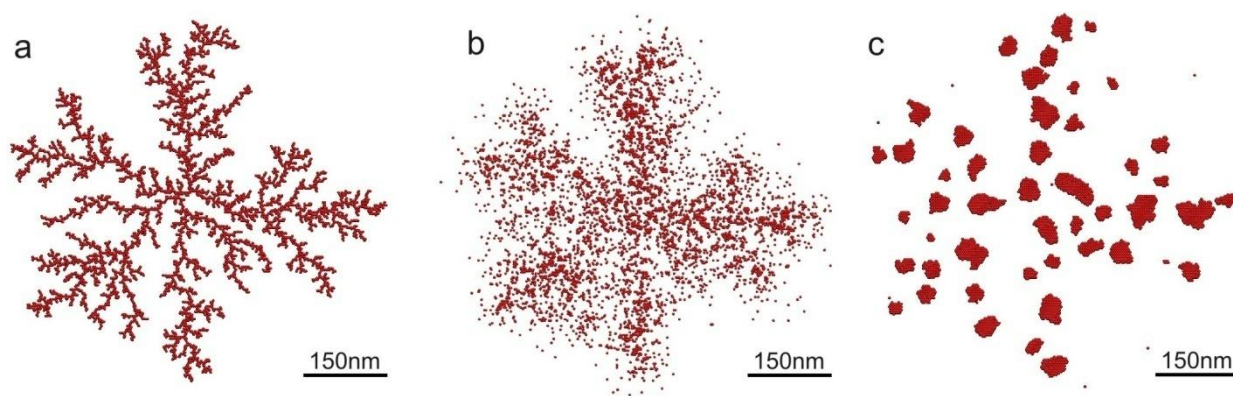
Fig. 1: Evolution of the fractal structure, calculated with accounting for the internal dynamics of the particles in the fractal: (a) initial structure of the fractal; (b) rapid fragmentation of the fractal (c) fragmentation of a fractal due to diffusion of the particles along the fractals branches

We consider the post-growth processes occurring in a nanofractal on surface by accounting for the diffusion and detachment processes in the system. We demonstrate that these kinetic

processes control the final shape of the islands on surface after the post-growth relaxation as illustrated in Fig. 1. Based on the analysis of the results of our simulations, we suggest a criterion which we apply to distinguish between different patterns on a surface.

Additionally, we analyze the diffusion of individual particles on the graphite surface using the classical molecular dynamics method. We investigate how various essential parameters influence the diffusion of clusters on a surface and establish the nature of the diffusion mechanism. In particular, we consider the following parameters: the cluster size, the binding energy between the silver and the carbon atoms in the system, and the system temperature.

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METAL CLUSTER ANIONS: PHOTOIONIZATION CROSS SECTION AND PHOTOELECTRON ANGULAR DISTRIBUTION

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The main goal of present study is to define the role of many-electron correlations in description of photoionization processes in clusters. In this contribution we present the results of calculations of photodetachment cross section and photoelectron angular distribution in metal cluster negative ions. The reason of this consideration is also related to the recent experimental study in which the measurements of angular resolved photoelectron spectra have been performed systematically for sodium cluster anions in a broad range of cluster size [1]. Our calculations demonstrate the dominant role of the many-electron effects in the formation of photoionization cross sections and angular distributions of photoelectrons emitted from sodium cluster anions.

The calculations are performed within the consistent many-body theory based on the jellium model. The single-electron energies and wave functions of valence-electron system are determined within the Hartree-Fock (HF) approximation. In a spherically symmetric field, the single-electron wave functions can be presented by the radial n_r, orbital l and magnetic m quantum numbers. For instance, in the case of Na_{19}^- the electronic configuration of the ground state has the form: $1s^2 1p^6 1d^{10} 3s^2$. The wave functions of excited states are calculated both in the field of a "frozen" electronic cluster core with the created vacancy and with entirely rearranged residual electronic structure of the cluster. The photodetachment amplitudes are calculated using both the HF method and the Random Phase Approximation with Exchange (RPAE) [2].

The concrete results have been obtained for the photodetachment from sodium cluster anions with closed electronic shells: Na_7^-, Na_{19}^-, Na_{39}^-, Na_{57}^-. It is shown that the dynamical many-electron interactions play a crucial role in describing photoionization processes, in particular the cross section in the vicinity of giant plasmon resonance and photoelectron angular distribution in negative ions of metal clusters. For example, the calculated photodetachment cross section $\sigma(\omega)$ and angular asymmetry parameter $\beta_{1d}(\varepsilon)$ for $1d$-shell electron in Na_{19}^- anion are presented in Fig.1, where ω and ε are a photon and photoelectron energies, respectively; $\varepsilon = \omega - I_{1d}$ (I − ionization potential). The outer $2s$- and $1d$-shell electrons give the main contribution to the giant plasmon excitation which lies in the continuum spectra for anions (Fig.1a). This resonance is related to a collective motion of electronic system and appears in calculations only due to the many-electron interactions taking into account within the RPAE.

The crucial role of many-electron correlation effects may be seen well from angular asymmetry parameter calculations for $1d$ electrons in Na_{19}^- (Fig.1b). The single-particle approach applied by the authors in [1] and our HF results [2] fail to describe the obtained experimental data: we have a completely different behaviour of asymmetry parameter just after threshold. The results obtained with dynamic correlations within the RPAE differ qualitatively from the single-particle

picture and are in a good agreement with the experimental data. Note that the account for the rearrangement of electronic shells during photoionization process does not change qualitatively the behaviour of asymmetry parameter and leads to the slight changes of β_{1d} values at the near-threshold region. On the other hand there are several experimental dependencies corresponding to
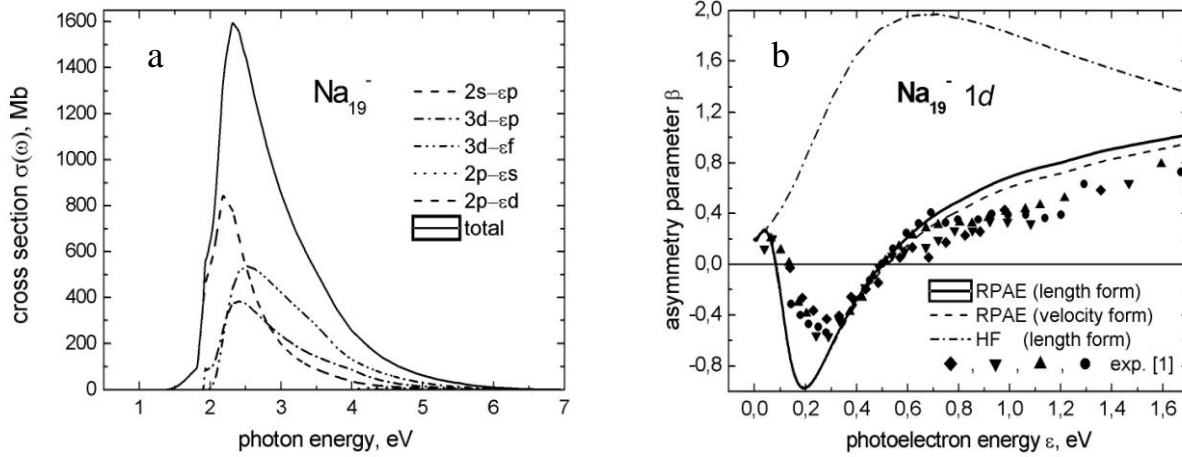
Figure 1: Partial and total photodetachment cross sections $\sigma(\omega)$ (a) and angular asymmetry parameter β_{1d} (ε) (b) for Na_{19}^- anion. Photoelectron energy $\varepsilon = \omega$ - I, Experimental data from [1].

the photoionization from the sublevels of the $1d$-orbital splitted by the crystalline field of the cluster. Therefore for the more accurate description of the photoionization one should take into account the detail geometrical structure of the ionic core.

The similar behaviour of asymmetry parameter with a deep minimum near threshold is obtained for $1p$ electrons in Na_7^-, $1f$ electrons in Na_{39}^- and Na_{57}^- sodium anions. Qualitatively different dependences of β parameter are found for $1g$ and $2p$ electrons in Na_{57}^-. There are no experimental data on photodetachment from this anion however the calculated β_{1g} and β_{2p} parameters are in qualitative agreement with the same parameters measured in Na_{55}^- [1].

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PHOTO-INDUCED PROCESSES IN FULLERENES

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The work is focused on the analysis of several peculiar phenomena, occuring in various photo-induced processes involving fullerenes and/or metallic clusters, which currently are subjects of intensive theoretical and experimental investigation. We present clear theoretical explanations of several experimentally obtained results as well as predict new phenomena which can be verified in experiments.

The following issues will be addressed at the Conference.

● Confinement resonances in photoionization of endohedral systems, $A@C_n$. We demonstrate [1] that the structure of confinement resonances in the photoionization of an encapsulated atom is very sensitive to the mean displacement $<a>$ of the atom from the cage center.The resonances are suppressed if $2<a>$ exceeds the photoelectron half-wavelength. We explain the results of recent experiments [2] which contradict the earlier theoretical predictions on the existence of confinement resonances in particular endohedral systems.

● Dynamical screening of endohedral complexes. The fullerene cage screens the endohedral atom from external electromagnetic fields and, thus, influences the photoabsorption rate of the atom. We demonstrate that this effect is strongly dependent on the photon energy. It was found that in the vicinity of the plasmon resonances of the fullerene, the photoabsorption of the confined atom is strongly enhanced from that of the free atom [3,4].

● Modification of the Auger decay of endohedral atoms. The Auger decay in an encapsulated atom strongly depends on its displacement from the cage center [5]. Using the developed formalism we explain dramatic broadening of the peaks in atomic photoionization measured recently [6] for $Sc_3N@C_{82}$.

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RESPONSE OF ENDOHEDRAL FULLERENES TO PHOTOABSORPTION BY THE ENCAPSULATED ATOM

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Numerous theoretical studies have explored the response of fullerenes to ionizing electromagnetic radiation [1]. Endohedral fullerene molecules, i.e., carbon spheres with one or several atoms encapsulated within the fullerene, have particularly stimulated the imagination of theorists as model systems for caged atoms and as a playground for the prediction of new phenomena [2]. Typically, in the calculations of photon interactions with fullerenes photoabsorption is considered to be equivalent to photoionization. This picture is already oversimplifying the situation with empty fullerenes. In the case of endohedral fullerenes the picture is shattered by recent experimental evidence for numerous additional important reaction channels available subsequent to inner-shell photo-absorption by the encapsulated atom within the fullerene cage. First conclusive experimental results on photon interactions with endohedral fullerenes in the gas phase are presently becoming available [3,4].

When a caged atom is photo-ionized, the emitted electron wave may be reflected by the cage, giving rise to multi-path interference and confinement resonances [2]. This phenomenon has been addressed theoretically mainly for rare gas atoms encapsulated within C_{60}, and most of the theoretical work was devoted to $Xe@C_{60}$. Predictions of the $Xe@C_{60}$ response to photons in the 70 to 150 eV range vary between very strong oscillations in the giant 4d photo-ionization resonance in the Xe atom [5] and only moderate excursions from a smooth cross section dependence [6-8], strongly depending on the model assumptions. Even energy shifts of the oscillations were calculated as a consequence of static polarization effects [9]. Clearly, the thickness of the fullerene shell and a possible displacement of the encapsulated atom from the center of the fullerene, e.g., by thermal motion, have substantial influence on the amplitude of the 4d cross section oscillation. Until very recently, no experiments were available to check which of the theoretical predictions of confinement resonances in $Xe@C_{60}$ is close to reality.

Due to serious limitations in the availability of endohedral fullerenes, the first conclusive experiments with such molecules in the gas phase were carried out with $Ce@C_{82}^{+}$ ions instead of the desirable $Xe@C_{60}$. In a first successful series of experiments on single and double photoionization of endohedral $Ce@C_{82}^{+}$ ions it was possible to extract the contributions of cerium 4d photoexcitation to net single and double ionization of the endohedral molecule [3]. Free Ce atoms or ions absorb photons with energies between 100 eV and about 170 eV almost exclusively via photoexcitation of the 4d subshell with subsequent single or double Auger decay. By that, they fully exhaust the available absorption oscillator strength $f_a=10$ through the net single and double ionization channels. Surprisingly, the experiments with the endohedral $Ce@C_{82}^{+}$ ions revealed a 4d oscillator strength originating from the encapsulated Ce atom of only about $f_a=3.4$ in the single and double ionization of the endohedral molecule.

In the search for the "missing oscillator strength", additional reaction channels of the $Ce@C_{82}^{+}$ ions have to be considered. In recent experiments [4], fragmentation plus ionization in collisions of

photons with $Ce@C_{82}^+$ and $Ce@C_{82}^{++}$ ions was investigated observing a selection of reaction channels:

$$h\nu + Ce@C_{82}^{q+} -> Ce@C_{82-2n}^{(q+m)+} + m\ e^- + n\ C_2 \qquad m=1,2\ ;\ n=1,2,\ldots 11\ ;\ q=1,2$$
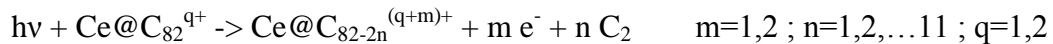
Beside pure electron emission (n=0) the presence of the cage around the absorbing cerium atom can give rise to additional decay mechanisms involving fragmentation of the fullerene cage. The experiments showed that the missing oscillator strength can be retrieved in the reaction channels, where a number n of C_2 dimers is ejected from the cage. In fact, the fragmentation+ionization channels by far dominate pure single and double ionization mediated by cerium 4d excitation. The most remarkable result discovered in the experiments is the large probability for the destruction of the fullerene cage when the photon is absorbed by the encapsulated cerium relative to the absorption by the cage itself. The probability of a 126 eV photon to result, for example, in the ejection of m=2 electrons and of n=6 C_2 dimers is more than 6 times higher when absorbed by the encapsulated cerium atom compared to absorption by the cage.

While the $Ce@C_{82}$ endohedral fullerene target material used in the above experiments was produced by a conventional arc burning and purification process, a recent set of experiments [10] made use of an implantation technique to produce $Xe@C_{60}$ for studying its response to synchrotron radiation. Small quantities of $Xe@C_{60}$ could be synthesized by bombarding thin layers of C_{60} with accelerated Xe^+ ions. Very dilute mixtures of $Xe@C_{60}$ with C_{60} and C_{70} were evaporated into the plasma chamber of an electron cyclotron resonance (ECR) ion source. Mass selected beams of $Xe@C_{60}^+$ ions with about a tenths of a nanoampere at 6 keV energy could be made available for photon-ion merged beam experiments. The measured cross section for the production of $Xe@C_{58}^{3+}$, i.e., for double ionization plus fragmentation of the parent $Xe@C_{60}^+$ ion, provides first experimental evidence for confinement resonances. Further experiments with better statistics are desirable and will be conducted in the future.

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Fr-III-1

FREE ELECTRON LASERS: DYNAMICS AND SRUCTURE TOWARDS FEMTOSECOND TIME AND NANOMETER SPATIAL RESOLUTION

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*F*ree *E*lectron *L*asers (FEL) are innovative, accelerator-driven light sources that now have been demonstrated to deliver, for the first time, intense coherent light in a wavelength regime from tens of nanometers down to even one Ångström. Pulse intensities surpass those of 4th generation synchrotrons by a factor of one billion and the light flashes, with a duration of less than ten femtoseconds (1 fs = 10^{-15} s), are more than thousand times shorter than achievable up to now. Thus, FELs penetrate a *terra incognita* in light-matter interaction opening a new chapter in science throughout all disciplines, in physics, material science, chemistry or biology.

The talk will highlight the working principles of FELs and the performance of the first machines operational worldwide, the FLASH in Hamburg, the SCSS in Japan and the LCLS in Stanford. Exploiting the capabilities of a new instrument, the *C*FEL-*A*SG *M*ulti *P*urpose (CAMP) end-station [1] (Figure 1) that allows the simultaneous momentum resolved detection of electrons, ions, scattered as well as of fluorescence photons, pioneering results of in atomic, molecular and cluster physics have been achieved pointing to the rich future potential. Can we record "the molecular movie", i.e., follow in time the motion of atoms and the rearrangement of electrons, e.g., at transition states during chemical reactions, for light-harvesting molecules and will it be possible to realize the vision determining the structure of single biomolecules − proteins, viruses − or nanoparticles in gas or liquid phases without the need of crystallization?
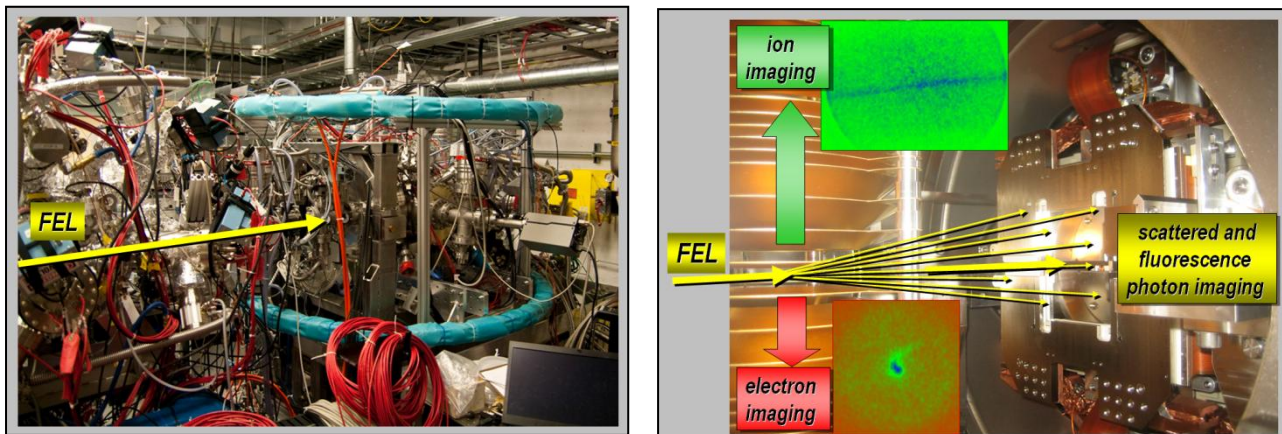

Figure 1: Left: The CAMP end-station operated at the LCLS at Stanford. Right: View inside with imaging spectrometers for electrons, ions and photons (large-area, fast read-out, low-noise X-ray CCDs).

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EXPERIMENTS ON CHANNELING IN CRYSTALLINE UNDULATORS

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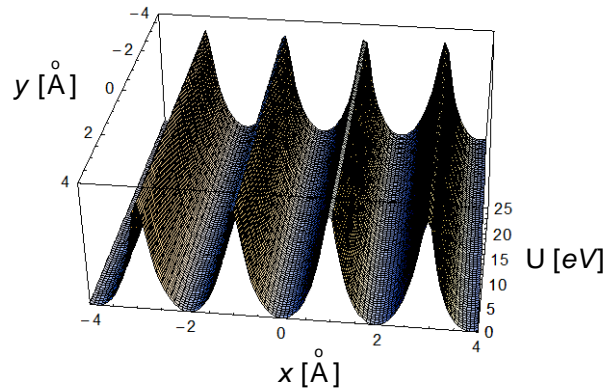

Figure 1: Transverse potential of (110) planes for positrons in a silicon single crystal.
The transverse motion of a positron in a bound state is called planar channeling.

If the crystal planes are periodically bent at the direction the particle moves, undulator-like radiation in the hundreds of keV up to the MeV region may be emitted in addition to channeling radiation. The possibility to produce such radiation by means of positron channeling was discussed in a number of papers, see e.g. Ref. [1]. However, the demonstration and utilization of such devices hampers from the fact that high quality positron beams in the GeV range are not easily available, in contrast to electron beams. It was suggested in Ref. [2] that by means of planar channeling of ultrarelativistic electrons in a periodically bent single crystal the production of undulator-like radiation should also be possible. The basic idea of this work is that similar dechanneling lengths as for positrons can also be achieved with electrons if their beam energy is chosen a factor of about 20 larger as for positrons.

There are several possibilities to realize crystalline undulator targets. Our approach is based on the production of graded composition strained layers in an epitaxially grown $Si_{1-x}Ge_x$ superlattice [3]. Because of the slight difference in the lattice constants between Si and Ge, adding a small content x of Ge to Si in a molecular beam epitaxy (MBE) growing process results in strain in the crystal and a bending of the crystal lattice. By varying the concentration x in the $Si_{1-x}Ge_x$ superlattice linearly and periodically [4], undulating (110) planes can be obtained (in the y-direction of Fig. 1).

Experiments have been performed at the Mainz Microtron MAMI to explore the radiation emission from 4-period epitaxially grown strained layer $Si_{1-x}Ge_x$ undulators with a period length λ_u= 10 µm and 50 µm. Electron energies of 195, 270, 855 and 1508 MeV have been chosen. The analysis for the short-period undulator indicates, in comparison with a flat reference crystal, a broad excess yield around photon energies of 36, 69 and 637 keV at incident electron energies of 195, 270 and 855 MeV, respectively.

The fact that the expected peak structures have not been observed experimentally prompted us to study also the dechanneling length of electrons, i.e., the distance an electron can be steered in a plane before it leaves the channel due to collisions with atoms or electrons. The experiments have been performed at the Mainz Microtron MAMI at various beam energies between 195 and 855 MeV for flat silicon single crystals only. In order to get a feeling for the dechanneling phenomenon in bent crystals, calculations on the basis of the Fokker-Planck equation have been initiated for which the centrifugal force will be taken into account.

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CRYSTALLINE UNDULATOR AS A SOURCE OF COHERENT RADIATION

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In the proposed talk recent advances in the theory of novel sorces of hard electromagnetic radiation: Crystalline Undulator (CU) and Crystalline Undulator based Laser (CUL) will be presented.

The operating principle of CU is based on the channeling phenomenon. Channeling takes place if a particle enter a crystal at a small angle to major crystallographic planes or axes. The particle becomes confined by the planar or axial potential and move preferably along the plane or axis following its shape.

If the planes or axes are periodically bent, the particles move along nearly sinusoidal trajectories. Similarly to what happens in ordinary undulator, relativistic charged particles radiate electromagnetic waves in the forward direction. The advantage of the crystalline undulator is an extremely strong electromagnetic field incide the crystal which can steer the particles much more effectively than the most advanced superconductive magnets. This allows to make the period of CU two or even three orders of magnitude smaller then that of the conventional undulator. As a result the frequency of the radiation can reach the hard X ray and gamma ray range.
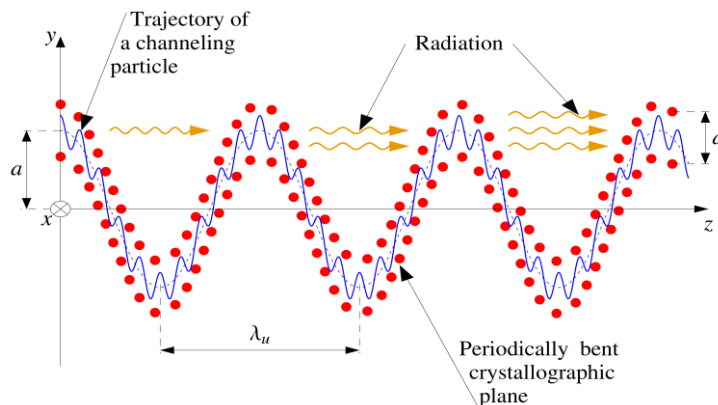

Figure 1: The scematic representation of the crystalline undulator.

The radiation becomes more powerful and coherent if the density of the particle beam that feeds the undulator is modulated along the beam direction with the period equal to the wavelength of the produced radiation. In this case the electromagnetic waves emitted by different particles have nearly the same phase and therefore the intensity of the radiation becomes proportional to the particle density squared in contrast to the linear proportionality in the case of unmodulated beam.

The beam can be modulated in ordinary (magnetic) undulator tuned to the wavelength of auxiliary light which is integer multiple of the wavelength of the crystalline undulator radiation (here called 'main radiation').

The auxiliary wavelength should be in the optical or soft X ray range which is attainable in the present state-of-the-art magnetic undulators and free electron lasers.The auxiliary radiation can be provided by an external source and should be directed along the axis of the magnetic undulator so that it can interact with the particle beam. Alternatively, the auxiliary radiation can be produced in the magnetic undulator itself if it operates as a self amplified spontaneous emission free electron laser (SASE FEL).

Due to the interaction with the auxiliary wave and the field of the magnetic undulator, the beam will be spatially modulated with the period equal to the wavelength of the auxiliary radiation. But the Fourier decomposition of the density profile will contain also higher harmonics with shorter wavelength including the wavelength of the main radiation. The necessary harmonic can be essentially amplified if the initial particle beam has a layered energy profile [2].In the recent patent application [3] we have described a device in which the crystalline undulator is placed near the exit from the magnetic undulator and therefore is fed by a modulated particle beam. This tandem of magnetic and crystalline undulators allows the intensive generation of coherent radiation in hard X-ray or gamma ray range. Thus we called the suggested device the Gamma-laser.

In the proposed talk these novel ideas will be presented and discussed in detail in the context of the earlier work of the group devoted to the theory of crystalline undulators and the development of the crystalline undulator based novel light sources [4,5].
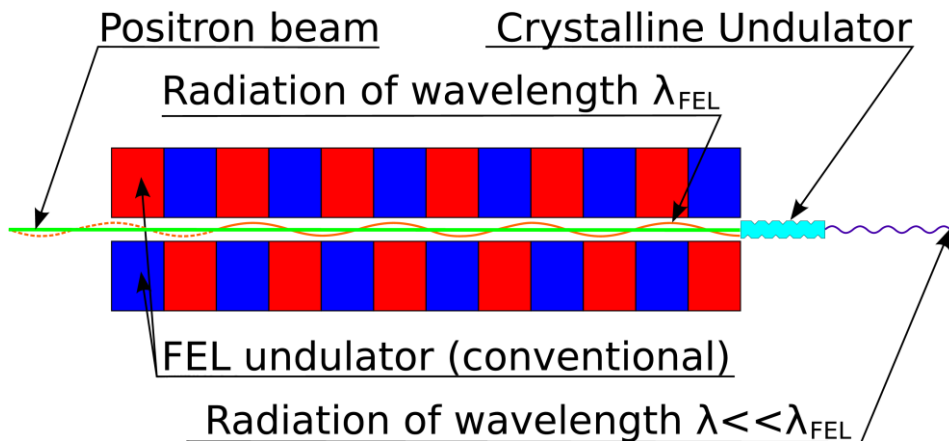

Figure 2: The scheme of the crystalline undulator-based laser.

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EXOTIC NUCLEAR CLUSTERS: SUPERHEAVY, NEUTRON-RICH, SUPERSTRANGE, ANTIMATTER

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The extension of the Periodic Table into new dimensions will be discussed. Nuclei can be superheavy, but also very neutron rich, i.e.nuclei like 42O or 270Pb are expected to be stable. Also nuclei with very many hyperons (containing s-quarks) or clusters consisting solely of hyperons are theoretically expected to exist. The same is true for antinuclei. We shall discuss wayshow to produce such exotic nuclear clusters, even in macroscopic quantities.

THE IMPORTANCE OF NANOSCIENCE FOR REVERSIBLE ENERGY STORAGE AND URBAN VEHICLES IN MEGACITIES

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In the megacities of today, a major concern is air quality and it is now well established that the nanoparticles in toxic exhaust fumes constitute an additional factor which multiplies the health risk due to petrol and diesel motors by virtue of a 'size effect' which embeds the toxins in the human lung tissue. Such particles disperse quickly in an open environment, but persist in confined spaces and tunnels, and the hazard due to fumes is therefore far greater in large cities where the concentration of population and density of traffic are maximised. Many cities are therefore turning to the two forms of clean power promoted as alternatives, namely (1) the electric car based on rechargeable or 'rocking chair' batteries and (2) the hydrogen car or electric car equipped with fuel cells. Unfortunately, both types of vehicle present weaknesses which suggest that much more research is needed into their weakest points, viz. the energy storage, which remains inefficient and the nature of the proposed fuel in the case of hydrogen, which is difficult to handle, store and distribute safely. While the electric and hydrogen-powered vehicles are locally clean, one must also consider the primary source of energy outside the city: there is little point in promoting locally clean vehicles which would aggravate the global problem and require a large consumption of fossil fuels in some other place to keep megacities clean. Therefore, efficient energy storage in the vehicles is the real (but as yet unachieved) goal. There are a number of requirements to be satisfied for the development of the clean cars of the future, all of which relate to the storage / recovery cycle, and these requirements point to nanotechnologies as the most promising source of new materials for the purpose. This talk will present a brief review of the current situation as far as can be gathered from published work, and will attempt to explain in simple terms why the interest in nanosciences for energy storage is so great at the present time, and what kinds of materials hold most promise.

Posters

HYDRATED CLUSTERS OF NUCLEIC ACID BASES IN SUPERSONIC BEAMS PROBED BY MULTIPHOTON IONIZATION MASS SPECTROMETRY

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The formation and UV multiphoton ionization (MPI using 220-230nm nanosecond laser pulses) of hydrated clusters of DNA/RNA bases are investigated by time-of-flight mass spectrometry. Clusters are formed in a continuous supersonic expansion of argon and water vapor seeded with sublimated nucleobases. The aim of this work is to contribute to understanding the effects of hydration on the excited and ionic states of UV-irradiated biomolecules.

Fig. 1(i) shows the first MPI mass spectrum of uracil-water clusters. The strong peaks for hydrated uracil monomer ions up to $U_1^+(H_2O)_7$ compared with the U^+ peak are consistent with IR spectroscopic evidence for particularly strong uracil-water hydrogen bonds [1]. By contrast, the non-hydrated adenine monomer ion is one of the most intense peaks in our equivalent adenine-water mass spectra (Fig. 1(ii)). Our data as a function of laser fluence (presented in the poster) demonstrates that at least 3-photon absorption is required for A^+ production in both dry and hydrated conditions. This implies internal conversion from the short-lived π^* excited state to the electronic ground state with extensive vibrational excitation, increasing the likelihood of cluster dissociation.
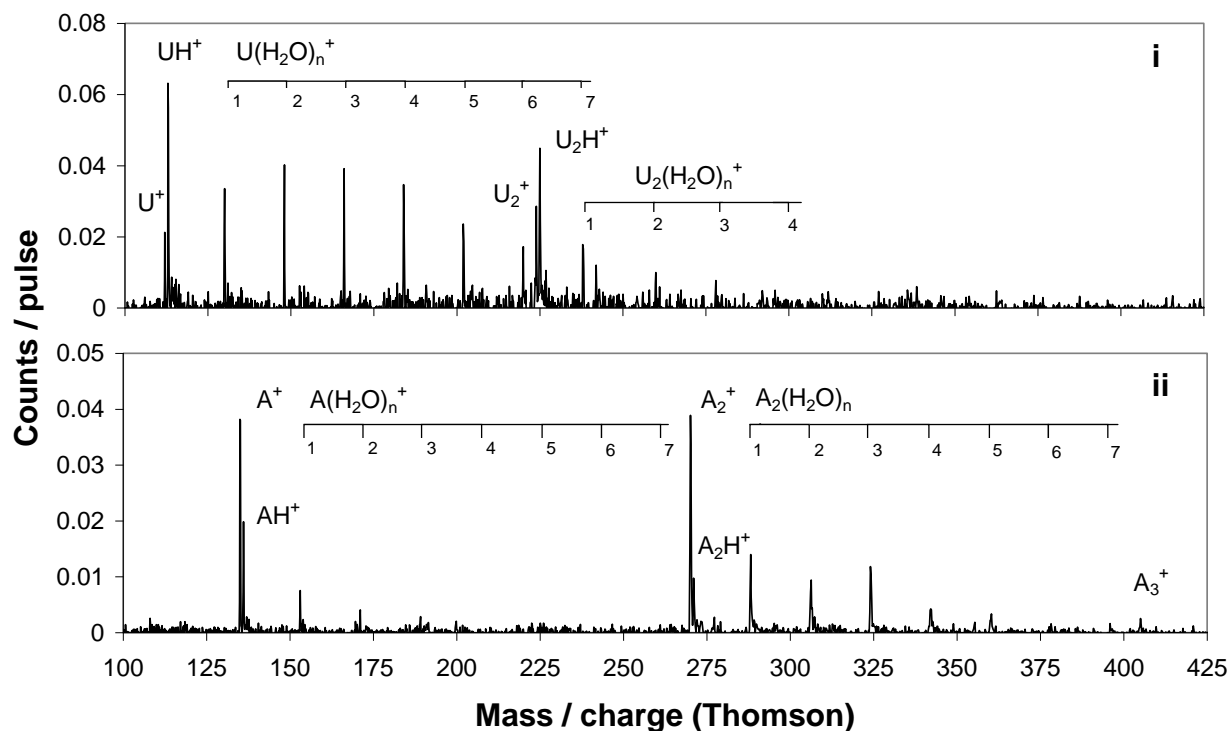

Fig. 1: One color (222 nm, 10^6 Wcm^{-2}) MPI mass spectrum of hydrated uracil (i) and adenine (ii)

PS-01

The mechanism for the production of protonated adenine ions depends on the ionization scheme. For non-hydrated adenine dimers, Hunig et al.'s [2] data for nanosecond excitation at 285 nm indicates hydrogen transfer in the neutral excited state, whereas time-resolved femtosecond photoelectron spectroscopy experiments at shorter wavelengths (266 nm) do not support this process [3]. In both cases, proton transfer in the ionic state has been confirmed. On the basis of the available thermochemical data [4], we suspect that the latter mechanism dominates in our experimental conditions; however hydrogen transfer in π-stacked structures of hydrated dimers is also possible and worth investigation.

The mass spectrum of hydrated adenine-uracil mixed clusters is shown in Fig. 2. Relatively strong $(AU)^+(H_2O)_n$ production indicates that the weakness of the U^+ signal is not due to scarcity of uracil in the neutral beam. We attribute the weak U^+ signal to extensive uracil-adenine clustering and proton transfer from uracil cations to neutral adenine within clusters. The 1,3-dioxo tautomer is the most stable uracil cationic form [5] with calculated acidity ranging from 198 to 220 kcal/mol depending on the proton site, compared with a proton affinity of 225 kcal/mol for neutral adenine [4]. Thus proton transfer from U^+ to A in a dimer cation is exothermic and cluster fragmentation is expected to produce a protonated adenine ion and a neutral deprotonated uracil radical. Regarding adenine ionization, the acidity of the adenine radical cation is 221 kcal/mol [4], compared with a proton affinity of 205 kcal/mol for the neutral uracil dioxo tautomer [6]. Hence proton transfer from adenine cation to neutral uracil is endothermic and the charge stays on adenine, producing A^+ and U upon cluster ion fragmentation. Our results indicate that the presence of water aids clustering but does not affect proton transfer processes in uracil-adenine cluster ions significantly.
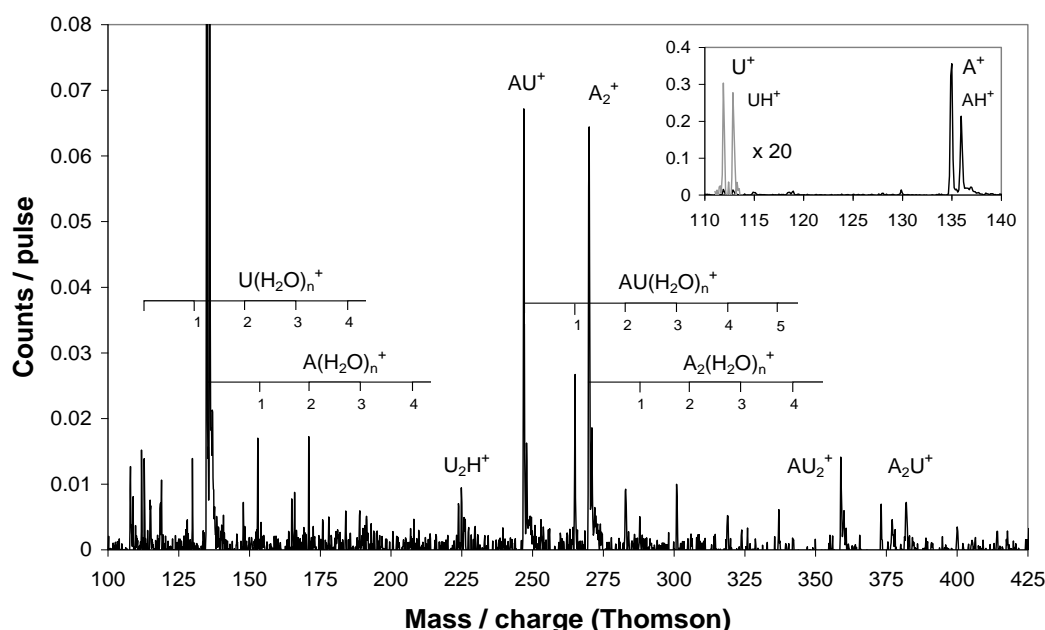

Fig. 2: One color (222 nm, 10^6 Wcm^{-2}) MPI mass spectrum of hydrated uracil-adenine complexes

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DEFECT-INDUCED SHIFT OF THE PEIERLS TRANSITION IN TTF-TCNQ THIN FILMS

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Organic charge transfer compounds represent a class of materials for interdisciplinary research on the borderline of correlation physics, material science and chemistry. In particular organic charge transfer compounds form a basis for extending the rapidly growing field of organic electronics towards binary donor-acceptor systems. In this regard thin film growth studies, as well as surface and interface-oriented research on the electronic properties of these materials become more and more important [1,2].

The interest in the electronic properties of organic charge transfer materials was boosted already in 1973, after the first successful fabrication of a novel organic conductor, tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ) [3]. TTF-TCNQ consists of parallel homosoric stacks of acceptor (TCNQ) and donor (TTF) molecules as illustrated schematically in Fig. 1. It was demonstrated that due to the interaction between the π-orbitals arising along the stack direction (corresponding to the b-direction in Fig. 1b) the electrical conductivity of TTF-TCNQ is strongly anisotropic with $\sigma_b/\sigma_a > 10^2$ at room temperature, where σ_b and σ_a are the electrical conductivities along the a- and b-directions, respectively. TTF-TCNQ single crystals show metallic behavior down to about 60 K and undergo a series of phase transitions at $T_H = 54$ K, $T_I = 49$ K and $T_L = 38$ K, which successively suppress the metallic conductivity of the TTF and TCNQ chains, turning the material into an insulator. The phase transition at 54 K is driven by a charge density wave (CDW) Peierls instability in the TCNQ chains and is usually referred to as Peierls transition.
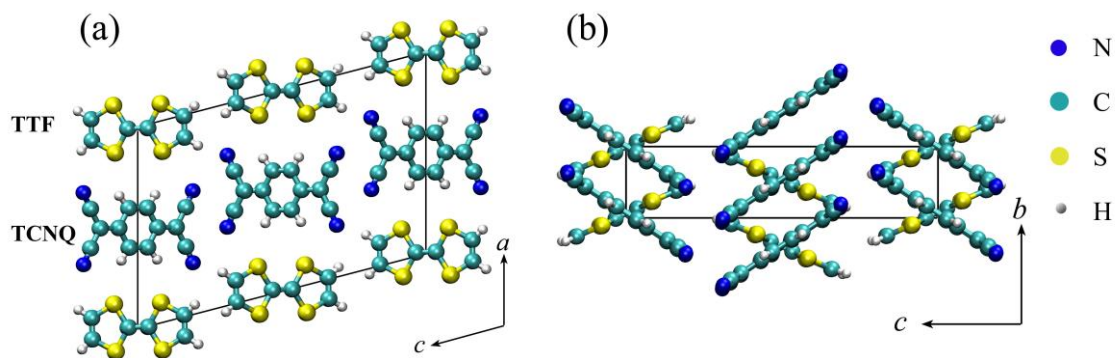

Figure 1: Crystalline structure of TTF-TCNQ in the monoclinic crystal system with space group P2$_1$/c. (a) Orthogonal view along the stacking b-axis. (b) Orthogonal view along the direction perpendicular to the *(bc)*-plane of TTF-TCNQ.

We investigate the influence of the substrate material and film thickness on the Peierls transition temperature in TTF-TCNQ thin films grown by physical vapor deposition. Different substrates were used for this purpose, such as SrLaGaO$_4$(100), SrLaAlO$_4$(100), MgO(100), MgF$_2$(001), MgF$_2$(100), Si(100)/SiO$_2$(285 nm), α-Al$_2$O$_3$(11$\underline{2}$0), and NaCl(100) substrates. X-ray diffraction data for all investigated films reveal that the *(ab)*-crystallographic plane of TTF-TCNQ

is aligned parallel to the substrate, while from SEM images it is evident that the substrate material and the growth conditions strongly influence the film morphology. (See Fig. 2).
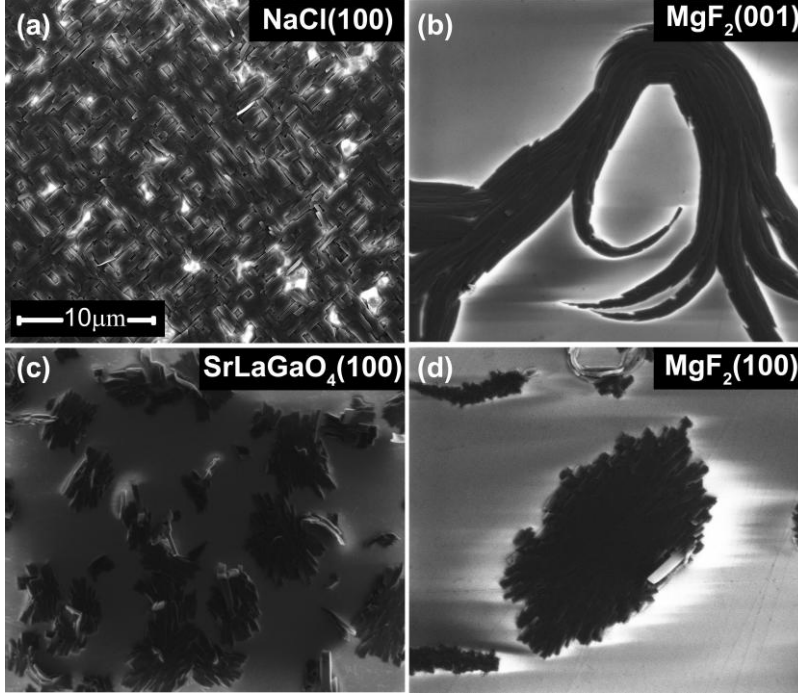

Figure 2: SEM images of TTF-TCNQ thin films grown on
(a) NaCl(100),
(b) MgF$_2$(001),
(c) SrLaGaO$_4$(100) and
(d) MgF$_2$(100)
substrates after 1 hour of deposition at 110 °C effusion cell temperature.

From electrical conductivity measurements we determined the Peierls transition temperature of the thin films under the influence of several critical factors. In particular, we demonstrate that the TTF-TCNQ film thickness and the substrate material do not cause significant changes of the Peierls transition temperature, while the defect density in the thin films introduced during the evaporation process is a factor which leads to a noticeable change in the Peierls transition temperature [4]. We observed that the Peierls transition temperature in thin films is lower than in TTF-TCNQ single crystals by 4 K. It was suggested that the decrease of the Peierls transition temperature due to defects obeys the following relation [5]:

$$\ln\left(\frac{T_{P0}}{T_P}\right) = \Psi\left(\frac{1}{2} + \frac{\hbar}{2\pi k_B T_P}\right) - \Psi\left(\frac{1}{2}\right),$$

where T$_{P0}$ and T$_P$ are the transition temperatures in the absence of defects and with defects, respectively. k_B is the Boltzmann constant, $\Psi(x)$ is the digamma function, τ is the scattering time due to the presence of defects and can be estimated from $l = \tau v_F$. Here l is the average distance between the defects and v$_F$ is the Fermi velocity. Using this approach we obtain 0.14 % defect concentration. This agrees favorably with the single crystal analysis performed in [6].

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HIGH FIELD EFFECTS IN NANOPARTICLES INDUCED BY X-RAY ABSORPTION

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Because of the high intensities available, synchrotron radiation offers a unique tool for studying the interaction of x-rays with nanoparticle structures. In an initial experiment, performed at the ESRF in 2002, our goal was to use x-ray induced ionization to map the density of nanoparticles in a hydrocarbon diffusion flame. The results obtained [1,2] were very surprising for instead of the expected weak ionization signal, a strong emission of electrons was observed when the flame was irradiated with a white beam of x-rays in the energy range from 5 to 30 keV.

This phenomenon can be explained by a model (coming from astrophysics) in which an x-ray photon leads to the ejection of an unreactive high energy primary electron and a second Auger electron (having for carbon, an energy of 262.4 eV) which scatters through the aggregated structure of a soot particle leading to multiple secondary electron emission. This electron loss leads to the buildup of high electric fields within the structure that causes further field emission of electrons and hence the high electron signal. This model is illustrated in figure 1.
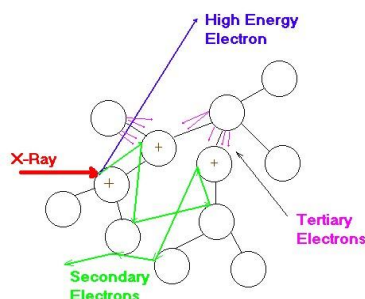

Figure 1: The primary, secondary and tertiary release of electrons due to the x-ray absorption by a aggregated nanoparticle structure.

In recent years we have concentrated on the use of small angle x-ray scattering (SAXS) to determine particle size distributions in flames [3] but a new apparatus is under construction that will explore the x-ray absorption by soot aggregates using both mass spectrometry and electron energy spectroscopy. A first experiment will be performed at SOLEIL in December of this year. The interest for astrophysics of this experiment will be highlighted.

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PHOTOELECTRON IMAGING IN PUMP-PROBE EXPERIMENTS COMBINING SYNCHROTRON AND LASER RADIATION

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Two-photon resonant photoemission, where the electron ejection proceeds via the excitation and subsequent ionisation of an intermediate state, is an efficient tool for the study of neutral excited states, for the complete understanding of the dynamics of photoionization and for the investigation of time-resolved photoelectron angular distributions (PADs). In our work the velocity map imaging (VMI) technique has been used to measure the PADs of electrons emitted from Rydberg states of rare gases excited by synchrotron radiation and then photoionised by a synchronised linearly polarised laser light. The analysis of the angular distribution

$$I(\theta) = \frac{\sigma}{4\pi}[1 + \beta_2 P_2(\cos\theta) + \beta_4 P_4(\cos\theta)]$$

allowed the extraction of the β_2 and β_4 asymmetry parameters which are related to the radial matrix elements and phase differences of the outgoing electron waves in the continuum.
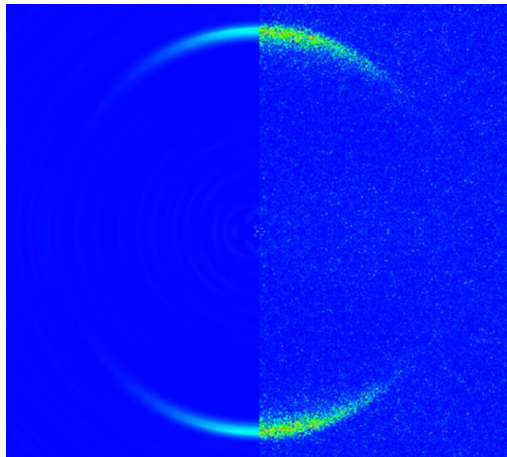continuum.

Fig.1: On the right side is the raw photoelectron image obtained following photoionization of the synchrotron prepared He 1s3p Rydberg states by a laser field with energy of 160 meV in excess of the ionization threshold. On the left hand side is the inverted image using the pBASEX method [2] from which the kinetic energy and angular distribution of the photoelectrons can be extracted.

In this work we studied the ionisation of several intermediate states in He, Ne and Ar for photoelectron energies from 20 to 100 meV. The geometry used in this experiment allows access to more parameters than revealed by previous methods [3] thus providing a better description of the photoionisation event. The experimental results have been interpreted via an angular momentum analysis method as well as compared with the predictions of a single channel quantum defect calculation.

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STUDY OF NANOMETER THICK FILMS BY SURFACE POLARITON SPECTROSCOPY

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We have used surface polaritons (SP) to study dielectric magnesium oxide films and conducting quasicrystalline Al-Pd-Re films on sapphire substrates. Surface polariton is the non-radiative interface electromagnetic mode, propagating along the interface of media and its field exponentially decays out of the interface [1, 2]. So it is very sensitive to the state of the surface and can be successfully used to characterize it and to estimate the film conductivity.

The introduction of a transition layer at this interface results in the shift and broadening of SP. This effect can be used to obtain film parameters (thickness and optical constants) in the region of SP existence and to evaluate the film conductivity.

Thin dielectric (10, 30, 100 and 300 nm thick) MgO films have been prepared by the chemical vapor deposition technique and conducting quasicrystalline Al-Pd-Re films (45 nm thick) have been deposited on sapphire substrates using layer-by-layer ion-plasma sputtering with subsequent vacuum annealing. The SP spectra have been measured by the attenuated total reflection (ATR) technique in Otto configuration [1], using IFS66v (BRUKER) infrared Fourier-transform spectrometer. The ATR unit NPVO-1 (LOMO, Saint-Petersburg) with KRS-5 prism was used for various angles of incidence (20-60 degree in the prism). Angular dependencies of the absorption bands in the spectra give the dispersion of SP on these structures. The measured SP dispersion is compared with one calculated using the literature film parameters and parameters obtained from the dispersion analysis of the external reflectivity spectra of 100 and 300 nm thick MgO films and quasicrystalline Al-Pd-Re films. For thinner MgO films there is almost no effect of the film deposition in the external reflectivity spectra. Due to the resonance interaction of the sapphire substrate SP (high frequency SP branch 635-810cm^{-1}) with the film vibrations [1] the splitting of the dispersion curve of the sapphire SP appears near 700 cm^{-1}. The splitting is present even for 10 and 30 nm films and is proportional to the square root of the film thickness in accordance with the theoretical predictions [1]. Optical constants of ultrathin MgO films and conducting quasicrystalline Al-Pd-Re films have been obtained from SP spectra measurements. In this region the sapphire SP in the presence of the quasicrystalline Al-Pd-Re film is broadening (due to the presence of metallic phase in the film).

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ON FLY PATH INTEGRAL MONTE CARLO STUDY ON H_5^+

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Since the experimental detection of H_5^+ in 1962 [1], the series of $H_{(2n+1)}^+$ ionic hydrogen clusters have attracted the attention of the astrophysicists, as these species and their deuterated isotopologues were found to play a key role in deuterium fractionation in the interestellar medium [2].

In order to assess the importance of quantum effects and anharmonicity present in H_5^+, we have performed Path Integral Monte Carlo (PIMC) simulations at a typical interestellar temperature of 10 K [3]. The electronic energy has been computed on the fly using the B3(H) DFT functional, specially designed for hydrogen-only systems, leading to a precise description of all aspects of the H_5^+ PES [4]. Based on this DFT/PIMC scheme full-dimensional converged results were obtained on the thermal equilibrium state and dissociation enthalpy of H_5^+ (see figure 1).

In particular, radial and angular distributions show that the internal proton is completely delocalised between the two H_2 units, which in turn, are almost freely rotating around the C_2 symmetry axis. These features show the quanttum nature of this hydrogen cluster and the importance of including anharmonic effects in the calculations. A result of particular relevance is the dissociation energy D_0 (see figure 1), which is in excellent agreement with the latest experimental results [5].
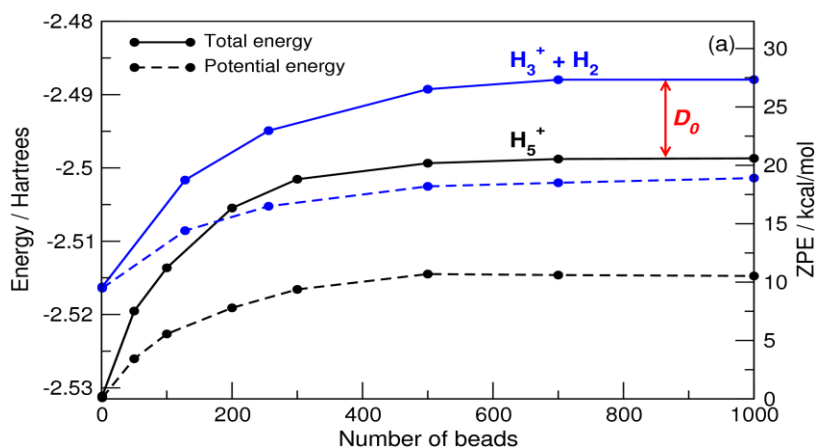

Figure 1: PIMC results for the zero point energy (ZPE) of H_5+ and its fragments, H_3^+ and H_2 (in Hartrees). The dissociation energy D_0 is also depicted (in kcal/mol). Note that a thousand beads were needed to reach convergence.

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CRITERIA OF NANOSCALE SURFACE PATTERN FORMATION

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

In the present work we investigate the process of fractal formation on a surface. For this we have developed a method describing the internal dynamics of particles in a fractal and accounting for the particle diffusion and detachment [2, 3]. We demonstrate that these characteristics determine the shape of the islands created on a surface. Based on the analysis of the results of our simulations, we suggest criteria which can be used to distinguish between different patterns on a surface.
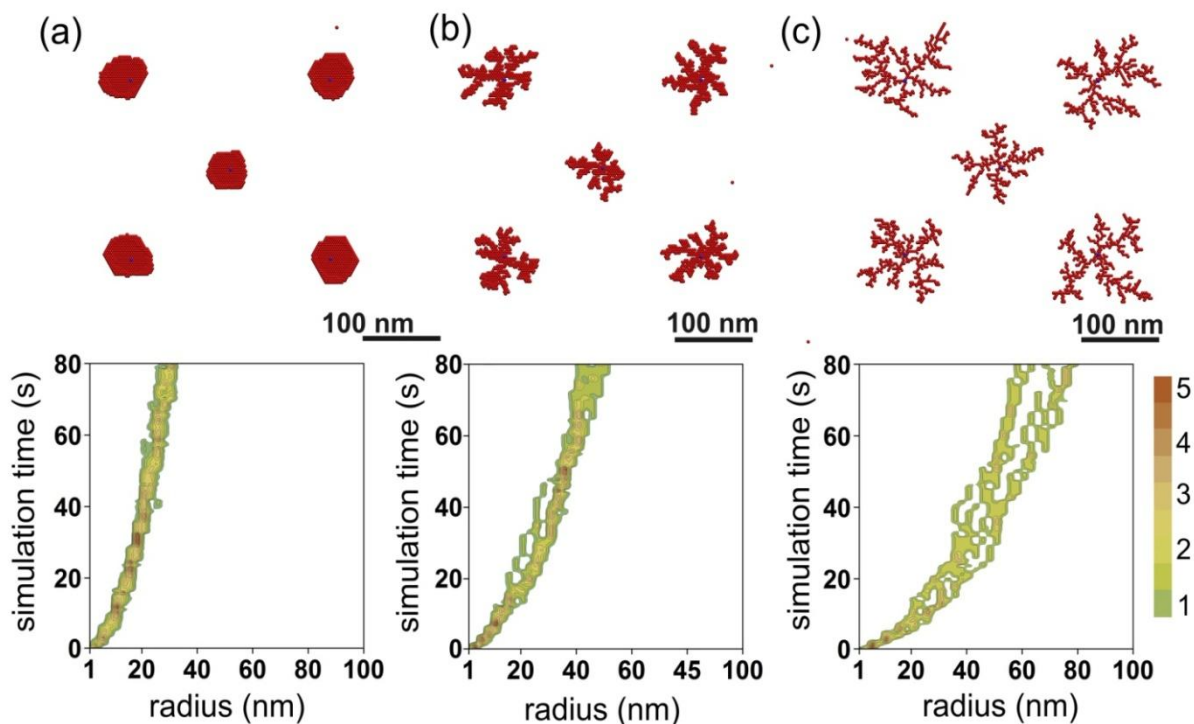

Figure 1: Formation of islands with different morphologies on a surface during the particle deposition process: (a) formation of compact islands; (b) formation of fractals with thick branches; (c) formation of the fractal structures with thin branches. The calculation was performed by varying ratio between the nucleation and the rearrangement time of the deposited particles, as discussed in the text below. Plots (a), (b) and (c) show the morphology of formed structures after t = 80 s of simulation. Contour plots illustrate the time evolution of the size distribution calculated for the emerging islands.

To illustrate the process of particle self-organization on a surface we consider three different scenarios shown in Fig. 2. We deposit the particles on a surface with the rate $F = 10^9$ particle/cm^{2}s being close to the experimental value [1]. The computation was performed with the use of the MBN Explorer Computer package [4]. As known from experiment the deposited particles nucleate more efficiently in the vicinity of point defects. Therefore, to speed up the nucleation process we have introduced five fixed point defects on the surface that become the island growth centers as illustrated in Figs. 1a-c.

We demonstrate that the morphology of islands on a surface is mainly governed by the characteristic time needed for the newly deposited particles to reach the growth region (nucleation time) and by the characteristic time needed for a particle to find an optimum position within an island (rearrangement time). When the rearrangement time is shorter than the nucleation time the compact structures are formed (see Fig. 1a). In the case of fractals with thick branches some peripheral particles have enough time to rearrange and form a more compact structure (see Fig. 1b), while in the case of fractals with thin branches the inner dynamics of particles in the fractal is almost frozen (see Fig.1c). The fact that fractals with thinner branches grow almost without any significant rearrangement leads to the formation of larger size structures, as compared to the more compact fractals with thicker branches during the same simulation time interval (see Fig. 1a-c). The compactness of an island can be characterized by the value of the fractal dimension [2] which is usually calculated by the box-counting method or using the mass-formula for dimension introduced in [5]:

$$N = \rho \left(\frac{2R}{d_0} \right)^{d_f} ,$$

where N is the number of particles in the system, R is the radius of the minimal circumscribed circle of the fractal structure, d_0 is the diameter of a particle and ρ is the ratio of the covered surface to the entire surface area (packing density). In the present work we quantify the emerged patterns on a surface using the calculated value of the fractal dimension.

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TOWARDS UNDERSTANDING THE MECHANISMS OF SILVER NANOPARTICLES DIFFUSION ON GRAPHENE

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The synthesis of metallic nanostructures (e.g. silver nanostructures) with the tailored size and shape has a number of practical applications. Different shapes of Ag nanostructures on a surface can be fabricated with the use of the silver cluster deposition technique under different external conditions [1-3]. The sizes and morphology of the synthesized Ag nanostructures strongly depend on the silver cluster mobility on a surface. In turn, the mobility of particles on a surface is governed by the particle diffusion mechanism on a surface [1].

This work is based on our earlier investigations where the evolution of the cluster structure on a surface and the clusters dynamics were studied with the use of the kinetic Monte-Carlo based models [4, 5]. Here we present the results of the classical molecular dynamics simulations performed for the silver clusters on graphene. We investigate how various essential parameters of the system influence the diffusion of clusters on a surface and establish the nature of the diffusion mechanism. In particular, we consider the following parameters: the cluster size, the binding energy between silver and carbon atoms in the system and the temperature.
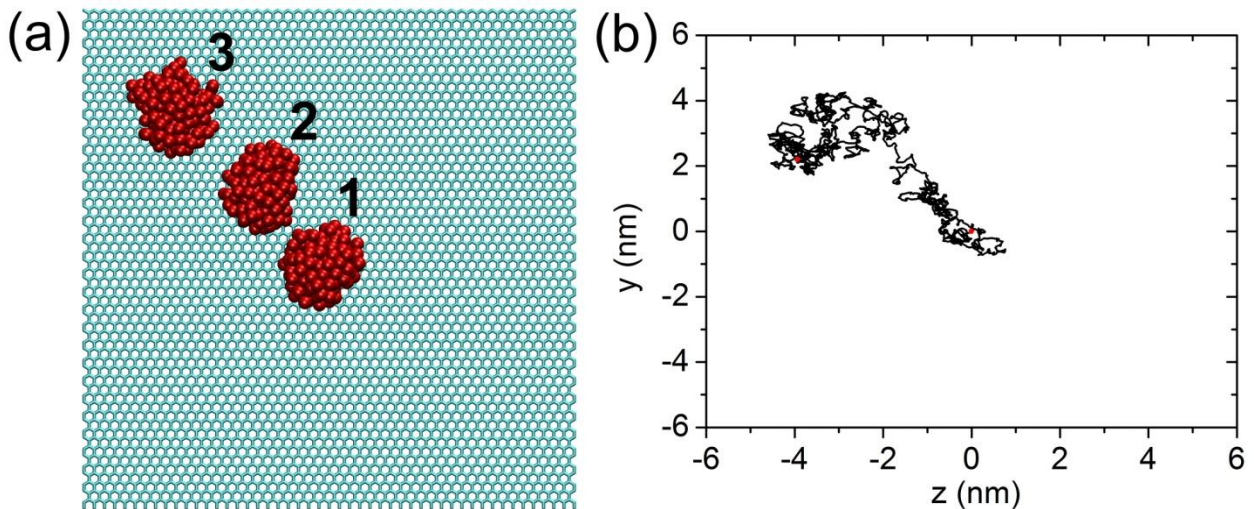

Figure 1: (a) Snapshots of the Ag_{135} cluster moving on graphene at different stages of the simulation, and (b) the trajectory of the Ag_{135} center of mass. The numbers 1, 2, 3 in (a) enumerate the cluster states in time, the time interval between these stages is 5 ns. The simulation time in (b) is 40 ns.

The Sutton-Chen potential was used to model the interparticle interactions inside of the silver cluster [6, 7]. The interaction between the silver and the carbon atoms was modeled by the pairwise Morse potential [6, 7]. The computations were performed with the use of the MBN

Explorer computer package, which is developed for structure optimization, simulation of dynamics and growth processes in various bio-nanosystems [8].

We analyzed the trajectories of the deposited nanoparticles and the evolution of their shape during the diffusion process depending on the system's temperature and the binding energy of silver and carbon atoms (see Fig. 1). The diffusion coefficient of a nanoparticle on graphene is defined as:

$$D = \frac{1}{4} \frac{d\langle r^2(t) \rangle}{dt}, \tag{1}$$

where $\langle r^2(t) \rangle$ is the mean square displacement of the particle on a surface as function of time

$$\langle r^2(t) \rangle = \frac{1}{n_t} \sum_{i=1}^{n_t} [r(t_{oj} + t) - r(t_{oj})]^2 \tag{2}$$

Here $r(t)$ is the radius vector of the particle center of mass at the instant t. Equation (2) assumes the splitting of the trajectory of a particle in n_t segments of equal duration. This is done in order to improve the statistics when evaluating the mean square displacement. We demonstrate that the diffusion coefficient of a silver nanoparticle on graphene strongly depends on the size of the cluster and the on temperature in the system.

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OSCILLATIONS IN PARTIAL PHOTOIONIZATION CROSS SECTION OF ENDOHEDRAL NOBLE GAS FULLERENES

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The oscillations in partial cross sections of photoionization of atomic clusters, in particular, of fullerenes C_{60}, at high photon energies was experimentally discovered more than 10 years ago [1]. These oscillations appear due to the reflection of photoelectrons at the borders of cluster potential and, as a result, the formation of spherical standing waves inside the cluster. From mathematical view, it can be explained in terms of the peaks which appear in the derivative of the self-consistent cluster potential dV/dr [1]. Besides, the oscillatory pattern strongly depends on the product $\left(\phi_{n_r l} \dfrac{dV(r)}{dr} \right)$, where $\phi_{n_r l}$ is the wave function of the initial-state wave with definite radial n_r and orbital l quantum numbers.

Recently, the similar oscillation was shown to occur in the photoionization cross sections of endohedral noble gas fullerenes, in particular $Ar@C_{60}$ [2]. In the cited paper the electronic structure of the complex was calculated within the Local Density Approximation (LDA) and the photoionization cross section within the Time Dependent LDA (TDLDA). Significant changes in the oscillatory behavior of the partial cross sections were found even for slightly hybridized $2p$ and $2d$ orbitals in the $Ar@C_{60}$ complex in comparison with C_{60}.

The present work is devoted to the application of the consistent quantum many-body theory to the description of photoionization of endohedral noble gas fullerenes. The unified electron system of $Ar@C_{60}$ contains 258 electrons, 240 of which are the valence electrons of the fullerene and 18 are from the argon atom. The single-electron energies and the wave functions are obtained within the self-consistent Hartree-Fock (HF) approximation. It is shown that the non-local exchange interaction leads to a significant hybridization of $2p$ and $2d$ orbitals. To compute the excited states wave functions we use the frozen-core HF approximation. The partial and total cross sections of the photoionization are calculated within the Random Phase Approximation with Exchange (RPAE). Self-consistent potential $V(r)$ of the endohedral system has a double-well profile in
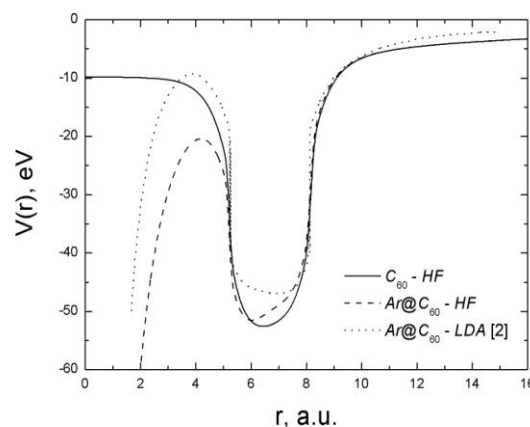

Figure 1: Self-consistent potentials of a fullerene C_{60} and endohedral fullerene $Ar@C_{60}$ calculated within HF (present work) and LDA [2].

contrast to the single-well potential of the empty fullerene C_{60}, see Fig. 1. Due to the additional well at the center of the system one may expect strong changes of the oscillations in the partial cross sections for endohedral fullerenes.

The comparison of the calculated partial cross sections of photoionization for $2g$, $2p$, $2d$ orbitals in the compound $Ar@C_{60}$ and in empty fullerene C_{60} is presented in Figs. 2a,b,c, respectively The calculation has been carried out within the RPAE both in the length (L) and the velocity (V) forms. Preliminary analysis of the obtained results shows that the changes in the oscillatory behaviour of the partial cross sections depend on the electron density distribution between embedded atom and fullerene shell, i.e. on the hybridization of ground state orbitals. Thus the calculations reveal the significant difference between the $Ar@C_{60}$ and C_{60} cases in oscillation behaviour of the photoionization cross section of the non-hybridized orbitals . For example, the partial $2g \rightarrow \varepsilon f$ cross section of the non-hybridized $2g$ orbital in $Ar@C_{60}$ differs significantly from that in empty C_{60} (Fig. 2a). The $2p$ orbital originated from Ar atom is strongly hybridized in $Ar@C_{60}$ complex and the essential part of $2p$ electron density is localized in the vicinity of fullerene shell. As shown in Fig. 2b, the oscillation behaviour of the partial $2p \rightarrow \varepsilon s$ cross section of photoionization of $Ar@C_{60}$ is also changed beside the C_{60} case but less than in the $2g \rightarrow \varepsilon f$ cross section. The electron density of the $2d$ hybridized orbital is sufficiently delocalized with respect to fullerene shell, and, as it is shown in Fig. 2c, there are no noticeable differences between oscillation behaviours in cross sections in cases $Ar@C_{60}$ and C_{60}.

Figure 2 (a,b,c): Calculated partial photoionization cross sections of a C_{60} and $Ar@C_{60}$ within the RPAE.

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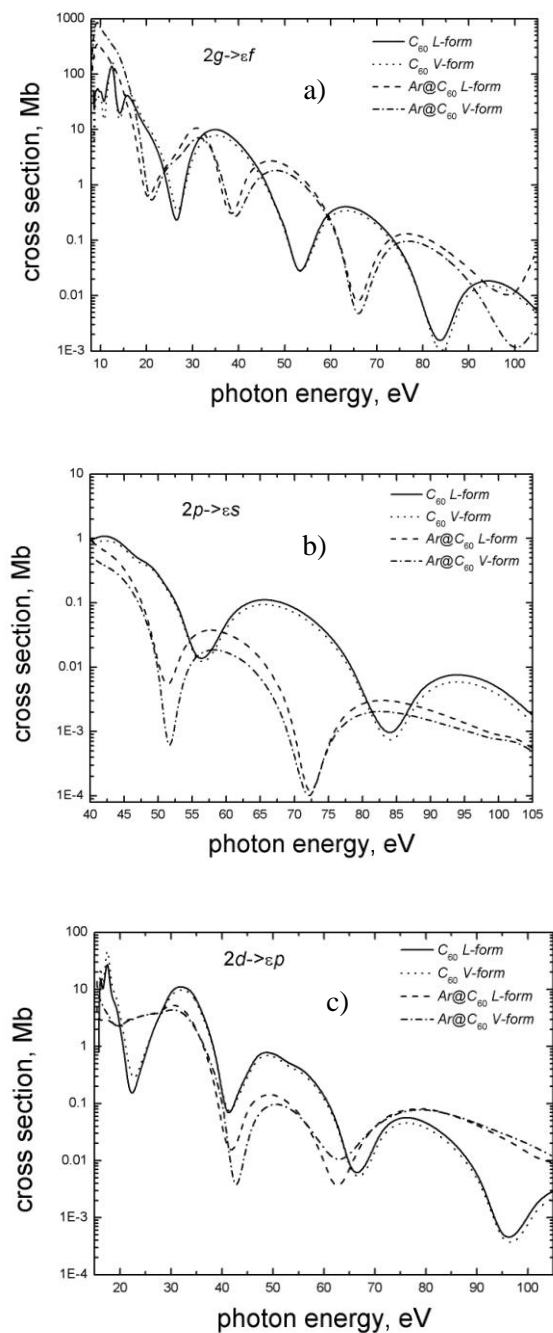
MICROMECHANICS OF DNA UNZIPPING

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The transition of DNA macromolecule from a double-stranded state to a single-stranded configuration *in vivo* is a key element in reading and reproduction of genetic information. In a course of this transition the hydrogen bonds in DNA complementary pairs become broken and the nucleic bases "open" to the external environment. The understanding of the mechanics of the DNA double-helix unzipping is one of the central problems of the DNA physics and molecular biology. In the last decade significant achievements in studies of DNA unzipping were obtained with the use of the single molecule manipulation techniques (atom force microscopy, optical and magnetic tweezers) [1,2]. In present communication the process of DNA strands separation is studied with accounting for the close-open transitions in complementary pairs, performed within the frame of phenomenological approach and also with the use of steered molecular dynamics (SMD).
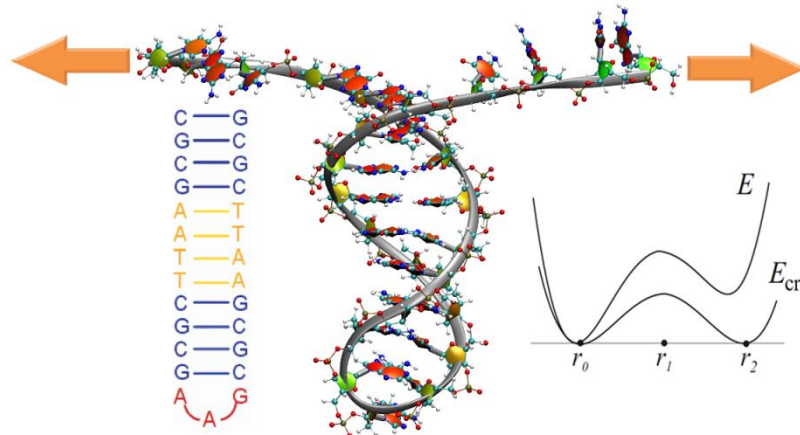

Fig. 1. Structure of a DNA double helix dodecamer. External unzipping forces acting on the DNA strands are shown with bold arrows. The inset on the right shows the characteristic profile of the potential energy for the complementary base pairs as a function of the interbase distance. At a critical value of the external force the potential energy profile has two minima with the same energy (E_{cr}). Thus, the topology of the potential energy surface can lead to the soliton-like regime of the unzipping fork propagation.

In order to describe the entire process of DNA unzipping we have proposed the most probable pathway of the mechanical strands separation in the double helix and have constructed a phenomenological model of DNA unzipping [3]. The model accounts for the stretch of the bases in complementary pairs and their rotation in the double helix. The proposed theoretical model allows predicting the kinetic parameters of base pair opening on different pathways in the double-stranded DNA [3] and the level of critical force for DNA strands separation [4]. The good agreement of the predictions of the theoretical model with the results of experimental measurements justifies the use of proposed model for the understanding and description of the DNA unzipping dynamics. Within the developed theoretical formalism the two-stage mechanism of the DNA unzipping by external

force is suggested. The proposed mechanism explains the cooperative nature of the unzipping process under the physiological conditions and the threshold character of the external force action. The process of DNA double helix unzipping is considered as a nonlinear dynamical process powered by an external force. On the first stage of the unzipping process the external force transforms the conformation of the double helix to the so-called "bistable" conformational state. During the second stage of the unzipping process the transition of the base-pairs from the closed to open state occurs and the unzipping propagates along the DNA molecule. The boundary between the open and the closed parts of the helix (so called 'unzipping fork') is demonstrated to move along the macromolecule chain as a step-like excitation (kink soliton). The moving unzipping fork consists of closed, preopened and open base pairs. An important element of the proposed unzipping mechanism is the transition of a closed complementary pair to its metastable preopened state under the action of an external force. It is suggested that the stability of the preopened pair state arises due to the interaction of bases with the surrounding water molecules.

To confirm our assumptions about the mechanism of unzipping process and the nature of base pairs stability in the preopened state, we have performed molecular dynamics simulations for the double stranded DNA in the water and counterions environment [5]. The investigated DNA duplex is constructed from Drew-Dickerson's dodecamer sequence and the hairpin (AAG) added at the end of the double helix. In the molecular dynamics (MD) simulations the dodecamer duplex is getting consequently unzipped pair by pair by the use of SMD type algorithm. Translational and rotational degrees of freedom of the base pairs in the unzipping dodecamer are analysed using the trajectories of the MD simulations. The analysis revealed that during the duplex unzipping each pair rotates relatively quickly together with the whole helix and then performs a slower rotation when the distance between the two bases increases. In order to allow the base pair unzipping in the fork the rest (closed) part of the helix has to rotate as a whole. In real DNA molecules with large contour length the free rotation of the helix is inhibited by the drag effect [6,7]. However, the rotational motion of the base pairs in the unzipping fork has to be the same as that of the considered dodecamer.

The MD simulations show that the opening of the base pairs occurs in the unzipping fork. The process of base pair opening consists of the untwisting of the base pairs (up to the zero value of helix rotation angle), and the stretching of H-bonds in pairs with the simultaneous incorporation of water molecules between the bases. Water molecules stabilize the preopened state of the base pairs in the fork. These stabilized intermediate states may lead to the formation of bistable transitional conformation of the helix before unzipping. The MD simulations showed that the trajectories of strands separation for different cases of unzipping are very similar for the regions of the duplex with predominant G·C content, and rather diverse for regions with A·T-pairs sequence. Comparison of the results of MD simulations with the predictions of our phenomenological model validate the assumption that under the action of external force the DNA base pairs undergo a transition to the metastable states, that are responsible for the threshold character of the unzipping process and can lead to the appearance of the cooperative effects in the strand separation of DNA.

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ELECTRONIC STRUCTURE OF ENDOHEDRAL FULLERENES WITH NOBLE GAS ATOMS

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Since the first experimental observation of endohedral fullerenes [1], series of theoretical studies dedicated to the investigation of these compounds and their interaction with photons within different models (see [2] and references therein) have arisen. In this work we apply for the first time the self-consistent Hartree-Fock (HF) approximation to calculate the electronic structure of noble gas endohedral fullerenes. As an example the compounds He@C_{60}, Ne@C_{60} and Ar@C_{60} are discussed in this contribution.

The total electronic system consisted of all electrons of the encapsulated atom and 240 valence electrons of fullerene C_{60} is considered in the spherically symmetric field created by the ionic core of a fullerene and the nuclear charge of embedded atom placed in the center of the spherical layer. Thus the electronic configuration, for example for Ar@$C_{60,}$ consists of 258 electrons:

$$1s^2 2p^6 3d^{10} 4f^{14} 5g^{18} 6h^{22} 7i^{26} 8k^{30} 9l^{34} 10m^{34} 2s^2 3p^6 4d^{10} 5f^{44} 6g^{18} 7h^{10} 3s^2.$$

The energy-level spectrum of this compound is presented on figure 1.
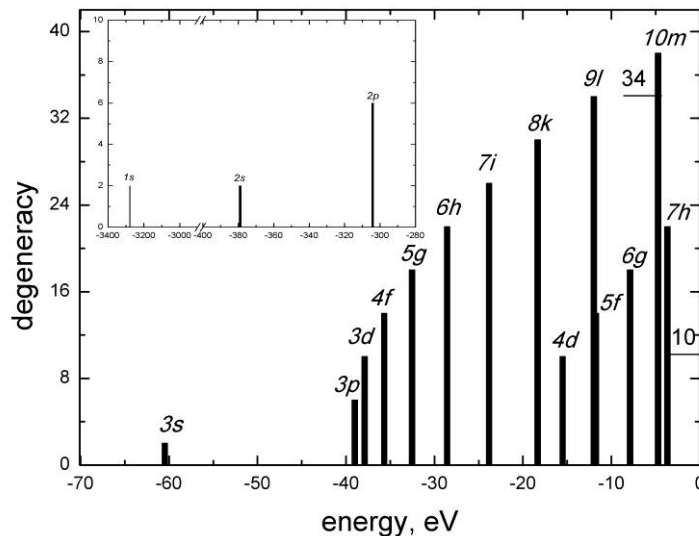
Figure 1: Calculated energy-level spectrum of the endohedral fullerene Ar@C_{60}.
None-nodes orbitals are occupied up to $l = 9$ (*10m* shell), one-node orbitals are
occupied up to $l = 5$ (*7h* shell). There is also one two-nodes state (*3s* shell).

The valence electrons of the fullerene are distributed in a usual way with ratio of 3 : 1 over the σ (none-node) and π (one-node) orbitals, correspondingly. The fullerene ionic core is presented by a uniform distribution of positive charge (Z=240) over spherical layer of the finite thickness [3]. Additional electrons from noble gas atom should be arranged either in a new shell which is absent in the configuration of the fullerene (for example, 3s in case of Ar@C_{60}) or in the partially filled fullerene orbitals by reason of minimal electronic energy principle.

Results of the calculations show that the inner-shell electrons (1s in He, 1s2s in Ne and 1s2s2p in Ar) remain to be the inner-shell electrons of the endohedral fullerene and they are located mostly near the embedded atom, while the behaviour of the outer atomic wave functions has revealed the strong hybridization of valence atomic and fullerene orbitals with the same values of angular momentum. For example, besides the ordinary near atom behaviour, the 3p electron density of Ar@C_{60} has additional maximum in the vicinity of the fullerene shell (see figure 2).

In conclusion, it has been found that there is a significant redistribution of the electronic density of hybridized states within the HF approximation beside the Local Density Approximation (LDA) (see figure 2). So it seems to be essential to take into account the non-local exchange interaction to calculate the electronic structure of endohedral complexes.
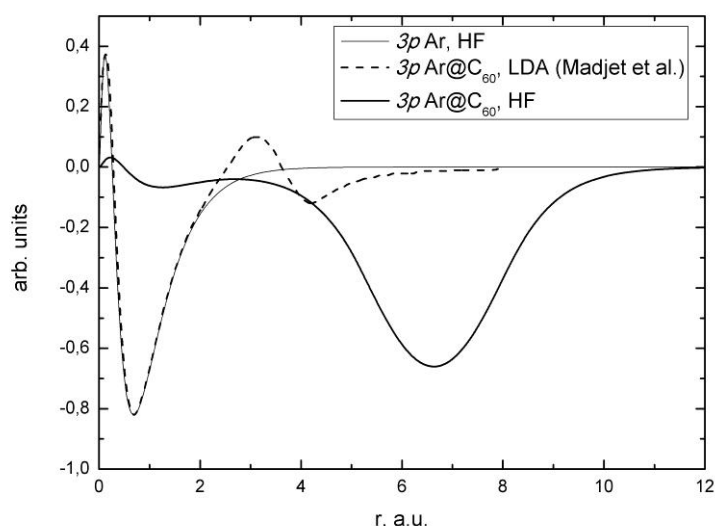
Figure 2: *3p* wave function of free Ar (HF) and hybridized *3p* wave function of compound Ar@C_{60} taking into account local (LDA) and non-local (HF) exchange interaction between electrons of the system. The LDA data is taken from [4].

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MBN EXPLORER - A FLEXIBLE PROGRAM FOR SIMULATING MOLECULAR AND NANOSTRUCTURED MATERIALS

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We present a multi-purpose computer code MBN Explorer. The developed package allows to model molecular systems of varied level of complexity. In particular, MBN Explorer is suited to compute the system's energy, to optimize structures, as well as to consider the molecular dynamics. MBN Explorer allows to use a broad variety of interatomic potentials, to model different molecular systems, such as atomic clusters [1], fullerenes, nanotubes [2], proteins, composite systems [3], nanofractals [4,5] etc. A distinct feature of the program, which makes it significantly different from the already existing codes, is its universality and applicability to a broad range of problems and molecular systems. Most of the existing codes are developed focusing on a particular class of molecular systems, and have severe limitations, while MBN Explorer goes beyond these drawbacks. On demand, MBN Explorer allows to group particles in the system into rigid blocks, thereby significantly reducing the number of degrees of freedom and simplifying the equations of motion. This algorithm is especially useful in studying of molecular dynamics of complex systems, consisting of large interacting building blocks, e.g. proteins or fullerene-based nanowires.
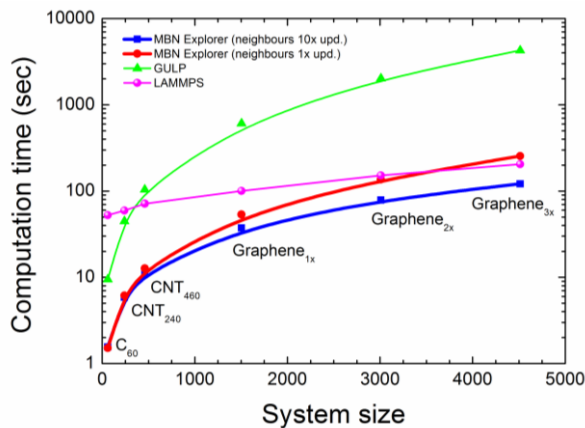
Despite the universality, the computational efficiency of MBN Explorer is comparable (and in some cases even higher) than the computational efficiency of the existing programs. The figure shows the computation time, needed to perform 1000 molecular dynamics simulation steps for a variety of carbon-based systems: C_{60}, carbon nanotubes (CNT) consisting of 240 and 460 atoms, graphene mono, di- and trilayers. The comparison shows that MBN Explorer is a promising alternative to the existing programs.

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