

ISACC 2008

International Symposium Atomic Cluster Collisions: Structure and dynamics from the nuclear to the MesoBioNano scale

St. Petersburg (Russia), June 3-7, 2008

Editor: Andrey V. Solov'yov



Abstracts

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Table of Contents

TABLE OF CONTENTS
PREFACE
ORGANIZING COMMITTEE
INTERNATIONAL ADVISORY COMMITTEE
ACKNOWLEDGEMENTS
OVERVIEW OF ABSTRACTS
INVITED SPEAKERS
Structure and properties of atomic clusters
CLUSTERS ON SURFACE
PHOTON-CLUSTER COLLISIONS AND CLUSTERS IN LASER FIELDS
ELECTRON AND ION CLUSTER COLLISIONS
CLUSTERING PHENOMENA AT NUCLEAR AND SUBNUCLEAR SCALES
PHASE TRANSITIONS, FUSION, FISSION AND FRAGMENTATION IN FINITE
<i>SYSTEMS</i>
STRUCTURE AND DYNAMICS OF BIOMOLECULES
Collision processes involving biomolecules
FROM BIOMOLECULES TO CELLS AND SYSTEM BIOLOGY
POSTERS
PARTICIPANTS
AUTHOR INDEX

Preface

The Third International Symposium "Atomic Cluster Collisions: structure and dynamics from the nuclear to the MesoBioNano scale" (ISACC 2008) will be held during June 3 - 7, 2008 in St Petersburg, Russia. The venue of the meeting will be the Saint Petersburg Scientific Center of the Russian Academy of Sciences. ISACC 2008 is organized by the A.F. Ioffe Physical-Technical Institute, St. Petersburg State University, St. Petersburg State Polytechnical University, A.I. Herzen State University, and Frankfurt Institute for Advanced Studies. ISACC is recognized by the European Physical Society (EPS) as a Europhysics Conference.

ISACC started as an international symposium on atomic cluster collisions in St. Petersburg, Russia in 2003. The second ISACC was held at the GSI, Darmstadt, Germany in 2007. The ISACC 2008 will promote the growth and exchange of scientific information on the structure and properties of nuclear, atomic, molecular, biological and complex cluster systems studied primarily by means of photonic, electronic, heavy particle and atomic collisions. In the symposium, particular attention will be devoted to dynamical phenomena, many-body effects taking place in clusters, nanostructures, molecular and biological systems, which include problems of fusion and fission, fragmentation, collective electron excitations, phase transitions and many more. Both experimental and theoretical aspects of cluster physics, uniquely placed between nuclear physics on one hand and atomic, molecular and solid state physics on the other, will be subject of the symposium.

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Conference Venue

The ISACC 2008 will be held in Saint Petersburg, Russia at the Saint Petersburg Scientific Center of the Russian Academy of Sciences located in the heart of St Petersburg, near the St. Petersburg State University and the Hermitage Museum. In this place the Russian Academy of Sciences was founded in 18th Century.

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Acknowledgements

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We acknowledge assistance from Ms. Stephanie Lo, FIAS Frankfurt am Main, in the preparation of the book of abstracts.

Conference Program

Tuesday, 03 June 2008

$9^{20} - 9^{30}$		ISACC-2008 Opening
9 ³⁰ - 10 ⁰⁰		Andrey Solov'yov – BioNano mechanics.
$10^{00} - 11^{30}$		Structure and properties of atomic clusters (part I) :
	Tu-I	Julius Jellinek – Atomic-level analysis of response properties of finite systems Vadim Ivanov – Spherical hollow cluster system: stability and electronic structure Dorin Poenaru – Interaction energy at the end cup of a deposited atomic cluster
$11^{30} - 11^{50}$		Coffee break
11 ⁵⁰ – 13 ²⁰	Tu-II	Structure and properties of atomic clusters (part II) Junfeng Geng – Metal and carbon at nanometer scale: the catalysis and growth Valentin Nesterenko – Population transfer process: from atoms to clusters and Bose-Einstein condensate Peter Toennies – Magic superfluid ⁴ He and para-H ₂ clusters
$13^{20} - 13^{30}$		Conference Photo
$13^{30} - 15^{00}$		Lunch
15 ⁰⁰ - 16 ³⁰	Tu-III	Clusters on surface (part I)Catherine Bréchignac – Deposition migration and coalescence of silver nanoparticles on carbon surfacesAtsushi Nakajima – Soft-landing isolation of transition-metal-benzene sandwich complexes into an alkylthiol self-assembled monolayer matrix Andrey Lyalin – Impurity effect on the melting of clusters
$16^{30} - 17^{00}$		Coffee break
17⁰⁰ - 18⁰⁰	Tu-IV	Clusters on surface (part II) Ziyou Li – Three-dimensional atomic-scale structure and stability of size- selected clusters on surfaces Radu Gheorgescu – Ground state and shape isomer deformations of alkali metal atomic clusters

Wednesday, 04 June 2008

$9^{15} - 10^{45}$	We-I	Photon-cluster collisions and clusters in laser fields (part I)
		Stefan Schippers – Collective excitations in (endrohedral) fullerene ions illuminated by synchrotron radiation
		Ulf Saalmann – Laser-driven rescattering for atomic clusters
		Thomas Fennel – Ionization dynamics of clusters in strong laser fields
$10^{45} - 11^{15}$		Coffee break
$11^{15} - 13^{15}$	We-II	<u>Photon-cluster collisions and clusters in laser fields (part II)</u>
		Andrey Belyaev – Photoionization of the fullerene C_{60} and its positive ions
		Andrey Korol – Collisional and radiative processes involving strongly
		polarizable cluster targets
		Stephanie Lo – Dynamical screening of an endohedral atom
		Oliver Hampe – Electron photodetachment and electron autodetachment
		from cluster anions
$13^{15} - 14^{45}$		Lunch
$14^{45} - 16^{15}$		Electron and ion cluster collisions
	We-III	
		Vitaly Kresin – Evaporative attachment of slow electrons to metal
		nanoclusters
		Henrik Cederquist – Fullerene stability
		Stephan Denifl – Inelastic electron interaction with doped helium droplets
$16^{15} - 16^{45}$		Coffee break
16⁴⁵ - 18¹⁵		Poster session

Thursday, 05 June 2008

$9^{30} - 11^{00}$		Clustering phenomena at nuclear and subnuclear scales (part I)
	Th-I	Yuri Oganessian – Superheavy elements Mikhail Itkis – Fusion-fission of superheavy nuclei and clustering phenomena Walter Greiner – Nuclei: superheavy – superneutronic – superstrange
$11^{00} - 11^{30}$		Coffee break
$11^{30} - 13^{00}$	Th-II	Clustering phenomena at nuclear and subnuclear scales (part II)
		Igor Mishustin – Clusterization of nuclear matter in supernova
		Matthias Hempel – A statistical model for the liquid-gas phase transition of
		hot hadronic matter
		Vasili Shaginian – Fermion condensation quantum phase transition in finite and two-dimensional strongly correlated Fermi-systems
		and two annensional strongly correlated rormin systems
13 ⁰⁰ - 14 ³⁰		Lunch
$14^{30} - 16^{00}$		Phase transitions, fusion, fission and fragmentation in finite systems
	Th-III	<u>(part I)</u>
		Alexander Yakubovich – From helix-coil transition in polypeptides to phase transitions in proteins
		Florent Calvo – Interplay between proton transfer and temperature effects in the conformation of isolated particles
		Martin Schmidt –Freezing-point depression by insoluble impurities: a nano
		effect
$16^{00} - 16^{20}$		Coffee break
$16^{20} - 17^{50}$		Phase transitions, fusion, fission and fragmentation in finite systems
	Th-IV	(part II)
		Vlasta Bonacic-Koutecky – Tailoring functionality of clusters and their
		complexes with biomolecules by size, structures and lasers
		Bernd Huber – Collisions with clusters of fullerenes and biomolecules
		Aunan Hussien – Flase transitions in functiones
19⁰⁰ - 21³⁰		Conference dinner on a boat

Friday, 06 June 2008

$9^{30} - 11^{00}$	En I	Structure and dynamics of biomolecules
	FF-1	 Franco Gianturco – Fragmentation paths in biosystems mediated by metastable electron attachment in the gas phase Michael Broyer – Spectroscopy of peptides and metal cluster-peptides complexes. Sergey Volkov – Deformation mechanisms of DNA-type macromolecule
$11^{00} - 11^{30}$		Coffee break
11 ³⁰ – 13 ⁰⁰	Fr-II	Collision processes involving biomolecules Thomas Schlathölter – Ionization and fragmentation of amino acids and their clusters – isomer effects and peptide formation Emanuele Scifoni – Nanoscale mechanisms of DNA damage initiated by energetic ions in tissue-like media Yoshihiro Takeda – Interaction of metal nanoparticles with biological molecules
$13^{00} - 14^{30}$		Lunch
14 ³⁰ - 16 ⁰⁰	Fr-III	From biomolecules to cells and system biology (part I) Ilia Solov'yov – Magnetic clusters in a beak of a bird: a mechanism of magnetoreception Eugene Surdutovich – Towards an inclusive approach to estimation of DNA damage due to incident ions Marc Thilo Figge – Molecular clustering at the immunological synapse
$16^{00} - 16^{20}$		Coffee break
16 ²⁰ – 17 ⁵⁰	Fr-IV	From biomolecules to cells and system biology (part II) Alexander Samsonov – Improved models for pattern formation in early development of drosophila Michael Petukhov - Molecular mechanisms of large scale conformational flexibility and thermostability in RecA protein filament Oleg Demin - Application of Computational Systems Biology for discovery of new anti-inflammatory drugs
$17^{50} - 18^{05}$		Symposium Closing

Saturday, 07 June 2008

Conference excursion to the Hermitage museum; Boat trip along channels of St. Petersburg.

Overview of Abstracts

Structure and properties of atomic clusters

Tu-I-1 . ATOMIC-LEVEL ANALYSIS OF RESPONSE PROPERTIES OF FINITE SYSTEMS <i>J. Jellinek</i>
 Tu-I-2. SPHERICAL HOLLOW CLUSTER SYSTEM: STABILITY AND ELECTRONIC STRUCTURE V. K. Ivanov, R. G. Polozkov, A. V. Verkhovtsev, V. S. Komarov and A. V. Solov'yov24
Tu-I-3 . INTERACTION ENERGY AT THE END CUP OF A DEPOSITED ATOMIC CLUSTER D. N. Poenaru, R. A. Gherghescu, A. V. Solov'yov and W. Greiner
 Tu-II-1. METAL AND CARBON AT A NANOMETER SCALE: THE CATALYSIS AND GROWTH J. Geng and B. F. G. Johnson
 Tu-II-2. POPULATION TRANSFER PROCESSES: FROM ATOMS TO CLUSTERS AND BOSE-EINSTEIN CONDENSATE V. O. Nesterenko, PG. Reinhard and F. F. de Souza Cruz
Tu-II-3 . MAGIC SUPERFLUID ⁴ He AND PARA-H ₂ CLUSTERS <i>J. P. Toennies</i>

Clusters on surface

Tu-III-1 . DEPOSITION MIGRATION AND COALESCENCE OF SILVER NANOPARTICLES ON CARBON SURFACES	S
N. Kébaïli, S. Benrezzak, Ph. Cahuzac, A. Masson, M. Schmidt and C. Bréchignac	33
Tu-III-2 . SOFT-LANDING ISOLATION OF TRANSITION-METAL-BENZENE SANDWICH COMPLEXES INTO AN ALKYLTHIOL SELF-ASSEMBLED MONOLAYER MATRIX <i>A. Nakajima</i>	I 34
Tu-III-3 . IMPURITY EFFECT ON THE MELTING OF CLUSTERS A. Lyalin , A. Hussien, A. V. Solov'yov and W. Greiner	35
Tu-IV-1 . THREE-DIMENSIONAL ATOMIC-SCALE STRUCTURE AND STABILITY OF SIZE-SELECTED CLUSTERS ON SURFACES 7 Li	36
Tu-IV-2 . GROUND STATE AND SHAPE ISOMER DEFORMATIONS OF ALKALI METAL ATOMIC CLUSTERS	50
R. A. Gherghescu, D. N. Poenaru, A. V. Solov'yov and W. Greiner	37

Photon-cluster collisions and clusters in laser fields

 We-I-1. COLLECTIVE EXCITATIONS IN (ENDOHEDRAL) FULLERENE IONS ILLUMINATED BY SYNCHROTRON RADIATION S. Schippers, A. Müller, R. A. Phaneuf, M. Habibi, D. Esteves, J. C. Wang, A. Aguilar, A. L. D. Kilcoyne, S. Yang and L. F. Dunsch
We-I-2. LASER-DRIVEN RESCATTERING FOR ATOMIC CLUSTERS U. Saalmann
We-I-3. IONIZATION DYNAMICS OF CLUSTERS IN STRONG LASER FIELDS T. Fennel, T. Döppner, J. Tiggesbäumker, L. Ramunno, T. Brabec, KH. Meiwes-Broer
We-II-1. PHOTOIONIZATION OF FULLERENE C ₆₀ AND ITS POSITIVE IONS A. K. Belyaev
We-II-2. COLLISIONAL AND RADIATIVE PROCESSES INVOLVING STRONGLY POLARIZABLE CLUSTER TARGETS <i>A. V. Korol</i> and <i>A. V. Solov'vov</i>
We-II-3. DYNAMICAL SCREENING OF AN ENDOHEDRAL ATOM S. Lo, A. V. Korol and A. V. Solov'yov
 We-II-4. ELECTRON PHOTODETACHMENT AND ELECTRON AUTODETACHMENT FROM CLUSTER ANIONS O. Hampe, M. Neumaier, M. Massaouti, B. Concina and M. M. Kappes

Electron and ion cluster collisions

We-III-1. EVAPORATIVE ATTACHMENT OF SLOW ELECTRONS TO METAL NANOCLUSTERS	
R. Rabinovitch, C. Xia, V. V. Kresin	.51
We-III-2. FULLERENE STABILITY H. Cederquist, Z. Berenyi, N. Haag, H. T. Schmidt, and H. Zettergren	.52
We-III-3. INELASTIC ELECTRON INTERACTION WITH DOPED HELIUM DROPLETS S. Denifl, F. Ferreira da Silva, H. Schöbel, F. Zappa, T. D. Märk, P. Scheier	.54

Clustering phenomena at nuclear and subnuclear scales

Th-I-1. SUPERHEAVY ELEMENTS Yu. Ts. Oganessian	59
Th-I-2. FUSION-FISSION OF SUPERHEAVY NUCLEI AND CLUSTERING PHENOMENA M. G. Itkis	50
Th-I-3. NUCLEI: SUPERHEAVY – SUPERNEUTRONIC – SUPERSTRANGE W. Greiner	51
Th-II-1. CLUSTERIZATION OF NUCLEAR MATTER IN SUPERNOVA ENVIRONMENTS <i>I. N. Mishustin</i>	52
Th-II-2. A STATISTICAL MODEL FOR THE LIQUID-GAS PHASE TRANSITION OF HOT NUCLEAR MATTER <i>M. Hempel and J. Schaffner-Bielich</i>	53
Th-II-3. FERMION CONDENSATION QUANTUM PHASE TRANSITION IN FINITE AND TWO-DIMENSIONAL STRONGLY CORRELATED FERMI SYSTEMS <i>V. R. Shaginyan</i>	54

Phase transitions, fusion, fission and fragmentation in finite systems

 Th-III-1. FROM HELIX-COIL TRANSITION IN POLYPEPTIDES TO PHASE TRANSITIONS IN PROTEINS A. Yakubovich, I. A. Solov'yov, A. V. Solov'yov and W. Greiner
Th-III-2. INTERPLAY BETWEEN PROTON TRANSFER AND TEMPERATURE EFFECTS IN THE CONFORMATION OF ISOLATED PEPTIDES <i>F. Calvo and Ph. Dugourd</i>
Th-III-3. FREEZING-POINT DEPRESSION BY INSOLUBLE IMPURITIES: A NANO EFFECT <i>M. Schmidt</i> , <i>C. Hock</i> , <i>S. Straβburg</i> , <i>H. Haberland</i> , <i>B. v. Issendorff and A. Aguado</i> 70
Th-IV-1 . TAILORING FUNCTIONALITY OF CLUSTERS AND THEIR COMPLEXES WITH BIOMOLECULES BY SIZE, STRUCTURE AND LASERS <i>V. Bonačić-Koutecký</i>
Th-IV-2 . COLLISIONS WITH CLUSTERS OF FULLERENES AND BIOMOLECULES B.A. Huber , V. Bernigaud, B. Manil, J. Rangama, N. Haag, H. Johansson, H. T. Schmidt, H. Cederquist, S. B. Nielsen, B. Liu, H. Zettergren, and P. Hvelplund
Th-IV-3 . PHASE TRANSITIONS OF FULLERENES: FRAGMENTATION ↔ REASSEMBLY OF THE CARBON CAGE <i>A. Hussien</i> , <i>A. Yakubovich</i> , <i>A. V. Solov'yov and W. Greiner</i>

Structure and dynamics of biomolecules

Fr-I-1 . FRAGMENTATION PATHS IN BIOSYSTEMS MEDIATED BY METASTABLE FLECTRON ATTACHMENT IN THE GAS PHASE	1
F.A. Gianturco	79
Fr-I-2. UV SPECTROSCOPY OF ISOLATED PROTEINS AND METAL CLUSTER/PEP COMPLEXES <i>M</i> Brover	TIDE 80
Fr-I-3. DEFORMATION MECHANISMS OF DNA-TYPE MACROMOLECULE	
S. N. Volkov	81

Collision processes involving biomolecules

Fr-II-1. IONIZATION AND FRAGMENTATION OF AMINO ACIDS AND THEIR CLUSTERS
– ISOMER EFFECTS AND PEPTIDE FORMATION
T. Schlathölter
 Fr-II-2. NANOSCALE MECHANISMS OF DNA DAMAGE INITIATED BY ENERGETIC IONS IN TISSUE-LIKE MEDIA E. Surdutovich, A. Kostyuk, I. Pschenichnov, I. Mishustin, A. V. Solov'yov and W. Greiner
Fr-II-3. INTERACTION OF METAL NANOPARTICLES WITH BIOLOGICAL MOLECULES Y. Takeda , F. Mafuné, T. Kondow

From biomolecules to cells and system biology

 Fr-III-1. MAGNETIC CLUSTERS IN A BEAK OF A BIRD: A MECHANISM OF MAGNETORECEPTION I. A. Solov'yov and W. Greiner	1
 Fr-III-2. TOWARDS AN INCLUSIVE APPROACH TO ESTIMATION OF DNA DAMAGE DUE TO INCIDENT IONS E. Surdutovich, E. Scifoni, I. Pschenichnov, I. Mishustin, A. V. Solov'yov and W. Greiner9 	3
Fr-III-3. MOLECULAR CLUSTERING AT THE IMMUNOLOGICAL SYNAPSE M. T. Figge and M. Meyer-Hermann	4
Fr-IV-1. IMPROVED MODELS FOR PATTERN FORMATION IN EARLY DEVELOPEMENT OF DROSOPHILA A. M. Samsonov, V. V. Gursky, K. N. Kozlov and J. Reinitz	6
Fr-IV-2. MOLECULAR MECHANISMS OF LARGE SCALE CONFORMATIONAL FLEXIBILITY AND THERMOSTABILITY IN RECA PROTEIN FILAMENT <i>M. Petukhov</i> , D. Lebedev, D. Karelov, E. Glazunov, A. Islamov, A. Kuklin, V. Lanzov, and V. Isaev-Ivanov	7
Fr-IV-3. APPLICATION OF COMPUTATIONAL SYSTEMS BIOLOGY FOR DISCOVERY OF NEW ANTI-INFLAMMATORY DRUGS O. V. Demin	F 8

Posters

 PS-01. MEMORY EFFECTS IN THE BREMSSTRAHLUNG EMISSION FROM A FERMION JET IN A NON EQUILIBRATED HOT PLASMA <i>F. Michler B. Schenke and C. Greiner</i>
PS-02 . ON THE INFLUENCE OF COLLISION MODELS ON THE RESULTS OF DIRECT SIMULATION MONTE CARLO OF FLOWS WITH CONDENSATION <i>N. Y. Bykov and D. V. Leshchev</i>
PS-03 . MODULATED POSITRON BEAM IN THE CRYSTALLINE UNDULATOR <i>A. Kostyuk, A. V. Korol, A. V. Solov'yov and W. Greiner</i>
PS-04 . ULTRAFAST DEMAGNETIZATION INDUCED BY FEMTOSECOND LASER PULSES <i>E. Maurat</i> , <i>E. Gigilio and PA Hervieux</i>
PS-05 . FINITE TEMPERATURE MAGNETISM OF METALLIC NANOPARTICLES <i>E. Maurat</i> and PA Hervieux
PS-06 . PINNING OF SIZE-SELECTED COBALT CLUSTERS ON HOPG V. N. Popok, S. Vučković and E. E. B.Campbell
PS-07 . DIPOLE MOMENT EFFECT ON WATER CLUSTER PROPERTIES S. V. Drozdov, D. Yu Dubov , V. A. Galichin, V. S. Rudnev, A. A. Vostrikov
PS-08 . ENERGY DISSIPATION UNDER ELECTRON-IMPACT EXCITATION OF MOLECULAR CLUSTERS S. V. Drozdov, D. Yu Dubov, V. A. Galichin, V. S. Rudnev, A. A. Vostrikov
PS-09 . SHELL EFFECTS ON FRAGMENTATION OF MULTIPLY CHARGED VAN DER WAALS CLUSTERS <i>M. Nakamura</i>
 PS-10. STRUCTURAL AND ENERGETIC ANALYSIS OF ALUMINUM MICROCLUSTERS: DENSITY FUNCTIONAL STUDY <i>M. Böyükata</i> and Z. B. Güvenç
PS-11 . GROUND STATE AND SHAPE ISOMER DEFORMATIONS OF ALKALI METAL ATOMIC CLUSTERS <i>R. A. Gherghescu, D. N. Poenaru, A. V. Solov'vov and W. Greiner</i>
 PS-12. SPHERICAL HOLLOW CLUSTER SYSTEM: PHOTOABSORPTION SPECTRUM V. K. Ivanov, R. G. Polozkov, A. V. Verkhovtsev, V. S. Komarov and A. V. Solov'yov
PS-13 . ELECTRON-POSITRON CLUSTER PROPERTIES: SIZE DEPENDENCE <i>V. K. Ivanov, R. G. Polozkov, P. I. Yatsyshin</i> and A. V. Solov'yov
PS-14. FORMULATION AND PROPERTIES OF CLUSTERS IN FULLERENE COATINGS OF FIELD EMITTERS
 PS-15. FABRICATION AND IN SITU XPS-DIAGNOSTICS OF A SYSTEM OF ISOLATED SILVER NANOCLUSTERS ON SILICON SURFACE V. M. Mikoushkin, S. Yu. Nikonov, Yu. S. Gordeev, S. L. Molodsov and Yu. S. Dedkov
PS-16 . SHELL ELECTRONIC STRUCTURE OF UNOCCUPIED STATES OF FULLERENES AND FLUOROFULLERENES $C_{60}F_X$ (x = 0, 18, 36)

V. M. Mikoushkin, V. V. Shnitov, V. V. Bryzgalov, Yu. S. Gordeev, O. V. Boltalina, I. V. Gol'dt, S. L. Molodsov and D. V. Vyalikh
PS-17 . COHERENCE PHEONMENA IN THE PHOTOELECTRON EMISSION FROM SYMMETRIC MOLECULAR SYSTEMS <i>A. Reinköster</i> , <i>S. Korica</i> , <i>M. Braune</i> , <i>R. Hentges</i> , <i>B. Langer and U. Becker</i>
PS-18. ELECTRONIC STRUCTURE AND PHOTOIONIZATION CROSS SECTION CLACULATIONS FOR THE FULLERENE C ₆₀ AND ITS POSITIVE IONS <i>A. I. Toropkin</i> , A. S. Tiukanov, A. K. Belyaev, R. G. Polozkov, V. K. Ivanov and A. V. Solov'yov
PS-19 . EXPERIMENTAL REVEALING OF ISOMERS FOR FULLERENE C ₆₀ V. I. Gerasimov, A. E. Kalabushkin, Yu. F. Titovets, O. S. Alekhin, Yu. N. Zelenskij and Yu. A. Nikonov
PS-20 . THE SUPERCONDUCTIVITY AND ELECTRICAL INSTABILITIES: STATISTICAL CORRELATION IN FULLERENE – COOPER CLUSTERS <i>A. V. Prikhodko and O. I. Konkov</i>
PS-21 . LIQUID SURFACE MODEL FOR CARBON NANOTUBE ENERGETICS <i>M, Mathew, I. A. Solov'yov and A. V. Solov'yov</i>
PS-22 . THE MECHANISM OF DNA MECHANICAL MELTING <i>S. Volkov</i> and A. V. Solov'yov
PS-23 . MECHANISM OF ANOMALOUS DEFORMATION OF BISTABLE DNA SITES P. P. Kanevska and S. N. Volkov
 PS-24. HIERACHY OF CHROMATIN ORGANIZATION IN INTERPHASE CELL NUCLEI OF EUKARYOTES BY SANS D. V. Lebedev, M. V. Filatov, A. I. Kuklin, A. Kh. Islamov, E. Kentzinger, H. Lauter, R. A. Pantina, B. P. Toperverg and V. V. Isaev-Ivanov
PS-25 . CANALIZATION OF GENE EXPRESSION IN THE DROSOPHILA BLASTODERM <i>M. Samsonova</i> , <i>Manu</i> , <i>S. Surkova and J. Reinitz</i>
PS-26 . MODELING THE ORGANIZATION OF THE <i>EVEN-SKIPPED</i> PROXIMAL 1.7 KB UPSTREAM REGULATOGY REGION IN TERMS OF BINDING SITES <i>A. D. Matveeva</i> , <i>J. M. C. Ionides, M. G. Samsonova, J. Reinitz</i>
PS-27 . STABLE BIOLOGICAL PATTERN FORMATION IN VARIABLE ENVIRONMENT: A MODEL OF SEGMENTATION GENE EXPRESSION IN <i>DROSOPHILA V. V. Gursky</i> , <i>S. A. Vakulenko</i> , <i>O. Radulescu and A. M. Samsonov</i>

Invited Speakers

Structure and properties of atomic clusters

ATOMIC-LEVEL ANALYSIS OF RESPONSE PROPERTIES OF FINITE SYSTEMS*

Julius Jellinek

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A new scheme for atomic-level analysis of the dipole moments and polarizabilities of finite systems will be presented and analyzed. The scheme is based on partitioning the space into volumes associated with the individual atoms of the system and defining the contributions of each atom to the total dipole moment and total polarizability from the charge density within its atomic volume. The atomic dipole moments and polarizabilities are then further decomposed into the so-called dipole and charge-transfer parts. The dipole parts of the dipole moments and the polarizabilities characterize dielectric types of responses of the atoms to the intrasystem bonding and to a small external electric field, respectively. The corresponding charge transfer parts represent the respective metallic types of responses. The systems total dipole moments and polarizabilities can also be partitioned into dipole and charge transfer parts. These are defined as sums of the atomic dipole and charge transfer parts, respectively.

The utility of the scheme will be illustrated through applications to atomic clusters of different sizes and elements. Its power as an analysis tool will be demonstrated through characterization of the site-specificity of the atomic moments and polarizabilities; through analyses of structure- (i.e., isomer-), shape-, and size-dependent trends in the total moments and polarizabilities, as well as their dipole and charge-transfer components; and through its use as a tool for comparative evaluation of the degree of nonmetallic *vs* metallic character of clusters of different materials and sizes.

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SPHERICAL HOLLOW CLUSTER SYSTEM: STABILITY AND ELECTRONIC STRUCTURE

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It is of sufficient interest to study the stability and structure of hollow cluster systems. In recent years investigations were mainly focused on the most familiar group of the hollow cluster systems- carbon fullerenes with various number of atoms $(C_{60}, C_{70}, C_{20} \text{ etc})$. However, one can pose a general question- what are the factors responsible for the stability of a hollow, fullerene-like cluster system? The main idea of this work is to investigate the stability and the electronic structure of a quantum metallic cluster system undergoing the transition from a spherical volume state to a hollow shell type of object.



Figure 1: HF total energies per particle for clusters of different size versus radius R_{min} of the hole. The Wigner-Seitz radius is equal to $r_s = 4.0$ a.u.

We consider metal clusters within the jellium model, which treats the cluster as a two component system: homogeneous positively charged ionic core and quantized valence electrons. It was proved that this model describes well enough the electronic structure of metal clusters and fullerenes [1, 2]. The ground state electronic wave functions, the single-electron energy levels and the total energies of the clusters have been calculated within both the Hartree-Fock (HF) and the local density approximations (LDA). The purpose of these model calculations is to investigate the dependence of the cluster energy upon the variation of the positive charge distribution of the ionic core ranging from a homogeneously charged volume sphere to a spherical

layer with the hole radius R_{min} . So, with the chosen Wigner-Seitz parameter r_s , we keep the cluster volume constant and vary the radius of the hole.

The HF total energies per particle for clusters with different numbers of valence electrons N versus R_{min} are shown in Figure 1. The Wigner-Seitz radius is equal to $r_s = 4.0$ a.u. As expected the energy curves have minimum in the vicinity of $R_{min} = 0$ demonstrating stability of the clusters against the bubble formation. However, with increase of R_{min} the energy curves pass over the barrier and acquire the second minimum corresponding to a stable state of the hollow cluster system. Note the radius R_{min} of the stable hollow cluster structure depends significantly on its size. The same result is obtained with the LDA formalism.



Figure 2: Single-electron energies of cluster with $N = 40(1s^22p^63d^{10}2s^24f^{14}2p^6)$ as a function of hole radius R_{min} .

The single-electron energy dependences calculated within the HF approximation for the N_{40} cluster versus radius R_{min} are shown in Figure 2. There one sees the crossing of the 2s and 4f single-electron energy levels. This means that the ground state electronic configuration of the cluster should be rearranged above the crossing point. Thus, in the vicinity of $R_{min} \sim 5a.u$. the N_{40} ground state electronic configuration changes from $1s^22p^63d^{10}2s^24f^{14}2p^6$ to $1s^22p^63d^{10}4f^{14}5g^8$. This rearrangement occurs due to the different dependence of the single-electron energy levels of the cluster upon the radius of the hole.

Finally we conclude that the stable hollow cluster structure is a result electron correlations in the system. The total energy of the system depends on density of the positive ionic background, the number of delocalized valence electrons and the electronic configuration.

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INTERACTION ENERGY AT THE END CUP OF A DEPOSITED ATOMIC CLUSTER

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The liquid drop model (LDM) was successfully applied to nuclear fission processes since 1939, and more recently it was adapted to the atomic cluster physics [1] because the delocalized electrons of a metallic cluster may be considered to form a Fermi liquid like the atomic nucleus. There is a growing interest in nanostructured coating of surfaces by cluster deposition. One of the simplest shape is a semi-spheroid with the z axis of cylindrical symmetry oriented perpendicularly on the surface plane. In a previous paper [2] we obtained analytical relationships for the deformation-dependent surface and curvature energies of the semi-spheroid, assuming no interaction with the substrate. The most stable shape was a superdeformed prolate semi-spheroid, which seems to be met in some cases as can be seen from the scanning probe microscope image of deposited cluster shapes. On the other hand, experimentally observed oblate shapes are not explained if we stick to this "free cluster" assumption. A more realistic approach (including the preceding one) would take care of the interaction, which may be simulated by changing the value of the surface tension of the end-cup contact surface. The multiplication factor, i, takes values in the interval (-1.98, 2). For i = 1 we obtain the semi-spheroidal case previously studied [2]. Typical results of equilibrium shapes are shown in figure 1: hyperdeformed prolate semi-spheroid ($\delta = 0.97, c/a = 2.9$); superdeformed prolate semi-spheroid ($\delta = 0.63, c/a = 1.9$), semi-sphere ($\delta = 0, c/a = 1$); superdeformed oblate semi-spheroid ($\delta = -0.68, a/c = 2$), and hyperdeformed oblate semi-spheroid ($\delta = -1, a/c = 3$) for i = 2, 1, 0, -0.58, -0.76, respectively.



Figure 1: LDM equilibrium shapes of Na₅₆ semi-spheroidal cluster corresponding to the minima of deformation energy.

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METAL AND CARBON AT A NANOMETER SCALE: THE CATALYSIS AND GROWTH

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Metal nanoparticles can be used as catalyst for growth of novel carbon nanostructures. Both types of nanomaterials have become increasingly interested by scientists working in the fields of chemistry, physics, and engineering because of their outstanding properties as quantum dots for fundamental exploration of physical problems, or as electron transport materials for semi-conducting industry. Here we present a brief survey of our recent works on metal nanoparticles and carbon nanomaterials, which comprises the following topics:

- *Metal nanoparticles as catalyst for carbon nanotube growth.* Several novel methods for the synthesis of metal nanoparticles as catalyst for large-scale production of single walled, multi-wall carbon nanotubes and carbon nanofibers have been developed. Among them, the production of single-walled carbon nanotubes is of a particular interest. We describe a straightforward method for the synthesis of high-quality single-walled nanotubes in high yields. In this case, we have found that nickel formate serves as an ideal precursor for the formation of Ni nanoparticles as the catalyst. By optimising the experimental conditions, the Ni nanoparticles are found to be catalytically highly active, with a small size (~ 1.0 nm) and a narrow size distribution.
- Patterned growth of carbon nanostructures on surface: Growths of patterned carbon nanotubes have been carried out on metal and semiconducting substrates. In this case, we have successfully developed a wet chemistry method for surface-bound growth of carbon nanotubes over a large area, with Ni or Co nanoparticles as catalyst. These tubes were grown vertically, with a patterned nanostructure. The experiments were carried out by a micro-contact printing technique associated with a suitable CVD deposition, which promises a wide range of engineering applications at low cost. Potential applications include the development of field emission devices and super-capacitors.
- Synthesis of nanoscale metal cluster single molecules. A family of Au, Ru, Fe and Co supercluster single molecules have been synthesised by a novel dendrimer-based route. These giant molecules as catalyst provide unique advantages, for example, in the preparation of monodispersed nanoparticles with a well-defined molecular structure and surface functionality. In contrast to the 'magic' number synthesis of colloids wherein metal particles are stabilised by a 'passivating' external layer of organic ligands, we have used large internal organic scaffolds such as [DAB-dendr-[N(CH₂PPh₂)₂]₁₆ to construct an array of metal clusters, thereby forming nanoscale self-ordering. Studies on these nanocluster single molecules have been further extended to their surface self-assembly, as uniform-size catalytic seeds for a diameter-controlled growth of single-walled carbon nanotubes.
- Crystal structure and growth mechanism of fullerene nanowires. Exceptionally long C_{60} nanowires, with a length to width aspect ratio as large as 3000, are grown from a 1,2,4-

trimethylbenzene solution of C₆₀. They have been formed to possess a highly unusual morphology, with each nanowire being composed of two nanobelts joined along the growth direction to give a V-shaped cross section. The crystal structure of these nanowires has been found to be orthorhombic, with the unit cell dimensions of a = 10.2 Å, b = 20.5 Å, and c = 25.6 Å. Structural and compositional analyses enable us to explain the observed geometry with an anisotropic molecular packing mechanism that has not been observed previously in C₆₀ crystal studies. The nanowires have been observed to be able to transform into carbon nanofibres following a high temperature treatment but their original V-shaped morphology can be kept unchanged in the transition. A model for the nanowire morphology based upon the solvent-C₆₀ interactions and preferential growth directions is proposed, and potentially it could be extended for use to grow different types of fullerene nanowires.

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POPULATION TRANSFER PROCESSES: FROM ATOMS TO CLUSTERS AND BOSE-EINSTEIN CONDENSATE

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Modern quantum optics delivers a variety of population transfer processes (PTP) for atomic and molecular spectroscopy (see for reviews [1]). They range from the familiar stimulated Raman scattering to fascinating adiabatic processes like stimulated Raman adiabatic passage (STIRAP) [1] and Stark-shift-chirped rapid adiabatic passage (SCRAP) [2]. We show that these methods can be recast for other systems: atomic clusters [3, 4] and multi-component Bose-Einstein condensate (BEC) [5].

Some properties of atomic clusters (plasmon modes, short lifetimes, ...) essentially hinder implementation of PTP. However, our recent TDDFT calculations show that in some cases it is possible to overcome the troubles and develop the successful techniques. As a result, we can get for clusters a valuable spectroscopic information, in particular, a direct access to the single-electron levels both below and above the HOMO-LUMO gap [3,4].

The analogy between two-photon PTP and tunneling opens intriguing perspectives for implementation of the processes like STIRAP for the transport of BEC in multi-well traps. We analyze the transport problem in the mean-field approximation and show that successful STI-RAP transfer can take place even in spite of the detrimental impact on the non-linearity (caused by interaction between BEC atoms) [5]. We consider BEC transport in linear and cyclic configurations of the wells and discuss perspectives of investigation of new BEC dynamics and various geometric phases (Berry phase, etc).

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MAGIC SUPERFLUID ⁴He AND PARA-H₂ CLUSTERS

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Whereas the spectroscopy of chomophore molecules embedded in small clusters of ⁴He or para-H₂(pH₂) molecules provides evidence for their "microscopic" superfluidity relatively little is known about the superfluidity of the small pure clusters [1]. Path Integral Monte Carlo (PMIC) calculations for pure ⁴He clusters, which are definitely liquid, predict that $N \approx 64$ clusters are superfluid below about 2 K [2], but do not exhibit magic stabilities. Thus it was surprising that the size distributions of small ⁴He clusters produced in free jet expansions measured with non-destructive matter-wave diffraction revealed 4 – 5 magic-like peaks [4]. Comparison with highly accurate Diffusion Monte Carlo calculations confirm that the peaks are not due to structural stabilities but instead occur whenever the cluster acquires an additional elementary excitation level. These particular clusters are favored during growth in the expansion. The comparison with experiment confirms the calculated energy levels and provides indirect evidence that the clusters are superfluid.

pH₂ clusters appear to be anomalous since they are predicted to be superfluid, while exhibiting "magic" icosahedral solid-like stabilities at N* = 13, 19 and 23. This apparent contradiction has been resolved by PIMC calculations which show that superfluidity is localized at the surface and only for $N \le 26$ [3].

Diffraction experiments [5] similar to those described above and Raman spectroscopy [6] of pH_2 clusters confirm the magic number N* = 13, but diffraction of normal-H₂(nH₂)-clusters (25 % j = 0 pH₂ and 75 % j = 1 ortho H₂) indicates a lack of any magic number up to N = 40 [5]. To understand this difference we are presently investigating theoretically the influence of the ortho molecules on the quantum behaviour of nH₂ clusters.

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Clusters on Surface

DEPOSITION MIGRATION AND COALESCENCE OF SILVER NANOPARTICLES ON CARBON SURFACES

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The diffusion and coalescence of metal nanoparticles on surfaces play important roles in the dynamics of growth process of nanostructures. The influence of surface preparation is one of the key parameter in the dynamics of the migration and the anchorage of the nanoparticles on the surfaces. Among the surfaces, Carbon is the prototype element that forms extensive 2D structures that thus can be bent, pleated and furled. Due to the pliability of the building block, nature has an exceptional liberty in forming 3D structures by graphitic layers. Beside graphite, there are the classes of Carbon nanotubes that are promising material for electronic devices.

We succeeded in the deposition of silver nanoparticles with a mean diameter of $3nm \pm 0.5nm$ on graphite terraces, pleated graphite surfaces, and multiwalled carbon nanotubes prealably deposited on HOPG. The purpose of our paper is to compare the silver nanoparticle interaction with these three kinds of carbon surfaces through the result of their diffusion on the substrates. The resulting patterns are interpreted by model calculations based on diffusion-limited aggregation with specific constraints to describe the surface curvatures and defects.

The free silver nanoparticles are formed from gas aggregation source [1]. They are mass analysed by a time of flight spectrometer before their deposition on the substrate. We analyze the islands resulting from the silver nanoparticle deposition by TEM, scanning electron microscopy (STM) and non contact atomic force microscopy (AFM). The deposition of the silver nanoparticles on graphite terraces lead to fractal islands isotropically distributed due to the diffusion-limited aggregation of the nanoparticles on a surface with a small number of defects (10^{-8} /cm²) [2]. At low flux deposition, only the graphite defects are decorated by the fractal islands in agreement with an heterogeneous nucleation. At higher flux deposition homogeneous nucleation takes place that increases the density of islands. The deposition on pleated graphite reveals interesting behavior. It show evidence of a strong anisotropy in the nanoparticles from the surrounding areas. The trapped nanoparticle aggregate linearly along the bend forming a quasi one dimensional rod. By contrast, deposition of silver nanoparticles on MWCNT's leads to a large density of islands (10^{-11} /cm²) that is drastically different than the deposition on pleated graphite with similar curvature. It can be interpreted as a high defect density in carbon nanotubes which are used to anchor the silver nanoparticles.

In summary, our results on silver nanoparticle diffusion on bent graphite and/or MWCNT show very different behaviors. Although bent graphite surfaces with a little number of point defects can be used as guides for nanoparticle diffusion and anisotropic growth, MWCNT's can be used to anchor the particles.

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SOFT-LANDING ISOLATION OF TRANSITION-METAL-BENZENE SANDWICH COMPLEXES INTO AN ALKYLTHIOL SELF-ASSEMBLED MONOLAYER MATRIX

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Gas-phase synthesized metal-benzene sandwich complexes have generated a great deal of attention due to their unique metal- and size-dependent characteristics, originating from their onedimensional (1-D) anisotropic structures. In particular, the complexes consisting of vanadium (V) and benzene, V_n (benzene)_{n+1}, efficiently form multidecker sandwich structures [1,2]. Gas-phase synthesized transition metal-benzene 1:2 cation complexes, $M^+(benzene)_2$ (M = Ti, V, and Cr), were size-selectively deposited onto a C18-SAM substrate with the hyperthermal collision energy of 10-20 eV [3]. All of the complexes were neutralized after soft-landing due to charge transfer from the SAM substrate, and retain their native sandwich structure intact. However, only the Ti(benzene)₂ complexes are dissociated after the hyperthermal deposition with 20-eV collision energy whereas the other V(benzene)₂ and Cr(benzene)₂ complexes are successfully landed on the SAM substrate. This may be due to the decrease in bond order in projectile Ti⁺(benzene)₂ complexes so that reducing collision energy to 10 eV is required to make a nondissociative depositon of Ti(benzene)₂ complexes on the SAM. The soft-landing process results in penetration of incoming complexes into the SAM matrix, while the extremely low energy (thermal) deposition (~25 meV) of Cr(benzene)₂ complexes via a PVD technique leads to physisorption of the complexes on top of methyl surface of the SAM. Although these complexes are weakly physisorbed on the SAM with random orientation, the complexes that are incorporated in the SAM matrix are highly oriented with their molecular axis canted $\sim 70^{\circ}$ off the surface normal, a phenomenon which is probably due to the attractive CH- π interaction between the capping benzene rings of the cluster and the lateral methylene groups of the alkanethiolates. In addition, the complexes penetrating into the SAM matrix exhibit unusual large activation energies for desorption of over 100 kJ/mol, with the result that the thermal desorption of the embedded complexes can be suppressed even at room temperature. The thermal desorption of matrix-isolated sandwich complexes is probably associated with the crystal-rotator phase transitions of the C18-SAM matrix. In this study, we evidently demonstrate that the soft-landing of the gas-phase synthesized M(benzene)₂ complexes with hyperthermal collision energy onto the alkanethiolate SAM result in matrix-isolation of the injected complexes inside the SAM matrix by comparing their thermal deposition studies. The soft-landing isolation technique using SAM matrices has advantage for trapping the gas-phase synthesized complexes and clusters as it is on the substrates and also utilizing their functionality for the nanoscale future materials [4].

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IMPURITY EFFECT ON THE MELTING OF CLUSTERS

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We report the results of a systematic theoretical study of impurity effects on the thermodynamic properties of Ni clusters [1]. The choice of transition metal clusters is stipulated by their high chemical reactivity and multiple applications in nanostructured materials, such as, the catalytically activated growth of carbon nanotubes (see, e.g., [2]). In the current work we performed classical molecular dynamics simulations using the many-body Sutton-Chen potential for the metal-metal interaction. The interaction with impurity (a carbon atom) was modeled by the Morse potential. It is shown that adding an impurity induces changes in the thermodynamic properties of Ni clusters. We demonstrate that a single carbon impurity can result in significant changes in the melting temperature of a Ni cluster consisting of hundreds of atoms. The magnitude of the change induced is dependent upon the parameters of the interaction between the Ni atoms and the C impurity. Hence, thermodynamic properties of Ni clusters can be effectively tuned by the addition of an impurity. We also show that the presence of a carbon impurity considerably changes the mobility of atoms in the Ni cluster, at temperatures close to its melting point. The knowledge of the thermodynamic state and the mobility of atoms in a cluster are important, for example, for estimation of the growth rate of carbon nanotubes or the diffusion and pattern formation of supported clusters.



Figure 1: Left: Caloric curve for pure Ni_{147} cluster (filled dots) and Ni_{147} cluster with C impurity (open circles); right: heat capacity for Ni_{147} cluster (solid line) and Ni_{147} cluster with C impurity (dashed line).

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Tu-IV-1

THREE-DIMENSIONAL ATOMIC-SCALE STRUCTURE AND STABILITY OF SIZE-SELECTED CLUSTERS ON SURFACES

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Clusters occupy special places in fundamental research and practical applications. As a form of matter intermediate between atoms and the bulk, they allow a study of the evolution of a physical property from atomic to solid-like. Today's advancements in nanocluster fabrication techniques enable us to control the size of the clusters with great precision. This presents new opportunities for high-quality characterization of nanocluster structures. We recently applied the state-of-art spherical aberration-corrected scanning transmission electron microscopy (STEM) to perform atomic resolution high angle annular dark field (HAADF) imaging of metallic nanoclusters. In the case of soft-landed size-selected Au clusters (Au₃₀₉), with the aid of quantitative image intensity analysis and molecular dynamics modelling, we not only determined the detailed atomic geometry of the gold clusters with atomic precision, but also revealed the possible signal for the fluctuating nature of the atoms in the surface layer of the clusters. The single shot microscopy illustrates a new, efficient and very promising way to study the atomic structure and stability of supported ultra-small metal clusters. Furthermore, I will present new results to show that these well-characterized size-selected nanoclusters have the potential to be employed as a mass standard in nanometrology using electron microscopy.
Tu-IV-2

GROUND STATE AND SHAPE ISOMER DEFORMATIONS OF ALKALI METAL ATOMIC CLUSTERS

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The spheroidal shell model is used to describe the deformed states of atomic clusters. The Hamiltonian is analytically solved in cylindrical coordinates. The angular momentum term is treated as deformation dependent. The asymptotic eigenfunctions are obtained for axially symmetric potentials without approximation. The energy levels are used as input data for shell corrections. Minima due to shell effects are obtained as a function of the number of atoms in the atomic cluster as well as of the deformation. Calculations are performed for atom number up to 200, and spheroidally deformed (oblate and prolate) shell closures are predicted.

Photon-cluster collisions and clusters in laser fields

COLLECTIVE EXCITATIONS IN (ENDOHEDRAL) FULLERENE IONS ILLUMINATED BY SYNCHROTRON RADIATION

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Mass selected fullerene ions have been exposed to synchrotron radiation in the 17–310 eV energy range. Selected absolute cross sections for single and multiple ionization as well as fragmentation were measured for ions of C_{60} , C_{70} , C_{80} , C_{82} , and C_{84} . Below the threshold for carbon K-shell excitation the measured cross sections exhibit two distinct giant resonance features which are attributed to the excitation of plasmon modes in the fullerene ion's valence shell where the valence electrons oscillate collectively with respect to the positively charged ionic cores of the atoms that form the fullerene cage. Especially, the second higher energy plasmon in C_{60} has received attention in the recent literature [1,2,3]. It can be strongly excited only because of the special geometry of the fullerene, i.e., because these molecules are *hollow*.

More recently, we have performed experiments with endohedral $Sc_3N@C_{80}^+$ and $Ce@C_{82}^+$ fullerene ions [4]. An interesting question is to what extent the plasmon excitations are influenced by the atoms inside the fullerenes' carbon cage. Additionally, many-electron atoms such as cerium support collective excitations themselves leading to giant resonances in atomic photoabsorption spectra. An intriguing prediction for Xe@C₆₀ is that the atomic giant resonance may become split because of interferences between outgoing electron wavefunctions that are partly reflected at the C₆₀ cage [5]. In our experiments we compare photoionization of free and encaged cerium ions and thereby aim at clarifying such issues.

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LASER-DRIVEN RESCATTERING FOR ATOMIC CLUSTERS

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Laser-driven rescattering of electrons [1] is at the heart of strong-field atomic physics. The basic principle is very simple: a bound electron is released from an atom with the help of the strong electric field of a laser, by which it is subsequently driven back. On return to the ion the electron may recombine (emitting harmonic radiation [2] with the access to attosecond laser pulses [3]), ionize other electrons (inducing multiple ionization [4]) or may be backscattered (gaining high kinetic energy termed above-threshold ionization [5]).

For atoms the rescattering process can be understood in classical terms by an electron elastically scattered at a zero-range potential in the presence of an oscillating electromagnetic field [6]. The absorption is particularly effective for a large momentum change, which is achieved through *backscattering*, and for scattering events taking place at a maximal vector potential (*minimal* electric field). For an extended scattering potential—as provided by a charged atomic cluster—we will show [7] that optimum energy absorption upon rescattering requires completely different conditions, namely *forward-scattering* at *maximal* electric field.

A simple model for the cluster potential allows for the corresponding electron dynamics to be solved analytically. We get a quantitative estimate of the acceleration of the electrons which depends on *both*, the laser field strength and the depth of the scattering potential. Interestingly, this situation is akin to the so-called *powered swing-by* (or gravity-assisted maneuver) of spacecrafts.

To illustrate the relevance of the rescattering mechanism in extended systems we present results of microscopic calculations for rare-gas cluster exposed to intense laser radiation [9]. The theoretical approach describes the laser-driven electronic nano-plasma and the ionic explosion dynamics by means of classical equations of motion [8] and has been successfully applied to study the absorption mechanisms for a wide range of clusters sizes and laser pulses.

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IONIZATION DYNAMICS OF CLUSTERS IN STRONG LASER FIELDS

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The continuing interest in intense laser cluster interactions is driven by both technological applications and the quest for fundamental insight into complex many-body processes. The highly efficient absorption of laser energy and subsequent emission of fast electrons, energetic highly charged ions, x rays, and neutrons is relevant for the generation of EUV light, energetic particles, and pulsed neutrons bursts. The created nanoplasma itself is of fundamental interest for studying strong-field-induced dynamics in dense media as the microscopic processes are also of key importance to other branches of many-body physics, including plasma physics, and laser modification of solids, such as dielectrics.

Much of the violent cluster response is related to the creation of a hot transient nanoplasma. In the talk two central aspects of the nanoplasma dynamics will be addressed. First, laser excitation of a temporarily resonant collective electron mode results strongly enhanced absorption. For excitation with delayed dual pulses this plasmon resonance can be directly measured, e.g. by analyzing the emission of highly charged ions [1] or fast electron [2], see Fig. 1, which exhibit a strong angular preference. On the basis of simulations the acceleration and angular preference



Figure 1: Electron emission from Ag_N exposed to 100 fs laser pulses of peak intensity $8 \times 10^{13} W/cm^2$. (a) energy spectra for emission parallel (E_{||}) and perpendicular (E_⊥) to the laser polarization axis for single– and optimal dual–pulse excitation. (b) parallel and perpendicular electron yield for different energy windows (as indicated) for dual pulse excitation as function of pulse delay.

of fast electrons emitted at resonance can be linked to surface-plasmon assisted re–scattering of highly excited electrons on the cluster (SPARC). Recent experimental results on metal clusters will be presented. Simulations further supports, that energetic electrons are emitted from the clusters in short sub-femtosecond bursts – details of the mechanism will be discussed.

Second, experiments show that intermediate and heavy atom clusters, e.g., Xe_N, Pt_N, and Pb_N, emit ions with charge states up to 20-30 for moderate laser intensities of 10^{14-15} W/cm². The mechanisms underlying the generation of these highly charged ions, however, remain debated. Our investigations support, that local-field effects on electron-impact ionization (EII) as



Figure 2: Predicted maximum charge state of atomic ions emitted from Xe_N (as indicated) exposed to a 250 fs laser pulse of peak intensity $4 \times 10^{14} W/cm^2$.

well as the electron-ion recombination dynamics in the exploding clusters have to be considered in detail to explain the observed highly charged ions. By taking both effects into account in molecular simulations a much better agreement with experiments is achieved when compared to previous studies. Local-field enhanced EII an frustrated electron-ion recombination together can augment the highest charge states by more than a factor of two, when compared to the conventional treatment of EII and total recombination of all quasi-free electrons [3], see an example for Xe_N in Fig. 2.

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PHOTOIONIZATION OF FULLERENE C₆₀ AND ITS POSITIVE IONS

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The analysis of the electronic properties and dynamical characteristics of fullerenes has attracted much attention over the years. Importance of investigations may be thought as apparent due to the intermediate position of fullerenes between atomic structures and solids. In this very specific form of matter the unique hollow cage structure sets off fullerenes from a cluster family.

The photoionization cross sections of the fullerene C_{60} and its positive ions C_{60}^+ , C_{60}^{2+} and C_{60}^{3+} are calculated within the photon energy range from the ionization thresholds up to 80 eV and compared with the recent experimental data [1] and other calculations, see, for example, [1,2]. The main features of the theoretical framework used in the present work has been developed earlier [3,4] and applied for the description of photoionzation of C_{60} , C_{60}^+ , and C_{60}^{2+} [2–4]. In the present work the theoretical approach is improved by means of using the Perdew-Wang parametrization [5] for the exchange-correllation energy functional.

The total photoionization cross section is calculated as a sum of partial cross sections for each orbital. The ionization amplitude of each orbital is calculated both within the singleelectron approximation and also by taking into account many-electron correlations. At the first stage, the frozen core model and the local density approximation (LDA) are used assuming that there is a single electron transition during the process. Then, the correlations between the transitions from different states are taken into account within the random phase approximation. Single-electronic states of a fullerene ion are calculated within the spherical jellium model with the self-consistent potential [3] determined within LDA. The basic Kohn-Sham equations are used for determining of the single-electronic wave functions. In the present study we are treating 2 models for the fullerenes: the spherical jellium model with the self-consistent potential and the spherical jellium model of a finite width.

The calculated photoionization C_{60} and C_{60}^{q+} (q = 1, 2, 3) cross sections indicate the giant plasmon resonances with positions of ≈ 20 eV for all fullerenes treated. This is in a good agreement with the classical Mie theory and the experimental data [1]. The photoionization cross sections calculated in the present work fulfill the sum rule for all fullerenes, so in contrast to the previous C_{60} calculations [2,3] they are not scalled by any factor.

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COLLISIONAL AND RADIATIVE PROCESSES INVOLVING STRONGLY POLARIZABLE CLUSTER TARGETS

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Specific role played by various plasmon excitations in collisional and radiative processes involving strongly polarizable targets will be discussed in this talk. The emphasis is made on the photoionization and electron scattering from metal clusters and fullerenes.

Recent experiments [1] indicate that the measured angular distributions of photoelectrons from strongly polarizable targets (in particular, metal clusters) may deviate noticeably from the predictions of conventional theory. We demonstrate that even within the dipole-photon approximation the profile of the angular distribution is modified:

 $1 + \beta(\omega) P_2(\cos \theta) \longrightarrow 1 + a_2(\omega) P_2(\cos \theta) + a_4(\omega) P_4(\cos \theta)$

due to the action of the field of alternating dipole moment $\mathbf{D}(t)$ induced on the residue target. The coefficients $a_2(\omega)$ and $a_4(\omega)$ depend on the cluster geometry and are proportional to the intensity $|E_0|^2$ of the laser field. We show that dramatic changes in the profile (the $P_4(\cos\theta)$ terms) can occur even at comparatively low intensities (~ $10^{-7} \dots 10^{-5}$ a.u.). This effect is sensitive to the target size and its dynamic dipole polarizability.

The processes of elastic and inelastic electron scattering from clusters and fullerenes are also strongly dependent on the dynamic response of the target. However, in contrast to the photoionization, which is governed solely by the contribution of a dipole surface plasmon, the collisional processes allow for the multipolar surface *and* volume plasmon excitations. In our work we elucidate the role of plasmon excitations in the formation of electron energy loss spectra as well as in the total inelastic scattering cross section. Special attention is paid to the interplay of various plasmon modes and to their manifestation in the profile of the cross section.

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DYNAMICAL SCREENING OF AN ENDOHEDRAL ATOM

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Fullerenes provide a unique platform for studying the effects of confinement. It is important to understand the impact of the confining fullerene shell on the photo absorption of the endohedral atom. A dynamical screening factor, $F(\omega)$, can be defined to relate the photo absorption cross section of the confined atom with that of the free atom:

$$F(\omega) = \sigma_{\text{confined}} / \sigma_{\text{free}}.$$

This has been performed with a semi-classical approach for fullerenes: the infinitely thin fullerene [1] and the fullerene of finite thickness [2]. Large enhancements of the photo absorption cross section of the confined atom occur near the fullerene's plasmon frequencies. This semi-classical model shows qualitative agreement with *ab initio* calculations performed in [3] for Ar@C₆₀.



The figure shows the dynamical screening factor for Argon confined within C_{60} . The dashed line is the limiting case where the interaction (resulting from the presence of the external light field) between the fullerene and the atom is negligible [2]. The solid line shows the effect of accounting for this mutual interaction. The dotted line indicates the position of the ionisation potential of argon.

The semi-classical model of [2] is generalised to include an atom located in an arbitrary position within the fullerene. The spatial dependence of the

dynamical screening factor will be presented. A method for spatial averaging over the possible positions of the endohedral atom will be discussed.

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ELECTRON PHOTODETACHMENT AND ELECTRON AUTODETACHMENT FROM CLUSTER ANIONS

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Multiply charged molecular and cluster anions (or multianions) in the gas-phase have attracted considerable interest over the past years [1-4] as they are ubiquitous building units in chemistry. Unlike singly charged anions, multianions exhibit a characteristic repulsive Coulomb barrier (RCB) towards electron/anion loss or transfer. We have investigated doubly charged fullerene anions C_{76}^{2-} and C_{84}^{2-} stored in a Penning ion trap of a Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer as generated by an electrospray ion source [5].

In this contribution we report on:

(i) Electron transfer kinetics of fullerene dianions with SF_6 as a function of collision energy. A pronounced threshold behaviour is observed for the formation of SF_6^- , which is a nominally exothermic reaction. Threshold energies obtained are discussed on the grounds of an electrostatic model of the Coulomb barrier. [6]

(ii) Photodetachment studies from fullerene dianions C_{76}^{2-} and C_{84}^{2-} [7].

Electronic excitation with a ns-pulsed laser at wavelengths of 355 and 532 nm using a Nd:YAG laser and concomittant photon absorption induces electron emission – without any fragmentation of the fullerene cage. Ion yields C_m^{2-} and C_m^{-} (m=76 and 84) as a function of laser-fluence were analyzed on the basis of Poisson statistics to give the number of photons required for electron detachment and the absolute absorption cross-sections. A statistical unimolecular rate model describing "over-the-barrier" electron emission is employed to derive activation energies from the experimental data. For the monoanions, the activation barriers obtained from the model are in good agreement with the first electron affinities when including effects of radiative cooling [7], which in turn strongly supports the underlying mechanism of an activated over-the-barrier process. In case of the dianions the activation energies reflect the strong Coulomb repulsion between the extra charges and are contrasted to an electrostatic charging model for dielectric spherical particles [8] as well as quantumchemical computations.

(iii) First results from a newly developed liquid- N_2 cooled Penning trap on electron tunneling from molecular multianions [9].

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Electron and ion cluster collisions

EVAPORATIVE ATTACHMENT OF SLOW ELECTRONS TO METAL NANOCLUSTERS

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We have carried out a measurement of the abundance mass spectra of Na $_{n-7-140}$ ions formed as a result of low energy (0.1 eV) electron attachment to a beam of free clusters. Both the anion (daughter) and the neutral (precursor) cluster mass spectra were recorded simultaneously, making it possible to follow and analyze their transformations without distortions due to beam variations.

The anion mass spectrum revealed significant restructuring with respect to that of the neutral precursors, including a downshift in the shell-closing magic numbers, as well as strong changes in the relative intensities of open-shell peaks. The latter effect cannot be explained by a simple pattern shift by one electron number, and requires an accurate treatment.

The restructuring of cluster abundances was analyzed theoretically on the basis of a threestage evaporative attachment picture: (1) electron capture by the polarization potential of the cluster; (2) prompt dissipation of electron attachment energy into the internal vibrational degrees of freedom (cluster heating); followed by (3) evaporative cooling. The last stage, comprising a cascade of monomer and dimer evaporations, is described within the statistical framework of evaporative ensemble theory. Convoluting the modeled evaporation chains with the mass spectra of the neutral precursors, we obtained detailed agreement of the predicted anion abundance patterns with the experimental data, without any adjustable parameters. Furthermore, being sensitive to the cluster dissociation energies, the data verified that the prior literature dimer binding energies need to be corrected by $\approx 25\%$.

Thus a picture of the entire process of evaporative electron attachment to metal clusters has been ascertained. The results demonstrate that slow-electron capture offers a useful window into the polarization, statistical and binding properties of nanoclusters. Conversely, they emphasize that in interpreting charge-capture and charge-transfer reactions involving clusters it is essential to account for accompanying evaporative dynamics.

FULLERENE STABILITY

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Fragmentation of multiply charged fullerene ions following collisions with slow highly charged ions has been studied in order to investigate: *i*, kinetic energy release distributions (KERD) in asymmetric fission processes $C_{60/70}^{q+} \rightarrow C_{58/68}^{(q-1)+} + C_2^+$; *ii*, possible differences in the fragmentation of C_{60} and C_{70} ; and *iii*, competitions with other dissociation pathways. To our knowledge, there are neither experimental nor theoretical studies of KER-*distributions* for asymmetric fission of multiply charged fullerenes in the literature. In the experiment, the energies of the fission fragments were determined by means of a recoil-ion momentum technique with a two-dimensional position sensitive detector located at the end of a linear time-of-flight mass spectrometer. With this set-up, we have performed measurements for charge states from q=4 to 8. The KERDs as functions of q were then deduced by fitting simulated position distributions to the measured distribution on the detector. The simulated distributions were obtained by means of ion optical calculations, with various assumed KER-distributions, of the position distributions on the detector. In figure 1, the KER-distributions yielding the best fits are shown.



Figure 1: Kinetic energy release distributions in asymmetric fission reactions of multiply charged C_{60} (solid curves) and C_{70} (dashed curves), as functions of q. The distributions shown are used in ion-optical simulation to yield optimized fits to the measured radial distributions at the end of the spectrometer (see text).

We find that the kinetic energy release distributions are lower, and narrower, in energy for C_{70} than for C_{60} which may be related to smaller changes in internal energies for C_{70} fragmentations. This, in turn, may be due to the larger number of vibrational degrees of freedom for C_{68} in comparison with C_{58} . In figure 2, the positions of the KERD-maxima are plotted as a function of q together with results from high level Density Functional Theory (DFT) calculations [1]. The most probable values of our KERD agree almost perfectly with [1].



Figure 2: The most probable KER values for asymmetric fission of C_{60}^{q+} (filled circles) and C_{70}^{q+} (filled squares). DFT results for C_{60}^{q+} [1] are shown by open circles and connected by lines in order to guide the eye.

Further, we have measured the intensity ratios between asymmetric fission and the competing C₂-evaporation processes, $C_{60/70}^{q+} \rightarrow C_{58/68}^{q+} + C_2$, for our experimental time frame of several microseconds. Combining the latter measurements with a statistical model for the competition between asymmetric fission and C₂-evaporation we extract semi-empirical values for the fission barriers. These semi-empirical results, compare very favorably with DFT results obtained by calculating the $(C_{58}^{(q-1)+} + C_2^+)$ transition-state [1] and somewhat simpler DFT calculations of C_{70}^{q+} fission barriers [2]. The agreement is surprisingly good and typically within a few tenths of an eV. Our semi-empirical results are only weakly dependent on model assumptions on the total excitation energies of the mother fullerenes and the pre-exponential factors in the rate constants.



Figure 3: Semi-empirical fission barriers for C_{60}^{q+} (filled circles) and C_{70}^{q+} (filled squares). Results from theory (DFT) [1,2] are shown by corresponding open symbols.

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INELASTIC ELECTRON INTERACTION WITH DOPED HELIUM DROPLETS

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The extensive number of spectroscopy studies with doped helium droplets shows impressively the ability of superfluid helium droplets for preparation of cold targets [1,2]. Any species embedded will be cooled down to 0.37 K which allows the preparation of complex fragile species. In contrast to optical spectroscopy, the inelastic electron scattering with doped helium droplets has been less studied. So far most investigations in this research field covered electron impact ionization of doped helium droplets (e.g. Refs. [3-5]). In this case an initial helium atom at the surface of the helium droplet is ionized and after subsequent charge transfer via several helium atoms the hole finally localizes at the dopant molecule or cluster inside the helium droplet. This different ionization mechanism compared to molecules in the gas phase can lead to substantial modification of fragmentation pattern upon electron impact ionization [3-5].

Our group has constructed a helium droplet source [6] which was initially used to study the electron impact ionization of pure helium droplets, as well as the metastable decays of small helium cluster ions. Recently we modified the helium droplet source by adding a pick up chamber with oven, pick up cell and external gas inlet which allows to dope cold superfluid helium droplets with various molecules. Currently the droplet source is mounted at a double focusing two sector field mass spectrometer (see Figure 1). The Nier type ion source of the mass spectrometer is capable to produce both positive and negative ions formed upon inelastic interaction of electrons with the doped droplets which are then mass analyzed with the two sector field instrument.



Figure 1: Experimental setup used for the experiments with doped helium droplets In the present contribution recent highlights of our electron attachment studies with doped helium droplets will be presented. For negative ion formation the intrinsically resonant attachment process is strongly altered compared to the free electron capture by bare molecules and clusters. At low

electron energies the captured electron forms a metastable bubble inside the helium droplet which finally localizes at the dopant. However, the electron distribution is shifted by the helium droplet which has important consequences for the abundance of low and high energy resonances as the attachment cross section has a 1/E dependence. Results will be shown for small biomolecules like DNA bases [6], amino acids and H₂O [7], for organic acids, for halogenated compounds [8] and for CO_2 . All of these compounds have been studied previously in the gas phase and for most species also bare cluster experiments have been carried out. From the comparison with these previous measurements we can deduce changes in the attachment process by the cold helium droplet environment and characterize the electron capture process for the various species embedded in He droplets.

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Clustering phenomena at nuclear and subnuclear scales

Th-I-1

SUPERHEAVY ELEMENTS

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The existence of transactinides is determined by the structure of the heaviest nuclei. Nuclear stability increases in the vicinity of closed proton and neutron shells. The nuclear shell model predicts stability islands in the domain of superheavy elements. Enhanced stability is expected for deformed nuclei near Z=108 and N=162, yet stronger effects are predicted for spherical nuclei close to Z=114 and N=184. This lecture is devoted to experimental verification of these predictions. Fusion reactions of 208Pb, 209Bi with 50Ti, 54Cr, 70Zn, etc. projectiles (cold fusion) produce nuclides with Z=104-113, N=151-165 in the region of deformed shells (Z=108, N=162). These nuclides undergo sequential alpha-decays to known transactinides. The synthesis of heavier, neutron-rich nuclei is carried out in reactions of 233,238U, 237Np, 242,244Pu, 245,248Cm and 249Cf with 48Ca projectiles (hot fusion), creating nuclides with Z=104-118 and N=161-177. These experiments show that adding six neutrons to isotopes with Z=110-114 results in an increased stability (about five orders of magnitude) as an effect of the spherical shell N=184. The nuclides undergo sequential alpha-decays ending in spontaneous fission of long-lived isotopes of Rf and Db. Energies and half-lives have been measured for 34 nuclei and are compared with theoretical calculations from various models. This lecture presents experiments on the detection of superheavy nuclides with in-flight recoil separators. Off-line liquid phase extraction of 268Db, the final product in the decay of (288)115, and the study of elements 112 and 114 by absorption gas chromatography will be discussed. The search for superheavy elements in nature and cosmic rays, as well as the search for spontaneous fission of Hs (Z=108) and its daughters under way underground in Modane (France), will be described. Results are from FLNR (Dubna, Russia) in collaboration with LLNL (Livermore, USA) and PSI (Villigen, Switzerland), GSI (Darmstadt, Germany), RIKEN (Wako-shi, Japan) and LBNL (Berkeley, USA).

Th-I-2

FUSION-FISSION OF SUPERHEAVY NUCLEI AND CLUSTERING PHENOMENA

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In the last decade big efforts were made in the field of superheavy elements synthesis with Z=112-118 in the reaction with heavy ions. However, the prediction of the formation cross section of superheavy nuclei and its survival probability is still open question. To solve this problem, the information on all possible processes in this type of reactions, such as evaporation residues, fission, quasifission, deep-inelastic and elastic scattering, is needed.

Results of the experiments aimed at the study of fission and quasi-fission processes in the reactions ³⁶S+²³⁸U, ⁴⁸Ca+^{144,154}Sm, ¹⁶⁸Er, ²⁰⁸Pb, ²³⁸U, ²⁴⁴Pu, ²⁴⁸Cm; ⁵⁰Ti+²⁰⁸Pb, ²⁴⁴Pu; ⁵⁸Fe+²⁰⁸Pb, ²⁴⁴Pu, ²⁴⁸Cm and ⁶⁴Ni+¹⁸⁶W, ²⁴²Pu, leading to the formation of heavy and super-heavy systems with Z=82-122 are presented. Cross sections, mass-energy and angular distributions for fission and quasi-fission fragments have been studied at energies close and below the Coulomb barrier. The observed peculiarities of the mass and energy distributions of reaction fragments are determined by the shell structure of the formed fragments.

The entrance channel effect plays an important role in the fusion-fission dynamics and the competition between the fusion-fission and quasi-fission processes. The target deformation is a dominant factor in the evolution of the composite system. It was found that the formation of quasifission fragments mainly determined by nuclear shells with Z=20, 82 and N=50, 126. The multimodal fission phenomena have been observed for the superheavy nuclei ²⁵⁶No, ²⁰⁶Sg and ^{266,274}Hs.

Th-I-3

NUCLEI: SUPERHEAVY – SUPERNEUTRONIC – SUPERSTRANGE

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The extension of the Periodic System into super heavy and extreme neutron rich domains is discussed. Also the sectors of strangeness and antimatter will be given attention.

Clusterization of nuclear matter in supernova environments

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In this talk I discuss clustering phenomena in stellar matter at sub-nuclear densities and moderate temperatures which are characteristic for supernova explosions. I demonstrate that thermodynamic conditions there are rather similar to those created in the laboratory by intermediate-energy heavy-ion collisions [1,2]. Theoretical methods developed for the description of multi-fragment final states in such reactions can be used also for description of the stellar matter. I present main steps of the statistical approach to the equation of state and nuclear composition [3], dealing with an ensemble of nuclear species instead of one "average" nucleus. I shall also present results concerning the structure and stability of nuclei embedded in the hot and dense stellar matter, calculated within a microscopic model [4]. The emphasis is made on possible formation of heavy and superheavy nuclei in supernova environments. The main conclusions of this study are:

- Statistical equilibrium approach is very useful for describing equation of state and composition of supernova matter. It can easily incorporate the empirical information concerning properties of hot heavy nuclei.
- Formation of heavy and superheavy elements (SHE) is favored by electron screening and reduction of symmetry energy in hot and dense stellar matter.
- If long-lived SHE do exist, they may be produced in supernova environments and injected in space in the course of explosions. If their life times are longer than 10⁷ years, they may even reach the Earth.
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A STATISTICAL MODEL FOR THE LIQUID-GAS PHASE TRANSITION OF HOT NUCLEAR MATTER

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We study the equation of state and the composition of nuclear matter at finite temperature with a grand canonical model which assumes nuclear statistical equilibrium. Matter is described as a thermodynamic ensemble of nucleons, photons, leptons and all possible nuclei. For the nucleons the relativistic mean field theory is used, the masses of the nuclei are taken from existing nuclear structure calculations, that were corrected for effects of finite temperature and the surrounding medium. The wide range of density, temperature and proton fractions which is present in astrophysical scenarios like supernova explosions is analysed. Emphasis is put on the liquid-gas coexistence region of nuclear matter where a broad fragment distribution can be seen. This density region is also accessible in terrestrial laboratories, namely by heavy ion collisions in form of multifragmentation experiments.

FERMION CONDENSATION QUANTUM PHASE TRANSITION IN FINITE AND TWO-DIMENSIONAL STRONGLY CORRELATED FERMI SYSTEMS

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It is shown that Landaus quasiparticle formalism continues to work in systems with a fermion condensate [1]. In the case of a finite system this formalism is suitable for describing the restructuring of states at the Fermi surface. It also works in an infinite system, and the idea of quasiparticles at low temperature as well-defined excitations at the Fermi surface remains valid. The quasiparticle lifetime is directly proportional to the temperature, and the density of states is inversely proportional to the temperature.

In the case of finite Fermi-system, the possibility of merging single-particle levels is examined. It is demonstrated that the opportunity for this behavior is widespread in quantum many-body systems. The salient feature of the phenomenon is the occurrence of nonintegral quasiparticle occupation numbers, leading to a radical alteration of the standard quasiparticle picture. The impact of nonintegral quasiparticle occupation numbers on the properties of nuclear, atomic, and solid-state systems is considered.

On the example of two-dimensional (2D) ³He we demonstrate that the main universal features of its experimental temperature T - density x phase diagram [2] look like those in the heavy-fermion metals. Our comprehensive theoretical analysis of experimental situation in 2D ³He allows us to propose a simple expression for effective mass $M^*(T, x)$, describing all diverse experimental facts in 2D ³He in unified manner and demonstrating that the universal behavior of $M^*(T, x)$ coincides with that observed in HF metals.

We obtain the marvelous coincidence with experiment in the framework of our theory. Moreover, these data could be obtained for ³He only and thus they were inaccessible for analysis in HF metals. This fact also shows the universality of our approach. Thus we have shown that bringing the experimental data collected on different strongly correlated Fermi-systems to the above form immediately reveals their universal scaling behavior [3].

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Phase transitions, fusion, fission and fragmentation in finite systems

FROM HELIX-COIL TRANSITION IN POLYPEPTIDES TO PHASE TRANSITIONS IN PROTEINS

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The phase transitions in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state or vice versa (also known as (un)folding process) occur or can be expected in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes.

We suggest a theoretical method based on the statistical mechanics for treating the helix random coil transition in polypeptides. We consider this process as a first-order-like phase transition in finite system and develop a theory which is free of model parameters and is based solely on fundamental physical principles. It describes essential thermo dynamical properties of the system such as heat capacity, the phase transition temperature and others from the analysis of the polypeptides potential energy surface [1,2].



Figure 1: Dependence of total energy and heat capacity calculated for Val_{30} polypeptide. The dots in the right plot show the dependence of heat capacity obtained from the analysis of polypeptides energy fluctuations; the solid line corresponds to the derivative of the interpolating function of the transition energy on temperature. Smaller peak at lower temperatures in the dependence of heat capacity on temperature corresponds to the order-disorder transition in side-chain radicals of valine.

We perform thorough comparison of the predictions of the statistical model with the results of molecular dynamics simulations. Two methods of calculation of heat capacity of the system are analyzed, namely method based on differentiation of energy on temperature dependence and method based energy fluctuations. We also investigate the influence of side chain radicals on the thermodynamic properties of the system [3].

The suggested theory is general and with some modifications can be applied for the description of phase transitions in other complex molecular systems such as proteins, DNA, fullerenes, etc. [4].

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INTERPLAY BETWEEN PROTON TRANSFER AND TEMPERATURE EFFECTS IN THE CONFORMATION OF ISOLATED PEPTIDES

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The fragmentation of gas-phase peptides is often experimentally addressed using mass spectrometry techniques. The molecules involved in such measurements are singly or even multiply charged with additional protons. In order to explain the fragmentation patterns, these protons are assumed to be highly mobile along the peptide sequence.

A fully atomistic model is presented to describe protonated isolated peptides in a sufficiently simple fashion for temperature effects to be directly simulated using conventional Monte Carlo or molecular dynamics techniques. More importantly, proton transfer between basic residues is included in the modeling, assuming that the most stable site is always protonated (adiabatic limit). Alternatively, the quantum mechanical delocalization of the extra proton over coupled basic sites can be described using an empirical valence-bond model, for which the adiabatic model is a particular case. We have developed a multistate molecular mechanics method along such lines, based on a standard force field (Amber ff96) for describing each protonated peptide, and simple potentials for the intersite couplings. The proton affinities needed to calibrate the different force fields to each other were obtained using static electronic structure calculations at the DFT/B3LYP level. These models were applied to the lysine-rich polyalanines A_4K , A_9K , and A_4KA_4K . In the small pentapeptide, the favored protonation site changes at about 400 K from the N-terminus to the lysine end, and coincides with the unfolding transition. Protonation at the lysine end is much more robust in A_9K due to a favorable interaction between the charge and the macrodipole arising from the helical secondary structure. In the A_4KA_4K peptide, the extra proton can be partially delocalized over the N-terminus and the first lysine end. Introducing attractive couplings can lead to proton-bound configurations stabilized through the formation of an ammonium-ammonia complex. These theoretical results [1] are comparable to recent measurements carried out in the Jarrold group [2].

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FREEZING-POINT DEPRESSION BY INSOLUBLE IMPURITIES: A NANO EFFECT

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Freezing point depression by impurities is usually an entropy-driven effect. By considering the system sodium – sodium oxide, we illustrate experimentally an additional mechanism, caused by insoluble impurities in nano-sized particles. Our experiments show that the oxide from two oxygen atoms in sodium clusters with 135-192 atoms causes a freezing-point depression by 17 ± 6 K. Additional oxygen amplifies the effect, while the corresponding bulk system shows no freezing point depression at all. First-principles density functional theory calculations reveal the interaction between a pure and an oxidized part of the cluster to be responsible for the effect. There is more structural freedom in a liquid cluster to optimize the interface between metal and impurity. This stabilizes the liquid phase and causes the observed, cluster-specific freezing point depression.

Th-IV-1

TAILORING FUNCTIONALITY OF CLUSTERS AND THEIR COMPLEXES WITH BIOMOLECULES BY SIZE, STRUCTURE AND LASERS

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Investigation of integrated metallic nanoparticle-biomolecule hybrid systems allows to gain fundamental knowledge about interactions among intrinsicaly different subsystems which produce novel properties and functions. This is due to the combination of unique electronic and catalytic properties of nanoparticles with the unique functional properties of biomolecules. Therefore a broad spectrum of applications in sensoric, bioanalytics and for bioelectronic devices is emerging. The aim of our contribution is to reduce the complexity of nanoparticle-biomolecules by studying structural and optical properties of metallic-cluster – peptide hybrid systems at molecular level in the gas phase. Therefore, by changing the size of the clusters in the nonscalable regime, removing or adding a single atom or/and changing the size of the peptide allows to tune structural and optical properties of hybrid systems and to probe their environments. The theoretical findings are supported by photofragmentation experiments.

In order to gain basic understanding about the nature of the interactions between small nanoparticles and biomolecules and to unravel the mechanism responsible for the optical processes, we first address the optical properties of size dependent cationic silver clusters interacting with tryptophan: $Trp-Ag_n^+$. Then we introduce a polyalanin chain with tunable length which links the tryptophan and silver subunits: $Trp - (Ala)_n - Ag_n^+$. This is a model system to study the interaction between silver clusters and proteins and offers the opportunity to investigate and to tailor the resonant fluorescence energy transfer (FRET) in hybrid systems in the future. For this purpose we developed a new strategy for the optimal pump-dump control in complex systems based on the "field induced surface hopping" method in which the nuclear dynamics is treated classically while the laser induced electronic transitions are treated fully quantum mechanically. Thus this should serve as theoretical basis for application of optimal control theory in the field of biosensories.

Th-IV-2

COLLISIONS WITH CLUSTERS OF FULLERENES AND BIOMOLECULES

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Large complex systems are able to store an amount of energy which may well exceed the energetic threshold of individual dissociation channels. This occurs as the energy is not necessarily localised but may be distributed among a large number of degrees of freedom allowing for long lifetimes of the excited system. When energy is transferred in collisions with other particles, this may lead either to the formation of differently structured systems (for example by fusion processes), or it may cause the fragmentation of the system on a shorter or longer time scale depending whether the whole system or only a part of it is involved in the energy deposition.

In the present contributions we will first discuss collisions of highly charged ions with clusters of fullerenes $(C_{60})_n$. In the case of the interaction of fs-lasers with these systems, the process of fusion has been identified for small cluster sizes[1]. We discuss whether these processes can be observed also in collisions with highly charged ions. Figure 1 shows a part of the measured mass spectrum in the range of small cluster sizes, obtained in collisions of Xe²⁰⁺ projectiles with (C₆₀)_n clusters.

In a second part, we will discuss results about the fragmentation of isolated and nanosolvated biomolecules. A particular aspect concerns the influence of the environment on dominant reaction channels and the fragmentation probability. The fact whether a 'protection effect' does exist or not is found to depend on the primary excitation process, i.e. whether only energy is transferred in the collision or whether electron transfer is involved in addition. Results for Porphyrin molecules as well as for AMP^{-*}(H₂O)_n clusters and dipeptides are discussed.

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Th-IV-2



Fig.1: Mass spectrum of fullerene clusters produced in collisions of Xe^{20+} projectiles with C_{60} _n clusters. Collision energy: 400 keV

Th-IV-3

Phase Transitions of Fullerenes: Fragmentation↔Reassembly of the Carbon Cage

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Figure 1: Snapshots of the fragmentation simulation of C_{60} . (a) Deformed C_{60} cage at T = 4500 K; (b) Broken bonds and evaporation of a C_2 from the cage at T = 5800 K; (c) Evaporation of a ring, leaving a window in the cage at T = 5800 K, 65 ps after the C_2 evaporation; (d) Cage unravels into a web-structure and short chains at T = 5800 K; (e) Web-structure has decomposed to chains and dimers, 61 ps later at T = 5800 K; (f) Only dimers and short C_3 chains at T = 6300 K.

Fullerene formation and fragmentation mechanisms have been intensely investigated over two decades. While it is known that fragmentation of the cage can be induced by pyrolysis [1], laser-irradiation [2] or collisions with charged/neutral particles [3–5], the mechanism of formation has remained unclear, with various proposed mechanisms of its assembly available in the literature [6,7]. In this work, we propose that thermal fragmentation and the assembly of fullerenes are related processes—both are mechanisms of phase transition. The former leads to the disintegration of the *solid*-like hollow cage to a *gas*-like state of dimers (C₂ units); while the latter reverses the previous process and recreates the fullerene cage from the hot carbon gas. By means of isothermal molecular dynamics (MD) simulations of fullerenes C₆₀ and C₂₄₀, we report the occurrence of fullerene sublimation above the phase transition temperature at 5855 K

Th-IV-3

for C_{60} and 5500 K for C_{240} . The loss of a C_2 unit rapidly leads to the breaking of the fullerene cage and its eventual decomposition into the gaseous phase, Fig. 1. In the region of the phase transition temperature, the system oscillates between two distinct phases: the *solid*-like cage and the *gas*-like state of the carbon dimers. Such oscillation corresponds to the consecutive back-and-forth fragmentation and re-assembly of the fullerene which can be seen clearly in the bimodal distribution of the total energy over time (at a single temperature). This coexistence behaviour, as well as the prominent peak of the temperature-dependent heat capacity and the abrupt jump in the temperature-dependent total energy, Fig. 2, are signatures of first-order phase transition in finite systems.



Figure 2: Total energy E of C₆₀ as a function of temperature for different C-C bond energy parameters of the forcefield we have developed $\epsilon_s = 2.38$, 3.25, 3.81, 4.12 and 4.99 eV. Each curve shows a distinct jump in energy corresponding to a phase transition in the system. The scattered plot is the time-average total energy and the solid thick line is the cubic B-spline interpolation.

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Structure and dynamics of biomolecules

FRAGMENTATION PATHS IN BIOSYSTEMS MEDIATED BY METASTABLE ELECTRON ATTACHMENT IN THE GAS PHASE

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The damaging effect of ionizing radiation has been known for a long time: it has been an accepted fact that high-energy tracks formed by α , β , γ particles and atomic ions can ionize cell components along the radiation track, thereby leading to various dissociation channels and to the formation of damaging radicals [1]. Recent observations by Sanche and coworkers [2] have also discovered that not only photons, but also electrons at energies below the ionization thresholds can generate damaged DNA strands by forming mutagenic, lethal DNA and RNA lesions which lead to single and double strand breaks [2]. Their data showed that electron attachment within an energy range between a few and less than 20 eV can indeed cause the above breaking processes [3] since the formation and ensuing decay of a broad variety of Transient Negative ions (TNIs) of the various components of the initial double helix structures.

The corresponding theoretical description, at the molecular level, of the rather complex energy redistributions which can lead to the final break-ups into stable fragment anions has been attempted by the calculations carried out in our group in Rome [4-6], where we analyse the quantum scattering process of low-energy electrons off the molecular components of DNA. In this approach we devise an essentially an initio model which allows us to locate and classify several low-energy resonances which then decay by different pathways of energy redistribution into the molecular nuclear networks. In particular, we shall show that detailed spatial analysis of the metastable electron wavefunctions at the initial geometry, and the study of the resonance changes following specific bond deformations, can allow to identify rather well the most likely dissociation pathways and the chemical nature of the final, neutral and ionic fragments to be compared with experiments [7].

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UV spectroscopy of isolated proteins and metal cluster/peptide complexes

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The spectroscopy of proteins is a very powerful method to determine their structures and related properties. In this paper we will present two series of recent results obtained firstly on proteins or polypeptides and secondly on metal cluster/peptide complexes. The anions or cations produced by an electrospray ionization source are stored in a quadrupole ion trap and excited by a tunable UV laser. The optical spectra are recorded by measuring the photodetachement or photofragmentation yields as a function of the laser wavelength.

For proteins, after laser irradiation of their multi-anions, we observe electron detachment from the proteins leading to the formation of radical ions. By measuring the detachment yield as a function of the laser wavelength, one can determine the electronic excitation spectrum of the isolated protein. Results have been obtained for different variants of Angiotensin, Insulin and Ubiquitin and compared to solution spectra and ab-initio calculations. The obtained spectra is mainly due to chromophores and we observe a bathochromic shift which is directly related to the ionization state of the tyrosine chromophore^[1].

In the case of Tryptophan silver complexes (WAg_n^+) a strong optical absorption is observed and the spectra are compared to ab initio theoretical calculations^[2]. Two classes of structures, zwitterionic and charge solvated ones can be identified. They are correlated not only to slightly different absorption spectra, but mainly to two different fragmentation channels which may be therefore considered as fingerprint of the structure. For larger Silver cluster (n=9), the photofragmentation yield is too low and the energy gained by photoabsorption might be dissipated by fluorescence or Internal Vibrational Distribution (IVR). The results have been recently extended to WGlyGlyAg_n⁺ clusters. These hybrid molecules are ideal models for investigating on a fundamental point of view the properties of biosensoring materials.

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DEFORMATION MECHANISMS OF DNA-TYPE MACROMOLECULE

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The deformations of the chain macromolecules are described usually with the help of the model of worm like chain (WLC) in accordance to which the macromolecule is presented as uniform and anisotropic chain with harmonic law for the energy of the deformation [1]. Such model is named also as the model of elastic rod and is frequently used for the interpretation of the experimental data on deformation of the macromolecules of DNA-type [1, 2].

Last years the experimental data about the anomalous (as to WLC model) deformability of DNA double helix have been appeared. It was found the large bendability of the short DNA fragments, the loop formation in the relatively short DNA, and the anomalous condensation of the double helix in a small volumes (see [3-6] and cited therein). In the molecular dynamics simulations [7] it was shown that anomalous deformability may be connected with the conformational degrees of freedom of DNA double helix.

Besides this, the experiments on single molecule manipulation show unexpected effect of overstretching of the double stranded DNA [8]. In the experimental works it was demonstrated the elongation of the macromolecule counter length in 1.7 times under some definite value of acted force (about 65 pN). One of the interpretations of the effect is the transition of the DNA double helix from B-form of the double helix to S-form (stretched) with appropriate change of the chain length [8]. So, here the macromolecule internal degrees of freedom are connected with the external degrees, as in the anomalous effects of bending.

For the interpretation of the effects with such large deformations of DNA macromolecule it is insufficient to use the WLC model. To understand the large-scale transformations of the double helix it is necessary to use the approaches of the nonlinear mechanics. To describe the deformability of DNA-type macromolecule in the frame of the double helix state the concept of the structure elements motion in the frame of double helix state is developed. The macromolecule is considered as a chain of monomer with the conformational degrees of freedom. The mobility of the structural elements in the frame of DNA monomer unit is described by generalized four-mass model [9-11] for the displacements of atom groups: two groups of backbone atoms, and two nucleosides. It is taken into account also the nucleotides motions, intranucleoside mobility, and H-bonds stretching in the base pairs.

For small amplitudes of the structural elements displacements the developed approach allows to describe the conformational vibrations of the double helix. The calculated frequencies of DNA double helix are in a good agreement with experiments at $< 200 \text{ cm}^{-1}$ and give the understanding of DNA low-frequency spectra, its dependence on helix conformation, temperature, nucleotide and counterion content [12]. For large-scale displacements due to the consideration of concert motions of DNA structural elements, the unifying model for the study of different conformational transformations is constructed in the two-component form. One component of the model is the degree of freedom of the elastic rod and another component – the effective coordinate of the conformational transformation.

The conformational excitations under *B-A* transitions in the double helix are found. The transition from DNA basic state (*B*-form) to metastable (*A*-form) and the transition between the forms in the conditions of conformation equilibrium are studied. For both types of the macromolecule structural transformations the static deformations were determined for internal and external components. The comparison of the data of the developed theory with the experiments on DNA deformability (presented in Nucleic Acids Database) shows a good accordance. It is seen that observed DNA deformations are occasioned by the intrinsically localized excitations – static conformational solitons by their nature. The correlation between the macromolecule deformation and the number of the intrinsic conformational excitations are shown.

The obtained results are responsible for explanation the mechanisms of anomalous macromolecule deformation under DNA-protein recognition, double helix overstretching, DNA compacting in viruses. Indeed the proposed nonlinear mechanism of double helix deformability depends on the bistability of DNA monomer, boundary conditions, and applied force. The analysis of the solitonic excitations occurrence in DNA double helix show that it is possible two mechanisms of the deformation: stepwise and threshold. Both these mechanisms of the deformation include the significant participation of the conformational degrees of freedom of the double helix and may work on DNA in different cases of external force applying and the conformational properties of the double helix section.

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Collision processes involving biomolecules

IONIZATION AND FRAGMENTATION OF AMINO ACIDS AND THEIR CLUSTERS – ISOMER EFFECTS AND PEPTIDE FORMATION

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Small amino acids have been found e.g. in meteorites and are predicted to exist in interstellar clouds. There, neutral molecules and clusters are constantly exposed to irradiation with keV and sub-keV ions, e.g. from supernovae. Mass spectrometric investigation of the charged collision products from keV ion collisions with amino acids can thus deliver important data for the gas-phase ion chemistry in space. Also in the context of biological radiation damage, amino acids play an important role. It is well established that DNA damage is the first step of almost all biological radiation effects. However, in the nuclei of eukaryotic cells, DNA is wound around protein spools - the so-called histones. The radiation action upon these proteins is of interest since secondary particles formed during the interaction might in turn damage the neighboring DNA.

We studied the ionization and fragmentation of α - and β -alanine molecules and clusters by keV multiply charged ions using coincidence time-of-flight spectrometry. Strong isomer effects and extensive fragmentation are observed for isolated molecules [1]. Similar results have also been observed for other small amino acids [2]. For the case of alanine clusters, we find completely altered mass spectra. Besides hydrogen-bound clusters and fragments, different polymerization channels are observed. In particular we could identify clusters containing alanine-dipeptide formed in the gas phase.



Figure 1: Mass spectrum of product ions from 40 keV He²⁺ collisions with α - (top) and β -alanine (bottom). **A** and **B** label the main interaction products NH₂CH₂⁺ and NH₂CH₃CH⁺.

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NANOSCALE MECHANISMS OF DNA DAMAGE INITIATED BY ENERGETIC IONS IN TISSUE-LIKE MEDIA

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The peculiar energy deposition profile of the highly energetic ion beams, has opened great perspectives for radiation biology towards the implementation of medical equipments treating in a very well spatially resolved way the internal tumors [1].

Then from a couple of decades is becoming very challenging the study of the processes involved in this ion therapy by the means of the nuclear, atomic, molecular and biological physics modelling. In fact this is a spectacular testfield for theory implementations at a high interdisciplinar level and, on the other hand, its results are directly connected to urgent applications in improving emerging facilities for this new sanitary tool. While a number of steps at a macroscopic scale are known, the analytical description of the process starting from the entrance of the beam particles in the tissue and the final biological damage is still far to be completely understood at a nanoscopic level. The whole process stems from steps characterized by very different time scales, kind of interactions, transport properties, energies, spanning from nuclear physics to chemical reactions, till enzimatic reactions [2]. That's why the methods employed are very different, from Montecarlo simulations [3] to quantum dynamics [4]. It is known that the main damage is due to attach to the DNA chain of relatively low energy secundary electrons and radicals [5]. These products are able to induce different type of such a damage to the macromolecule, the most important one being the Double Strand Break (DSB), that stays for the occurrence of a break on both opposite strands within a given distance. Thus, detailed description of the spectrum of this secundary products generated by the ion passage is a key point, and our approach starts from the latter [6,7].

An overview is presented about existing methods studying the propagation of these electrons in the medium and their links to the possible estimations of the DSBs in a DNA molecule and a new approach [7] is proposed for an elucidation of nanoscale mechanisms of radiation damage.

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INTERACTION OF METAL NANOPARTICLES WITH BIOLOGICAL MOLECULES

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Gold nanoparticle has wide utilities as a bioanalytical probe because of its characteristic optical phenomena, and good affinity and appropriate sizes to any biomolecules concerned. For instance, an interaction of a gold nanoparticle with a protein molecule in an aqueous solution changes critically with the pH of the solution, because the net charge of the protein and the surface potential of the nanoparticle change on the pH of the solution and hence the affinity of the protein to the nanoparticle changes as well.

Moreover a high temperature and pressure reaction field is generated by laser irradiation in a close vicinity of a gold nanoparticle in an aqueous solution. In addition, by taking the characteristic protein interaction with the nanoparticle and the reaction field into consideration, we have demonstrated selective degradation of Lysozyme and BSA (bovine serum albumin) in the solution containing the nanoparticle under laser irradiation [1]. A typical result obtained is shown as follows: Lysozyme and BSA do not interact with gold nanoparticles in a pH > 11.0 region because their net charges and surface potentials are negative, and hence their degradation does not proceed efficiently. On the other hand, in a 7.0 < pH < 11.0 region, only Lysozyme having a positive net charge interacts with the nanoparticles and degradation of Lyzozyme selectively proceeds. In a pH ~ 4.0 region. Lysozyme is not aggregated on the particles under such a higher net charge of Lysozyme. On the other hand, BSA having a positive net charge a pH of ~ 4 region interact with the nanoparticles, and are efficiently degraded. In a pH < 4.0 region, Lysozyme and BSA can not interact with the nanoparticle, because the surface potential of the nanoparticles is nearly zero. Therefore, Lysozyme and BSA are not degraded in such an acidic solution. These findings lead us to conclude that the reactions occurring in the unique field can be utilized as useful and powerful tools in a bioanalytical chemistry.

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From biomolecules to cells and system biology

MAGNETIC CLUSTERS IN A BEAK OF A BIRD: A MECHANISM OF MAGNETORECEPTION

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Many birds are able to orient themselves accurately when the sky is not visible (e.g. covered with clouds). This requires non-visual sources of information. Many studies have established that birds are sensitive to the Earth's magnetic field. European robins, pigeons and other bird species use the geomagnetic field as a compass, and are also sensitive to slight temporal and spatial variation in the magnetic field that is potentially useful for determining location.

We study a putative avian magnetoreception mechanism, which is based on the interaction of two iron minerals (magnetite and maghemite) experimentally observed in subcellular compartments within sensory dendrites of the upper beak of several bird species [1,2]. The iron minerals in the beak form platelets of crystalline maghemite and clusters of magnetite nanoparticles. We develop a theoretical model [3,4] to quantitatively describe the interaction between the ironmineral containing particles, and demonstrate that depending on the external magnetic field the external pull or push to the magnetite clusters may reach a value of 0.4 pN. This might be principally sufficient to excite specific mechanoreceptive membrane channels leading to different nerve signals and causing a certain orientational behavior of the bird.

Experimental analyses of birds' behavior showed that if the vertical component of the magnetic field vector was inverted (see Figure 1): birds heading North in the geomagnetic field reversed their heading, now preferring South [5]. This is how the inclination compass in birds was discovered. Reversing the horizontal component and inverting the vertical component alter the axial course of the field lines in the same way; an animal not perceiving the polarity of the magnetic field will not realize any difference. Hence birds reverse their headings in both situations alike.

We suggest [3,4] that the iron-mineral-based magnetoreception mechanism might be involved in the magnetic-compass sense of birds. We show that the magnetoreceptor system observed in Ref. [1,2] and theoretically studied in [3,4] possesses all features of a polarity compass (see Figure 1). We also study how the number of maghemite platelets in the magnetoreceptor affects the compass properties of the system. We demonstrate that if the magnetoreceptor has only one maghemite platelet the polarity compass can become a bidirection inclination one. We outline the problems which should be considered experimentally in order to check our assumptions.



Figure 1: Principle of the polarity (a) and of the inclination (b) compasses. The polarity compass is similar to our technical compass, using the polarity of the magnetic field to distinguish between magnetic 'North' and 'South'. In the inclination compass the polarity of the magnetic field vector is irrelevant since birds obtain directional information from the axial course of the field lines. That way, birds cannot distinguish between northward and southward, but between poleward and equatorward. \vec{B} represents the vector of magnetic induction, B_v and B_h are its vertical and horizontal components. Note, that in the northern hemisphere the vertical component of the induction of magnetic field is inverted in respect to the southern hemisphere. The images of a bird show the tentative flight direction determined according to the polarity (a) and inclination (b) compass.

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TOWARDS AN INCLUSIVE APPROACH TO ESTIMATION OF DNA DAMAGE DUE TO INCIDENT IONS

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Ion-beam therapy is one of the most advantageous types of radiation treatments of malignant tumours because the ions being effective in a desired location, may cause less damage to the regions surrounding tumours and thus induce fewer side effects. This is especially important if the side effects are crucial for the patient's quality of life [1].

We are designing an inclusive approach to estimation of efficiency of irreparable damage to the DNA due to incident ions. In our mind, this estimation should be based on microscopic effects in the biological medium from analysis of propagation and stopping of projectiles to interaction of secondary electrons and produced free radicals with the DNA rather than on the energy deposition in the region. At this time, the understanding of these effects is very limited both theoretically and experimentally.

An incident particle, whether it is high-energy hadron, or electron, or photon, produces secondary electrons as a result of interactions with a medium. These are secondary electrons that are believed to be responsible (directly or indirectly) for the ultimate DNA damage. In order to set up a problem of secondary electron interactions we need physical characteristics of these electrons, such as their number density and energy and angular distributions. In the first part of our project [2,3], we have analysed the track of a single ion: we calculated the linear energy transfer (LET). The dependence of LET on the penetration depth indicated the Bragg peak, the position where the energy loss by the projectile reaches its maximum. In order to correctly predict the position of the Bragg peak, we had to treat the projectile relativistically. In order to obtain the shape of the Bragg peak, we had to take into account the process of charge transfer in which the ion, initially fully stripped off electrons, acquires some electrons as it slows down. Then, after accounting for scattering of the ion that results in straggling of its energy, our results indicated good agreement with Monte Carlo simulations using GEANT4 tool kit.

The final estimates will be related to the energy deposition by the projectiles, but this should be a result of the microscopic analysis. Then more accurate predictions may contribute to the protocol of cancer therapy. They will be formulated in the language of dosages, energies, radiation rates, etc. This is the definition of the inclusive approach that we are attempting to develop in the ongoing work.

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MOLECULAR CLUSTERING AT THE IMMUNOLOGICAL SYNAPSE

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Intercellular communication is central to immunity and is realized by the physical interaction between molecules on the surface of immune cells. Antigen-presenting cells process pathogen-derived molecules and present them at their surface together with major histocompatibility complexes (MHCs). Scanning T-cells in lymphoid tissue bind with their specific T-cell receptors (TCRs) to peptide-MHC (pMHC) on antigen-presenting cells, and on cognate encounter this interaction initiates the dynamic formation of an immunological synapse. The immunological synapse is an adhesive cell–cell junction with a nanometer scale gap between the cells and the sustained signaling via mutually bound receptor-ligand complexes is a vital process that sets T-cells into a variety of possible activation states.

The molecular structure of a prototypical immunological synapse forms within minutes into a well-organized bull's-eye pattern that may remain stable for hours (see Figure 1A). This molecular pattern is composed of an outer ring - the so-called peripheral supramolecular activation cluster (p-SMAC) – consisting of complexes of the adhesion molecule leukocyte functionassociated antigen-1 (LFA-1) and the intercellular adhesion molecule-1 (ICAM-1). The center of the bull's-eye pattern – the so-called central supramolecular activation cluster (c-SMAC) - consists of TCR-pMHC complexes. During recent years, the hypothesis that the bull's-eye pattern is required for enhanced and sustained TCR signaling and thus for T-cell activation has become a matter of controversy. In fact, immunological synapse formation does not seem to follow a fixed plan for a common molecular structure but adopts very different topologies that, for example, are dictated by the cellular diversity of interaction partners or are related to different phases of the dynamic T-cell scanning. Therefore, rather than being a necessary condition for information processing, the bull's-eye pattern might well be the signature of the underlying molecular interactions. A new category of experimentation is currently developing, where the spatial positions of cell surface molecules in living cells are directly manipulated and reproducibly controled through mechanical means [1-3]. These experiments allow to uncover the mechanisms behind the self-organization of the molecular clustering at the cell-cell interface.

We perform computer simulations of the immunological synapse formation using an agentbased model approach that monitors the motion and interaction of individual molecules and takes the binding kinetics of receptors and ligands explicitly into account [4,5]. The combination of *in vitro* experiments and computer simulations has the potential to pinpoint the kind of molecular interactions involved in the immunological synapse formation, which is achieved by the fact that *in silico* experiments allow with relative ease to manipulate individual mechanisms of the immunological synapse formation while monitoring their impact on the system as a whole. A comparison between the *in vitro* experiments [1] and the emerging molecular patterns in the simulations (see Figure 1B-D) as well as the formation dynamics (see Figure 1E-H) reveals that three interaction mechanisms are essential during the immunological



Figure 1: Simulation results of the molecular clustering at the immunological synapse in terms of TCR-pMHC complexes (light-gray) and LFA-1-ICAM-1 complexes (dark-gray). (A) Bull's-eye pattern in the absence of geometrical repatterning. (B-D) Repatterning of the immunological synapse by mechanical barriers (black) for the same geometries as in the experiments [1]. (E-H) TCR-pMHC microcluster dynamics during the formation of the immunological synapse after 30 seconds (E), after 2 minutes (F), after 5 minutes (G), and after 10 minutes (H).

synapse formation: (i) adhesion between neighboring TCR–pMHC complexes, (ii) repulsive short-range interactions between TCR–pMHC and LFA-1–ICAM-1 complexes, and (iii) either a centrally directed motion of TCR–pMHC complexes, or a long-range attractive interaction between them. In order to determine the relevant type of TCR–pMHC aggregation mechanism, novel experiments on geometrically repatterned immunological synapses are proposed.

Furthermore, our simulations predict that the observed diversity of molecular patterns, including dynamic and multifocal structures, is directly related to the receptor-ligand binding affinity [5]. In particular, we observe multifocal patterns of TCR–pMHC complexes for sufficiently low but still realistic binding affinities between TCRs and pMHCs. This result is a consequence of the interplay between the binding kinetics and the attractive long-range interaction between these complexes. The interaction attracts TCR-pMHC complexes to form local clusters, however, due to their low binding affinity, the complexes unbind and re-bind on a time scale that does not allow microclusters to coalesce and form a c-SMAC. We conclude that computer simulations represent a fruitful theoretical approach to study immunological synapse formation.

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IMPROVED MODELS FOR PATTERN FORMATION IN EARLY DEVELOPMENT OF DROSOPHILA

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We present a new model of pattern formation that correctly describes the spatiotemporal dynamics of gene expression domains in early Drosophila embryo. The simplest diffusion is caused by the Brownian motion of non-inertial particles, completely independent and free of interaction with others. Being based on the Fick law of diffusion, the RD equation has an unrealistic feature: motion has an infinite velocity. Indeed, the general solution to it has the form $u \sim (1/D)exp[-x^2/(4Dt)]$, where x is space, t is time and D is the diffusion coefficient, and describes an exponential growth/decay only. Almost all the RD models are based on competitive action of three biomolecular processes: diffusion, synthesis, and decay of products of biochemical reactions, say, proteins [1]. The complexity of a particular formal description varies and mostly depends upon how sophisticated is the model of synthesis, [2]. Despite of excellence in mathematical treatment and richness of ideas the models of highly nonlinear RD processes are not enough to describe many real problems arisen in systems biology. The most restrictive formal feature of models considered before is in the studies of just one, however complex, equation, and with nonlinearity traditionally containing a polynomial. We discuss a natural generalization of the problem statement and introduce a diffusive non-local term:

$$u_t = D \int_0^t f(t - t') \Delta u(x, t') dt' + g(u).$$
(1)

Some transformations yield the Hyperbolic Reaction-Diffusion (HRD) equation:

$$\tau u_{tt} + [1 - \tau g_u] u_t = D u_{xx} + g[u(x, t)], \tag{2}$$

which can be reduced to the standard RD equation model in the limit $\tau \to 0$. Physically it means that the *correlated motion* is now assumed in corresponding system of nuclei, that results in finite velocity of disturbances. The regulatory function is defined as in [1]:

$$g\left(\sum_{b=1}^{N} T^{ab}u_i^b + m^a u_i^{\text{Bcd}} + h^a\right) - \lambda^a u_i^a,\tag{3}$$

where a = 1, ..., N and N is a number of zigotic genes. Value and sign of the T^{ab} matrix elements show the regulatory action of gene b product on expression of gene a.

The generalizations lead to new results in modelling of patterns in early development of Drosophila embryo, that show unexpectedly good agreement with experimental data.

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MOLECULAR MECHANISMS OF LARGE SCALE CONFORMATIONAL FLEXIBILITY AND THERMOSTABILITY IN RECA PROTEIN FILAMENT

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RecA protein is central enzyme in homologous DNA recombination, repair and other forms of DNA metabolism in bacteria [1]. It functions as a flexible helix shaped filament bound on stretched single-stranded and double-stranded DNA. It was shown that the RecA filament can exist in several different conformations but it can catalyze DNA strand exchange reactions in its active form only having significantly different geometry characteristics such as helix pitch and gyration radius

In this work we present atomic level model for conformational transitions of the RecA filament. The model describes small movements of the RecA N-terminal domain due to coordinated rotation in two pairs of main chain dihedral angles (psi23/phi24) and (psi268/phi269) preserving unchanged inter-subunit interface. It is found that the model is capable to reproduce a wide range of observed changes of the helix pitch in transitions between compressed and stretched conformations of RecA filament and conformational flexibility of RecA C-terminal domain. Predictions of the model are in agreement with measurements of the filament helix pitch in RecA::ADP-AlF4 complex at various salt concentrations carried out by Small Angle Neutron Scatting (SANS) [2-4].

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APPLICATION OF COMPUTATIONAL SYSTEMS BIOLOGY FOR DISCOVERY OF NEW ANTI-INFLAMMATORY DRUGS

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Two approaches of computational systems biology are presented: pathway reconstruction and kinetic modeling. Pathway reconstruction collects all information about players of interest, processes interconnecting them and their stoichiometry and can be considered as a powerful tool to search for drug targets, discover possible biomarkers and attribute them to particular cell state or phenomenon. In framework of kinetic modeling approach we mine, collect and integrate quantitative *in vitro* and *in vivo* experimental data produced by classical biochemistry, genomics, proteomics and metabolomics and use them to build and verify kinetic models [1,2]. These kinetic models when considered as a repository of all information about the system of interest can be applied to different problems of drug discovery and production such as screening optimization [3], investigation/prediction of drug safety [4] and optimization/maximization of yield of drug precursors.

We have applied these approaches to develop workbench for discovery and safety assessment of anti-inflammatory drugs. All signaling pathways associated with inflammatory processes proceeding in platelets, endothelium cells, neutrophils and macrophages have been reconstructed and annotated. Kinetic models of metabolic pathways involved in synthesis and degradation of arachidonic acid and signaling networks initiated by prostaglandins in platelet and endothelium cells have been developed to understand/predict the mechanism of NSAID-stimulated adverse cardiovascular effects (clot formation). These models quantitatively describe the changes in dynamics and regulations of the pathways caused by the following NSAIDs: aspirin, celecoxib, diclofenac, naproxen, indomethacin, ibuprofen. Experiments assisting modeling efforts have been design to generate data for verification of the models and test model predictions. Software packages based on these kinetic and static models have been developed. This software allows to predict IC50 and clot formation risk for any anti-inflammatory drugs which are able to inhibit prostaglandin H synthetase.

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Posters

PS-01

Memory effects in the Bremsstrahlung emission from a fermion jet in a non equilibrated hot plasma.

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Radiative processes have been found to be one main reason for the energy loss of high p_T partons in a quark gluon plasma. Since the quark gluon plasma produced in heavy ion collisions expands and cools down before it hadronizes, the density of scattering centers is decreasing in time, which makes the radiative behavior of the jet time dependent. We use the Schwinger Keldysh formalism to describe such a non equilibrium process including the Laundau Pomeranschuk Migdal effect. As a first step, we restrict our calculations to QED-like interactions, i.e., to ordinary photon emission. A comparision of our results to a quasistatic calculation shows that the radiative behavior follows the changes in the medium almost instantaneously.

PS-02

ON THE INFLUENCE OF COLLISION MODELS ON THE RESULTS OF DIRECT SIMULATION MONTE CARLO OF FLOWS WITH CONDENSATION

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The direct simulation Monte Carlo (DSMC) method is the powerful technique for numerical investigation of near-continuum and rarefied gas flows [1]. The method may be employed for simulation of flows with complex physic-chemical processes in a volume including cluster formation phenomena. Recently DSMC technique was used for calculation of flow of laser ablated material by nanosecond scale laser pulse of moderate intensity with taking into account condensation process [2].

The kinetic approach suggested in [2] employs for description of collision processes socalled hard sphere model (HS model). The use of the model may be explained by the absence of reliable data for about cross-sections of monomer-cluster and cluster-cluster collisions.

In this work we developed our simulation technique toward use of more complex approach described in [3]. This approach allows to receive the dependence of the collision cross section from the collision energy on *ab initio* calculations. The influence of application of different approaches for cross-section description on simulation results is demonstrated for the flow of laser ablated in vacuum niobium particles. The important features of gasdynamics of such free non-stationary laser plumes are large gradients of parameters and wide range of parameters variation. Such behavior of flow gives us perfect opportunity to test different model of particle cross-section. The analysis of application of different collision models is presented.

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MODULATED POSITRON BEAM IN THE CRYSTALLINE UNDULATOR

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Developing radiation sources in the hard X ray and gamma ray range is an important goal of the modern physics. Such sources could have many applications in basic science, technology and medicine.

The present state-of-art lasers are capable for emitting electromagnetic radiation from the infrared to ultraviolet range of spectrum. X-ray free-electron lasers (xFEL) are currently being built. Moving further, i.e. into gamma-ray band, is not possible without new technologies.

One of the most promising prospective technologies is using the phenomenon of charged particle channeling in single crystals. The electrostatic fields inside a crystal are extremely strong. They are able to steer the particles much more effective than even the most advanced superconductive magnets. A single crystal with periodically bent crystallographic planes can be used as a compact undulator that forces particles to move along nearly sinusoidal trajectories and radiate in hard X ray and gamma ray frequency range. Such a device is known as crystalline undulator.



Figure 1: A schematic representation of the crystalline undulator.

The feasibility of gamma-ray generation by means of spontaneous emission from ultrarelativistic positrons due to their planar channeling through a periodically bent crystal was demonstrated a decade ago [1] (see also [2] and references therein). Recently, the feasibility of electron-based crystalline undulator was demonstrated [3].

PS-03

Even more powerful, monochromatic and coherent gamma-rays would be emitted if charged particles in a crystalline undulator are correlated in such a way that the distance between the particles along the beam direction is an integer multiple of the wavelength $\lambda_{\rm r}$ of the emitted radiation. Saying it another way, the beam density has to be *modulated* in the longitudinal direction with the period $\lambda_{\rm r}$. In this case, the electromagnetic waves emitted by different particles have approximately the same phase and the intensity of the radiation emitted in the forward direction becomes proportional to the beam density squared (in contrast to the linear proportionality for an uncorrelated beam). Because initial (seed) radiation is needed for the modulation (the process is termed as *bunching* or *microbunching*), this phenomenon is a classical counterpart of the stimulated emission in quantum physics. Therefore, it referred to as a lasing effect in crystalline undulator. The feasibility of crystalline undulator-based gammalaser was considered in [1, 2]. Recently, a two-crystal scheme - gamma klystron - has been proposed [4]. In the both mentioned papers a simplified model was used which does not take into



Figure 2: The longitudinal distribution of the particles that leads to the lasing effect: the distance between the particles along the beam direction is an integer multiple of the wavelength $\lambda_{\rm r}$ of the emitted radiation.

account the particle oscillations within the channel (i.e. between the crystallographic planes or axes). Because different particles have different amplitude of the channeling oscillations, this leads to demodulation (debunching) of the beam. Additional contribution to the beam demodulation comes from incoherent collisions of the channeling particles with the crystal constituents. After the demodulation, the laser effect disappears and the beam radiates as in usual crystalline undulator. Therefore, beam demodulation is the major limiting factor of the crystalline undulator based gamma laser.

In the proposed presentation, the radiation of the modulated beam in the crystalline undulator will be considered. The demodulation process and its influence on the parameters of the produced radiation will be studied. The physical limits of the crystalline undulator based hard X ray and gamma ray lasers will be investigated.

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Ultrafast demagnetization induced by femtosecond laser pulses

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In 1996, the team of Jean-Yves Bigot [1] has highlighted the existence of ultrafast demagnetization (within few tens of femtosecond) processes induced by femtosecond laser pulses in ferromagnetic thin films. These demagnetization processes are not yet fully understood. They involve microscopic interactions such as spin-orbit coupling (SO), the excitation of Stoner pairs, the scattering of d electrons by conduction electrons,

From a theoretical point of view, the main difficulty is to provide an adequate description of the interplay between electronic and spin degrees of freedom in the metal. So far, only two theoretical models have been proposed to explain this effect [2, 3]. These works are based on two different mechanisms. In [2], the spin-orbit coupling implying only the electronic degrees of freedom is invoked while in [3], phonon or impurity mediated spinflip scattering is privileged. Unfortunately, the parameters employed in [2] are not realistic and the model developed in [3] is a phenomenological approach which does not allow quantitative predictions.

The question about the good mechanism has been debated intensively until the publication of a recent experimental work employing time resolved X-rays Magnetic Circular Dichroism (XMCD) techniques [4]. According to the authors, their measurements unambiguously excludes that the original spin momentum is transferred to electronic orbital momentum via spin-orbit coupling. They claim that their data are only compatible with a substantial femtosecond angular momentum transfer from the spins to the lattice within few tens of femtosecond.

Within the framework of the Time Dependent Density Functional Theory (TDDFT) which has been extended to include the SO [5], we confirm that the SO alone is not sufficient to lead to a clear demagnetization of the system. However since we strongly believe that the ultrafast demagnetization process implies only the electronic degrees of freedom (and not the ones of the ions which are frozen within this ultra-short time scale), we propose a new scenario which is based on two ingredients: (i) spin-orbit coupling and (ii) electron-electron collisions between quasi-particles (going beyond the mean-field approximation used traditionally in TDDFT). We will present all the theoretical ingredients of our model at the conference.

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Finite Temperature Magnetism of Metallic Nanoparticules

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Enhancement of magnetism in clusters of elements that are ferromagnetic as bulk solids such as cobalt or nickel has been lengthy discussed in many theoretical and experimental works and demonstrated through Stern-Gerlach experiments [1]. However, magnetism in clusters of nonmagnetic elements such as simple or noble metals is still not well understood [2]. The magnetism of these clusters is caused by finite size effects and by the exchange-correlation interaction between valence electrons. This interaction originates from the Pauli exclusion principle and favors spin polarization. Recently, magnetization measurements of small, mass-selected Platinum clusters embedded in zeolite matrix have been reported and confirmed the high spin polarization of these species [3]. A fundamental issue concerns the evolution of magnetic properties of such systems as a function of temperature. Do they undergo a ferromagnetic-paramagnetic phase transition ? At which temperature ?

On the theoretical side, spin density functional theory, and in particular the local spin density approximation (LSDA) is a well suitable model for studying itinerant magnetism in metals. Finite-size and thermal effects have been incorporated within the framework of the spherical jellium model [4] allowing us to study finite temperature magnetic properties of open-shell simple metal clusters. We have been able to identify a magnetic phase transition which has the characteristics of a second-order phase transition. The critical temperature vanishes in the bulk limit as expected and strongly depends on electron correlations and cluster size. The magnetic susceptibility is found to obey the Curie-Weiss law which is in agreement with recent experimental measurements reported in [3]. Many results will be presented at the conference.

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PINNING OF SIZE-SELECTED COBALT CLUSTERS ON HOPG

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The possibility of designing and mastering the physical and chemical properties of nano-structured materials has led to considerable interest and activity in the academic and industrial domains. Size reduction effects on the electronic, optical and magnetic properties of nanometric systems are key parameters to develop novel advanced devices. Cluster beam technique opens a way to manipulate agglomerates of atoms, control cluster (nanoparticle, NP) size and impact energy. Control of cluster deposition energy is one of the advantages of cluster beams because the soft landing of NPs often leads to their surface diffusion followed by the agglomeration or coagulation that ruins the advantage of size selection. This problem can be solved utilising energetic cluster deposition when the cluster deposition energy is increased facilitating its slight embedding into the substrate (so-called pinning) thus immobilising the deposited cluster [1].

Clusters of cobalt were produced using Laser Ablation Cluster Source [2]. The Cluster Implantation and Deposition Apparatus [3] gives the possibility to manipulate the positively charged clusters, in particular, to size select them with precision up to $n/\Delta n=40$ (*n* is the number of atoms in the cluster) for the sizes used in the experiments and to control their energy from meV level (correspond to supersonic velocity) up to 20 keV per cluster. The mass-selected clusters from the size interval n = 20-80 were used for the energetic deposition. The deposition energy for every selected size varied between 4 and 100 eV per atom in the cluster. The deposition was done on a freshly cleaved surface of highly-ordered pyrolytic graphite (HOPG) in ultra-high vacuum of $(1-5)\times10^{-9}$ Torr. The samples were studied using atomic force microscopy (in tapping mode) and scanning tunnelling microscopy. The obtained results show how the cluster-surface interaction mechanism changes from soft landing to pinning and further to implantation with increase of the deposition energy.

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PS-07

DIPOLE MOMENT EFFECT ON WATER CLUSTER PROPERTIES

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Large electric dipole moment is one of the most important features of water molecule determining its physico-chemical activity in both gaseous and bulk state. In a similar manner, the issue of the dipole moment of water clusters, μ_c , directly affects their properties. Moreover, it is of apparent importance for understanding the mechanisms that form the structure of the condensed state of water.

The value of μ_c is governed by two factors. The first one is the average value of the dipole moments of clustered molecules, $\mu_{1,c}$ which significantly exceeds that of a free molecule [1]. The second factor, i.e., the relative orientation of molecular dipoles in the cluster, is quite clear only for clusters consisting of a few water molecules, whose structure is unambiguously known from both the experiments and the quantum chemistry calculations. With the increase of cluster size, the molecular dynamics (MD) simulation becomes the only suitable technique. It results in large number of almost isoenergetic configurational isomers (conformers) with the dipole moments corresponding mostly to a random orientation of molecular dipoles and proton-disordered cluster structure, although some locally stable structures with the larger values of μ_c were also obtained for clusters of a hundred molecules [2, 3].

The recent molecular-beam studies for attachment of a slow electron to a water cluster $(H_2O)_{n \approx 1000}$ have shown that the capture of the electron by a long-range field of the permanent dipole moment of the cluster is responsible for the anomalously large attachment cross section [4]. The dipole moment of the cluster was estimated as a function of its size *n*. The obtained values of noticeably exceed the "random-orientation" dipole moments and provided the evidence of molecular dipole ordering and ferroelectricity of some cluster conformers [5].

This report discusses the possible values of $\mu_{1,c}$ and their impact on the optical activity of cluster in infrared spectral region. For this purpose, the MD simulation of large water clusters was performed, the special attention focussing on the conformers with higher dipole moments. The sizeand temperature-dependent spectral densities of energy radiated by water cluster and its spectra of IR absorption have been obtained as Fourier transform of the dipole autocorrelation function. These values are compared with the molecular ones.

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ENERGY DISSIPATION UNDER ELECTRON-IMPACT EXCITATION OF MOLECULAR CLUSTERS

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The appearance of molecular clusters in weakly ionized media affects strongly on the media properties. This report presents the results of crossed-beams investigation into the inelastic interaction of pure and mixed clusters of N₂, H₂O, CO₂, N₂O molecules with low-energy (0 < E < 100 eV) electrons. Clusters were formed under homogeneous condensation of gas in supersonic free jet [1]. The variation of expansion condition allowed the generation of clusters with the average size ranging from 2 to several thousands molecules per cluster [2–4]. In this manner the size effects of studied processes were manifested. An electron beam was generated by a Pierce gun with an indirectly heated oxide-coated cathode [5]. The total ion currents of formed positive and negative ions, as well as visible and UV radiation were measured. The composition of small clusters was determined by quadrupole mass spectrometer.

It is well known that under electron-cluster collision considerable portion of electron energy can be absorbed within cluster

 $(AB)_N + e^- \rightarrow (AB)_N^{l^*} + (l+1)e^-,$

here l = 0, -1, + n is possible charge state of cluster. Dissipation of excitation energy occurs through a variety of secondary processes:

$(AB)_N^{l^*}$	\rightarrow	$(AB)_{N-j}^{l}$ + $j AB$	(fragmentation/evaporation)	(1)
	\rightarrow	$(AB)_{N-1}^{l} + AB^{*}$	(nonequilibrium fragment ejection)	(2)
	\rightarrow	$(AB)_{N}^{l} + hv$	(radiative deexcitation)	(3)
	\rightarrow	$A^{l}(AB)_{N-1} + B$	(dissociation and ion-molecular reactions)	(4)

The following processes received our main attention:

- the equilibrium and nonequilibrium cluster fragmentation at electron impact ionization and cation formation was studied;

- the energy loss of primary and secondary electrons within cluster resulting in dissociative or direct capture of electron and stable anion formation was analyzed;

- the channels of radiative deexcitation and radiationless quenching of excitation of clustered molecules were revealed;

- the dissociative ionization of clustered molecules and a number of ion-molecular intracluster reactions were studied.

An example of the last processes is the suppression of intracluster dissociation for mixed H_2O/CO_2 cluster ions. The primary ionization of pure water clusters is known to be accompanied with $(H_2O)_j^+$ ion dissociation to $H^+(H_2O)_{j-1} + OH$ [6]. Due to large proton affinity of water molecule the energy effect of this process is small, and even negative for larger *j*. For this reason, under the electron impact ionization of pure water cluster even the $(H_2O)_2^+/H_3O^+$ current ration was as low as 0.03. By contrast, in case of H_2O/CO_2 binary condensation the fraction of unprotonated water

cluster ions increases greatly, so that $(H_2O)_j^+$ and $(H_2O)_jCO_2^+$ ions are detected to j = 6 and 8, correspondingly (see four families of clustered ions in Figure).



In this case an alternative channel of energy dissipation may be Penning ionization of H_2O molecule with highly excited CO_2^* molecule followed by CO_2 evaporation:

 $(\mathrm{H}_2\mathrm{O})_j\mathrm{CO}_2 + e^- \rightarrow (\mathrm{H}_2\mathrm{O})_j\mathrm{CO}_2^* + e^- \rightarrow (\mathrm{H}_2\mathrm{O})_j^+ + \mathrm{CO}_2 + 2e^-.$

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SHELL EFFECTS ON FRAGMENTATION OF MULTIPLY CHARGED VAN DER WAALS CLUSTERS

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In this report, we discuss on the stability and fragmentation of multiply charged van der Waals clusters. In particular, we focus on the role of geometrical shell effects.

A multiply charged cluster is stable if its size is larger than the *appearance size*, which is obtained from the condition that the energy barrier exists for every fragmentation channels. About 20 years ago, Echt et al. [1] estimated the appearance sizes for many kinds of multiply charged van der Waals clusters. Their calculation has been in good agreement with the most of experimental measurements. In their calculation, the parameters of the LDM were those given by Brian and Burton [2] through a molecular dynamics simulation carried out at the temperature T = 40 K.

Recently, two groups [3] have calculated the energy of the global minimum of Lennard-Jones clusters up to size n = 1000. This situation corresponds to T = 0 K. Using their calculations, we propose a new set of parameters for the LDM at T = 0 K.

We calculate the appearance sizes from these global minimum energies and with using the liquid drop energy at T = 0 K. Through a comparison of these two types of calculations, we can study the role of *geometrical shell effects*. Calculated results are listed in Table I and are compared with experimental data as well as with previous LDM calculation at T = 40 K. [1]. In general, the appearance sizes at T = 0 K are than those at T = 40 K since the surface energy at T = 0 K is 3/2 times larger than that at T = 40 K. As for Ar clusters, the present calculation gives in good agreement with the experimental measurements. In most cases, the LDM at T = 0 K gives nearly the same appearance sizes as those obtained using the shell corrected energies. In the case of Xe_n^{4+} , shell effects considerably change the appearance sizes. Furthermore, due to shell effects, multiply charged clusters may be unstable even though their sizes are larger than the appearance size.

It should also be pointed out that shell effects play a significant role in the decay process of multiply charged clusters. Figure 1 shows the energy barriers for fragmentation of Kr_{53}^{2+} as a function of a fragment size. Calculations are performed using the two methods mentioned above. Predicted decay pattern will be completely different with the two models. Although LDM predicts that fragmentation is possible for a wide range of fragment size. If we take into account shell effects, however, emission of a cluster with the size of magic number (13) becomes the only energetically accessible channel.

Detailed report is presented in [4] as for rare gas clusters and [5] for those of fullerenes.

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STRUCTURAL AND ENERGETIC ANALYSIS OF ALUMINUM MICROCLUSTERS: DENSITY FUNCTIONAL STUDY

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In this study, Density Functional Theory (DFT) B3LYP at 6-311++G(d,p) [1] level is employed to optimize the structures of the aluminum microclusters. Detailed analysis of the energetic and structural stability of Al_2 - Al_{13} clusters and their isomers are presented. Attention is also paid to the determination of their lower-lying electronic states. The total and the binding energies of the clusters with their isomers have been investigated. The first and the second energy differences, harmonic frequencies, point symmetries, and HOMO-LUMO (highest occupied molecular orbital-lowest unoccupied molecular orbital) energy gaps in their neutral, anionic and cationic complexes have been determined. Moreover, a simple growth path is discussed for the studied sizes and isomers. Results are compared with previous works [2,3].

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GROUND STATE AND SHAPE ISOMER DEFORMATIONS OF ALKALI METAL ATOMIC CLUSTERS

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The spheroidal shell model is used to describe the deformed states of atomic clusters. The Hamiltonian is analytically solved in cylindrical coordinates. The angular momentum term is treated as deformation dependent. The asymptotic eigenfunctions are obtained for axially symmetric potentials without approximation. The energy levels are used as input data for shell corrections. Minima due to shell effects are obtained as a function of the number of atoms in the atomic cluster as well as of the deformation. Calculations are performed for atom number up to 200, and spheroidally deformed (oblate and prolate) shell closures are predicted.

SPHERICAL HOLLOW CLUSTER SYSTEM: PHOTOABSORPTION SPECTRUM

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The results of photoabsorption cross section calculations for cluster systems with a spherical hole in the center are presented. We consider metal clusters within the jellium model, which treats the cluster as a two component system: homogeneous positively charged ionic core and quantized valence electrons. The purpose of these model calculations is to investigate changes in the photoabsorption spectra of the clusters caused by the variation of the positive charge distribution of the ionic core ranging from a homogeneously charged sphere to a spherical layer with the hole radius R_{min} . With the chosen Wigner-Seitz parameter r_s , we keep permanent the cluster volume and vary the radius of the hole.

The ground state electronic wave functions and the single-electron energy levels of the clusters have been obtained within both the Hartree-Fock (HF) and the local density approximations (LDA). The single-electron wave functions of discrete and continuum excited states have been calculated in the frozen-core field. The HF electron wave functions have been used for the calculation of the dipole amplitudes and cross sections within the random phase approximation with exchange (RPAE) accounting for the many-electron correlations. Within the LDA formalism the amplitudes and cross sections have been calculated using the random phase approximation (RPA). These calculations allowed us to perform a detail comparison of the photoabsorption cross sections of the ordinary and the hollow metal clusters.

The main attention is paid to the well-known plasmon resonances in photoabsorption spectra of metal clusters [1]. It is well known that both HF and LDA theories fail to describe plasmon resonance excitations and one needs to use the RPAE or RPA respectively in order to account for the collective response of the electronic subsystem to an external electromagnetic field.

For the homogeneous distribution of the ionic charge within a sphere, it turns out that surface plasmon excitations belong to the discrete spectrum. But for the hollow cluster system the plasmon excitations get shifted to the continuous spectrum. The presence of the outer and inner surfaces in the hollow system results in two surface plasmon excitation modes, symmetric and antisymmetric, in accordance with recent calculations and measurements of photoionization of fullerenes [2–4]. Preliminary calculations show that the lower energy surface plasmon resonance is much stronger than the higher energy one. The results for the hollow clusters with N = 40 and N = 80 valence electrons will be reported at the conference.

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ELECTRON-POSITRON CLUSTER PROPERTIES: SIZE DEPENDANCE

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In this contribution we present recent advances in studies of electron-positron clusters (EPCs) started in [1]. Here we focus on the investigation of evolution of the cluster properties with the growth of the cluster size. The metallic phase of EPCs consists of a number of delocalized electrons and positrons bound together by the attractive Coulomb potential and the potential of the particles mutual polarization. The EPCs possess the shell structure similar to that of metal clusters [2]. Unlike metal clusters the motion of negatively and positively charged subsystems in EPCs is identical and quantized.



Figure 1: Density distributions for electron-positron clusters with different numbers of electronpositron pairs N = 2, 8, 18, 20, 34, 40.

Our calculations have been performed within the Hartree-Fock (HF) approximation. Due to the local Electro-neutrality of the system the Hartree term for electrons compensates that for positrons. Hence the wave functions for both the electron and the positron subsystems can be obtained from the following equation:

$$-\frac{\Delta}{2}\varphi_i(\mathbf{r}) - \sum_j \varphi_j(\mathbf{r}) \int \varphi_j(\mathbf{r}')\varphi_i(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' = \varepsilon_i \varphi_i(\mathbf{r})$$
(1)

Similar calculations but with the static, ionic core charge distribution of the variable shape, called the optimized jellium model, have been performed in [3]. As follows from equation (1), EPCs are bound in the HF approximation by the nonlocal exchange interactions (including self-interaction). The energy level structure of the system is obtained self-consistently. Due to the charge symmetry it is identical for the electron and the positron subsystems. Numerically this condition has been met by solving the HF equations iteratively. Such procedure allowed us to obtain the single particle energies ε_i and wave functions φ_i . Figure 1 shows the electronpositron densities calculated within the HF approximation for EPCs of different sizes.



Figure 2: Average radius of EPCs as a function of number of electron-positron pairs N.

The energy level structure has been calculated for EPCs with different numbers of electronpositron pairs N = 2, 8, 18, 20, 40, 58, 68, 70 filling the closed shells $1s^2, 1p^6, 1d^{10}, 2s^2, 1f^{14}, 2p^6, 1g^{18}, 2d^{10}, 3s^2$ correspondingly, and thus, forming the spherically symmetric charge density distributions. The calculated EPC average radii as a function of N are plotted in Figure 2. Nonmonotonous behavior of the radius with N is a consequence of the EPCs shell structure.

A next possible interesting step in this research could be an application of the Dyson equation method [4] accounting for many-electron (positron) correlations to the problem considered, and the comparison of the results obtained with those following from the local density approximation theory [1].

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FORMULATION AND PROPERTIES OF CLUSTERS IN FULLERENE COATINGS OF FIELD EMITTERS

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Electric fields exceeded 10⁷ V/cm ought to be realized near the cathode surface in order to obtain field emission currents that are necessary in practice. Such electric fields are reached at moderate value of operating voltage, if some kind of clusters (nano- or microprotrusions) are formed at the emitter surface and enhance the electric field. Small clusters on the cathode surface often demonstrate properties that differ from ones of bulk material. Besides, the clusters exist at extreme conditions. They are exposed to the action of strong ponderomotive electric field forces and suffer bombardment of the residual gas ions that is intensive in technical vacuum conditions. Understanding of the cluster formation and destruction regularities on the field emission cathodes, their physical nature and properties presents great interest not only for emission electronics but also for other branches of science and technique.

At present time, the possibilities of carbon or containing carbon protective coatings creation for field emitters are intensively investigated. It is possible to hope that such coatings ought to be stable upon gas medium action and ion bombardment. The authors developed methods of fullerene protective coatings creation and investigated the tip field emitters having such coatings. The regularities of C_{60} cluster formation on the fullerene coating surface and their properties were studied. There was investigated influence of nonuniform electric fields and ion bombardment on structure and emission characteristics of clusters.

Main experiments were performed in the universal high vacuum chamber that included systems for coating deposition and treatment. The structure of the surface of created emitters was investigated by means of field emission microscope that had magnification factor $\sim 10^6$. During the main experiments, the residual gas pressure in chamber was about 10^{-9} Torr. A potassium ion source was used for modeling of processes under the action of ion bombardment and for treatment of the field emitter and fullerene coating by the ion flow. The ion flow density on the tip emitter surface was changed during the experiments approximately from 10^{-8} up to 10^{-6} A/cm².

Having investigated fullerene coatings 0.1- 5 of monolayer thick the spontaneous generation of nano-formations was noticed on the coating surface. These nano-formations had emission images in the form of a spot with ordered structure, namely, in the form of doublet, quadruplet, semicircles, hollow rings and others. When the current from the emitter was collected the cross-sectional dimensions of the spots with ordered structure were varied during observation. Sometimes the changes of emission image structure (for instance, the transition from doublet to quadruplet and back) were observed. The cross-section and height of these formations were estimated. These estimations showed that nano-formations are 3D nano-clusters consisting of no more than a few tens of C_{60} molecules. For instance, the formations having image in the form of doublet were found to have cross-sectional dimension of 3.0 and a height of 1.5 nm approximately. Transformation of doublet into quadruplet practically did not change height of cluster but reduced its cross-sectional dimension approximately down to 1.5 nm. Received data showed that cluster dimension reduction may be caused by decrease of the number of fullerene molecules in nano-formation as a result of ion bombardment. The reverse process of increasing dimensions is probably the result of additional C_{60} molecules joining the structure. The mechanism of this process is supposedly as follows. Nonuniform electric fields, existing near the emitter surface, polarize the C_{60} molecules and displace them along the field gradient to the cluster.

The structure of the ordered images can be explained taking into account the wave nature of the electrons and the regularities of de Broglie electron wave propagation in the cluster. The cluster represents itself original resonator (three dimensional potential well) for de Broglie electron waves. According to the estimations, the well linear dimensions (a height and base value) are approximately equal to one quarter of de Broglie wave length λ_{DB} or a multiple of $\lambda_{DB}/4$. Spatial distribution of electron flow exiting from the external boundary of resonator into a vacuum is evidently defined by the distribution of standing electron wave amplitude in the resonator. The view of distribution shall change itself with variation of resonator geometric dimensions because of the change of oscillation mode in it.

Besides described small clusters, it was possible to form enhancing electric field protrusions on the coating surface that have essentially more dimensions. Usually, protrusions of this type had almost equal a transverse dimension and a height $\geq 10-15$ nm and were formed by essentially more $(10^2 - 10^4$ times as large) quantities of C₆₀ molecules. Method of creation of such type clusters contained complex procedure of thermal and field treatment of fullerene coating. The possibility was demonstrated to create emitter with single protrusion at the surface as well as distributed cluster structure with a few tens almost equal formations at submicron tip top. The clusters with typical dimensions $L_c \gg \lambda_{DB}$ were seen at the screen as bright spots of different dimension, but their image did not contain any distinctive ordered structure. Our measurements showed that clusters in distributed structure are steady to high electric field action. Distributed multi-cluster system yields currents up to 100-150 µA in the continuous regime.

The effect of the bombardment by ion flow of different nature on the characteristics of fullerene coatings was investigated. The bombardment of the coating by the flow of potassium ions with the energy of <200-300 eV provided the stable decrease of the fullerene coating work function. In result, the voltage corresponding to some fixed emission current was decreased more than twice. The noticeable change of surface structure was not observed. The structure of activated fullerene coating was possible to change in the result of treatment by the flow of ions with the energy of \geq 1500 eV. Preliminary treatment of the substrate surface by so fast potassium ions flow influenced on the coating formation, increasing the adhesion between the coating and substrate. It increased the hardiness of fullerene coating to the high field action and provided great emission current extraction. The bombardment of formed coating by fast potassium ions flow made it possible to increase the uniformity of created distributed cluster structures that also rised their hardiness to the extraction of high currents.

To obtain the information about the influence of residual gas on the operation of cathodes with activated by the potassium ion flow fullerene coating, the measurements were performed in the wide range of residual gas pressures approximately from 10^{-9} up to 10^{-6} Torr. Besides, the effect of prolonged exposition of cathodes with activated fullerene coating at residual gas pressure about 10^{-4} Torr was studied. It was demonstrated the high hardiness of cathodes to the action of gas medium and ion bombardment. The steadiness to the ion bombardment was explained taking into account the existence of self-organization processes in distributed cluster structures on the surface of coatings in the strongly nonuniform electric fields.

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FABRICATION AND IN SITU XPS-DIAGNOSTICS OF A SYSTEM OF ISOLATED SILVER NANOCLUSTERS ON SILICON SURFACE

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Designing new technological approaches to fabrication of systems of metallic nanoclusters and development of new ways of cluster size diagnostics are the actual tasks of nanotechnology. We give in this report an example of possible solution of these tasks by fabrication of silver clusters on silicon. Fig.1 illustrates the idea of the technique. It includes deposition of a metallic film with hilly relief and the uniform etching the film by ions. This etching makes the film thinner and, at some stage, develops Ag-clusters. Further etching diminishes clusters. It enables fabrication of electrically isolated supported nanoclusters of comparable sizes and variation of their average size. Diagnostics of the average cluster size was performed by X-ray photoelectron spectroscopy with using synchrotron radiation (SR). Information about sizes of nanoclusters was obtained despite the

fact that photoelectron spectroscopy has no lateral resolution.

Fig. 2 shows the dependence of the Ag3d_{5/2} binding energy on the effective thickness of the silver layer $E_B(d)$. It is a monotonously decreasing dependence with some peculiarities probably connected with errors of the measurements. The binding energy of the initial film just after the metal deposition is close to the value $E_{Ag} = 368.3$ eV of the bulk metallic silver. The binding energy increases of about 1 eV when the effective thickness. According to the assumed model of the cluster system fabrication, the effective thickness of the layer is connected with the average size of clusters created at some stage of the ion etching the deposited silver.





b). System of Ag-clusters on Si surface. Clusters are isolated from the conductive Si- surface by individual dielectric SiO_2 - layers.

We studied transformation of electronic structure of silver clusters supported by conductive surfaces due to size confinement effects earlier and revealed that the corresponding $Ag3d_{5/2}$ binding energy shift does not exceed 0.2 eV in going from the bulk metal to the extremely small clusters consisting of only two atoms [1, 2]. Therefore, another hypothesis of the line shift was chosen taking into account that the clusters under consideration are particles electrically isolated by rather thick dielectric layer which radically diminishes interaction of clusters with the conductive silicon bulk. Isolated clusters of nanometer sizes are characterized



Fig.2. Dependence of the Ag3d core level binding energy on the silver amount or the average number of atoms in the system of silver clusters on the Si/SiO₂ surface.

by low capacity providing significant positive potential due to charging by one phoelectron. This potential retards photoelectron and results in "red" line shift: the smaller cluster, the larger shift. The model of free (the permittivity $\varepsilon = 1$) spheroidal clusters with effective radius R and capacity $C = \varepsilon R$ was considered. Fig. 2 shows the dependence of the binding energy on the effective thickness calculated in the frame of the model: $E_B(d) = E_{Ag} +$ $e^{2}/R(d)$. The arrows point at the values of the effective thickness of the silver layer corresponding to the average radii of clusters R = 5, 4, 2nm. One can see a reasonable

agreement between the model and the experimental dependencies both in the shape and values. The observed agreement confirms the assumed model. The suprizing fact is that the capacity of the fabricated clusters can be approximated by the capacity of a conductive sphere in vacuum. This fact evidences formation of spheroidal silver nanoclusters on the inert silicon oxide surface due to restructuring the dome-type clusters initially created under ion bombardment. In the case of the flat basis of clusters the effective permittivity should be larger at list two times as well as the capasity, and the agreement of the model and experimental energy dependencies would be hardly possible.

Thus, silver nanoclusters in the size range $R = 6 \div 1$ nm were fabricated on silicon surface at high vacuum conditions by ion etching a thin silver film deposited on the oxidized silicon surface. A unique feature of the system is that the metallic clusters are electrically isolated from the surface by individual SiO₂-layers. It was shown that ion etching resulted in reduction of the average cluster size of the system. Transformations of some properties of clusters were studied *in situ* in variation of the cluster size. The 1 eV size related "red" shift of the Ag3d_{5/2} photoelectron line was observed and dependence of Ag3d_{5/2} core level binding energy on the average cluster size was obtained. The model of charging the clusters by one electron in photoemission was suggested. It was shown that the observed "red" shift and the experimental binding energy dependence can be quantitatively described in the frame of this model. The suggested model enabled estimation of the average cluster sizes.

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SHELL ELECTRONIC STRUCTURE OF UNOCCUPIED STATES OF FULLERENES AND FLUOROFULLERENES $C_{60}F_x$ (x = 0, 18, 36)

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Fluorination of fullerenes seems to be interesting at the point of view of fundamental properties of carbon molecules and nanoclusters, as this process makes possible to clarify the role of different electron subsystems, π and σ , in forming the electronic structure of the cluster. During the last decade, electronic structure of different fluorinated fullerenes $C_{60}F_x$ have been extensively studied by different methods. Of particular interest is the comprehensive research of the dependence of electronic structure of fluorinated fullerenes $C_{60}F_x$ and $C_{70}F_x$ on the number of fluorine atoms in molecule (x = 11 ÷ 48) which is inversely proportional to the number of the valence π - electrons in molecule [1]. Synchronous reduction of the density of all of the unoccupied π^* - states and enhancement of the density of σ^* conjugated states were reported. This behavior evidences for the local type of the electronic structure of fullerenes typical for



molecules and excludes the shell type structure typical for metallic clusters. The aim of this work was searching the signs of the shell structure of unoccupied states in and flluorofullerenes fullerenes using molecules $C_{60}F_x$ with well defined number of fluorine atoms (x = 0, 18, 36) and the method of high resolution near edge X-ray absorption fine structure (NEXAFS) spectroscopy. The experimental evidence was found that unoccupied π^* - states of fullerenes and fluorofullerenes are delocalized ones and form cluster shells.

Fig.1. NEXAFS spectra of ordinary fullerene C_{60} and of fluorinated fullerenes $C_{60}F_{18}$ and $C_{60}F_{36}$.

Fig. 1 shows the C 1s edge NEXAFS spectra of $C_{60}F_{18}$ and $C_{60}F_{36}$ measured at the photon incidence angle $\alpha \sim 45^{\circ}$ in comparison with C_{60} spectrum. The spectra correspond to the dependence of probability of photoabsorbtion due to excitation of C1s core-level electron into unoccupied π^*



(sharp peaks) or σ^* (broad peak) states on the photon energy. Intensities of broad σ^* peaks of the spectra proved to be close to each other after these normalizations. Positions of the lowest energy π^* - peak (state 1 or lower unoccupied molecular orbital (LUMO) state) of all of the spectra coincide just as in Ref. [1], though the energy of the LUMO (284.5 eV) proved to be 0.4 eV higher. Fig. 1 illustrates transformation of electronic structure of unoccupied states due to fluorination. Creation of C-F bond must modify the bonding states of carbons from sp^2 to sp^{3} hybridization type. As a result, the number of π -electrons and the density of π^* -states should diminish in molecule proportional to the fluorine content, and the density of σ^* -states should increase. Such a transformation was reported in Ref. [1] in which increase of σ^* peak and drastic (more than two times) reduction of all of the relative intensities of LUMO - peaks were observed.

Fig. 2. Scheme of the shell electronic structure of unoccupied states of fullerene C_{60} and fluorofullerenes $C_{60}F_{18}$ and $C_{60}F_{36}$.

However, Fig.1 shows a somewhat different behavior. Relative intensity of LUMO peak (1) diminished only by 20% in attachment of 18 fluorine atoms by C_{60} and remains the same after attachment of additional 18 fluorine atoms which results in 60% exhaustion of the π conjugated system. To explain the observed NEXAFS spectra transformation, the following assumption was made. The π^* - states of fluorofullerenes are delocalized at large extent and form cluster shells analogous to the shells of metallic clusters according to the scheme drown in Fig. 2. These shells are created in the course of enlargement of the π - electron system starting from low energy states and disappear in the course of the π -electron system exhaustion starting from the high energy states. Indeed, π^* - high energy states 2 and 3 rapidly disappear when π -electron system is reduced due to fluorination whereas the intensity of low energy state 1 (LUMO) remains practically constant even at high degree of fluorination. Fig. 1 also shows that states 1, 2 and 3 are pure π^* - states and the state 4 is the mixture of π^* and σ^* orbitals because this state weakly depends on the number of π -electrons. The property of fullerene and fluorofullerenes, which differs these clusters from the metallic ones, is that the adding or removal of π -electrons does not change the energy of the shells because the already existing cluster field is formed by the large number of σ -electrons. The surprising fact is that covering the fullerene surface by the rather dense layer of fluorine atoms does not destroy the shell structure of molecule.

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COHERENCE PHENOMENA IN THE PHOTOELECTRON EMISSION FROM SYMMETRIC MOLECULAR SYSTEMS

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Orbitals of symmetric molecules are eigenstates of the parity operator and hence either gerade or *ungerade* states regarding their behavior under reflection. This gives rise to equal probability density of the bound state electrons at each atomic site of the molecule. The electrons, even the strongly bound core-electrons, are non-localized. Photoelectron emission from such molecules gives rise to partial cross section oscillations with a phase shift of π between the gerade and ungerade final ionic states. The oscillation period is proportional to the bond lengths R in case of diatomic molecules or the diameter D in case of spherical systems such as clusters and fullerenes. It was regarded that the oscillation behavior is described for all systems by l-dependent Bessel functions. However, a close analysis of the oscillations revealed that the Bessel-type behavior is realized for the spherical systems only. For all diatomic molecules a pure sinusoidal function describes the oscillation well down to very low kinetic energies in the near-threshold region. In this regime with de Broglie wavelengths larger than the bond lengths or sphere diameter of the ionized system, shape resonances appear at $\lambda_{de Broglie} = \frac{1}{2}, \frac{1}{4}R$ (or D). In case of C_{60} with its large diameter this would be at very low kinetic energies. New measurements in this energy region have been undertaken in order to prove the validity of the Bessel-type behavior for the partial cross section oscillations and the existence of a shape resonance at the expected position. These results will be compared with the behavior of other systems and interpreted in the larger context of coherence phenomena in photoelectron emission from symmetric systems of different kind.

ELECTRONIC STRUCTURE AND PHOTOIONIZATION CROSS SECTION CALCULATIONS FOR THE FULLERENE C_{60} AND ITS POSITIVE IONS

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The electronic structures and the photoionization cross sections are calculated for the fullerene C_{60} and its positive ions C_{60}^{n+} n = 1, 2, 3. The theoretical framework used in the present work has been mainly developed earlier by us [1–3] and applied for the description of photoionzation of C_{60} , C_{60}^+ , and C_{60}^{2+} [1,3,4]. In the present work the theoretical approach is improved by means of using the Perdew-Wang parametrization [5] for the exchange-correllation energy functional.

At the first stage, the frozen core model and the local density approximation (LDA) are used assuming that there is a single electron transition during the process. Then, the correlations between the transitions from different states are taken into account within the random phase approximation. Single-electronic states of a fullerene ion are calculated within the spherical jellium model with the self-consistent potential [1–3] determined within LDA. The basic Kohn-Sham equations are used for determining of the single-electronic wave functions. The ionization amplitude of each orbital is calculated both within the single-electron approximation and also by taking into account many-electron correlations. Finally, the total photoionization cross section is calculated as a sum of partial cross sections for each orbital. In the present work the photoionization cross sections are calculated within the recent experimental data [6] and other calculations for C_{60}^+ , see, for example, [4,6].

In the present study 2 models for the fullerenes are treated: the spherical jellium model with the self-consistent potential and the spherical finite-layer jellium model with an extra term in the self-consistent potential. The width of the layer has been varying to get the best agreement with the most accurate electronic structure calculations. In both models the calculated photoionization C_{60} and C_{60}^{n+} (n = 1, 2, 3) cross sections indicate the giant plasmon resonances with positions of ≈ 20 eV for all fullerenes. The second giant resonances are also found in visinity of the photon energy ≈ 35 eV. The example of the total photoionization cross sections calculated in the present work within the jellium layer model is shown in Fig. 1 for the fullerene ions.





Figure 1: The energy dependence of the photoionization cross sections for the fullerene ions calculated in the present work within the jellium layer model.

The calculated cross sections are in a good agreement with the classical Mie theory and the recent experimental data [6]. The photoionization cross sections calculated in the present work fulfill the sum rule for all fullerenes, so, in contrast to the previous C_{60} [1,4] and C_{60}^+ [6] calculations, they are not scalled by any factor. The physical background of the giant resonances will be discussed at the conference.

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EXPERIMENTAL REVEALING OF ISOMERS FOR FULLERENE C₆₀

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In the present research we have studied carbon soot after Krechmer-like carbon arc discharge process for fullerene production. The soot was separated by use of chromatography column into several fractions with different processing times. All the fractions were tested with mass spectrometry and show the same atomic weight of fullerene C_{60} . But in solution the fractions show quite different colors, which were controlled by optic spectrometry. X-ray tests of the fractions show that one of them has exactly the same structure as fullerene C_{60} and the others give different x-ray pictures. Also the infra-red spectrometry gives different specters for the fractions. Because the carbon black was carefully filtered out from the solutions of the fractions, we can conclude that we have a deal with different isomers of fullerene C_{60} .

THE SUPERCONDUCTIVITY AND ELECTRICAL INSTABILITIES: STATISTICAL CORRELATION IN FULLERENE – COOPER CLUSTERS

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The complex of studies carried out on Cu_nC_{60} polycrystalline samples, including electrical and Meissner measurements, clearly support the existence of a superconducting phase with T_c near 78K [1]. In this paper we present a detailed study of the nanosecond voltage-current characterization including statistical resistance distribution on above mentioned samples. The results of structural studies of a bulk polycrystalline fullerene sample were caried out [1]. The samples that were investigated were in the form of cylinder 2 mm diameter and 0,5 mm thick [2]. Square pulses of 10 ns and 0,4 ns rise time were used for I-V and hystogram dependence. Typical I-V curves for the Cu_nC₆₀ samples are presented in Fig. 1.



Fig. 1.

The detailed shape of I-V curves near U ~ 0 in I section (Fig.1-insert) was typical for superconductive state. It can be concluded that the physics of the statistical processes change radically near U_N from gomogenious statistical spreading to normal (Fig. 2). A possible mechanism for this behavior is considered on the basis of the concepts of percolation network and pinchlike current distributions.

The detailed shape of I-V curves near U_{t1} in II section was typical for S-VACH in glasses. It was found (Fig. 3) that a junction from normal statistical spreading (U=U_{t1}) to gomogenious

 $(U=U_{t2})$ of the resistance in II section perhaps is the result of sufficient heating of current channel and channel rising with constant current density.



Fig. 2. Histograms G(R) in I section. T= 78 K.

a - U= $U_0 = 0.3$ V, b-0.5, v-0.7, g-1.2, d - U= $U_N = 1.7$.

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LIQUID SURFACE MODEL FOR CARBON NANOTUBE ENERGETICS

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We develop a model to describe the energetics of single walled carbon nanotubes. According to this model, the total energy of a nanotube can be expressed as a sum of three terms, namely, surface area, curvature of the surface and the edge as follows

$$E = E_s + E_c + E_e = \sigma_i S + \sigma_c \frac{L}{R} + 2\sigma_e S_e.$$

Here σ_{i} , σ_{c} and σ_{e} are the energy densities corresponding to surface area, curvature of the nanotube and the edge of the nanotube. *L* and *R* are the length and radius of the nanotube. *S* is the area of the inner region of the nanotube while S_{e} is the area of the edge. Due to the similarity of our model to the liquid drop model which is well known in the fields of nuclear physics and cluster physics [1-3], we call our model as liquid surface model. We demonstrate that the liquid surface model predicts the energy of arbitrary nanotube with an accuracy of 0.1%, provided the chirality and the total number of carbon atoms in the nanotube are known.

Using the liquid surface model, we could predict the energetically favorable chiralities that correspond to a given radius of the catalyst nanoparticle on top of which carbon nanotubes grow during chemical vapor deposition [4]. This study explains one of the possible reasons for the preference of some particular chirality during the growth of nanotubes.



Figure 1: Possible chiralities evaluated for various radii of the nanoparticles on which a carbon nanotube grows. Different lines represent different radii of the nanoparticles. Each grid point corresponds to an integer value of chiral indices and hence represents a real nanotube. Squares indicate the chiralities which represent nanotubes of radii closest to the given value R.

As an example, in Fig. 1 we have considered nanoparticles of four different radii and calculated the corresponding possible values of nanotube chiral indices n and m. Since chiral indices are integer

numbers each grid point in the graph represents a nanotube. The squares in the graph show the chiralities which represent nanotubes of radii closest to the given value R.

Figure 2(b) shows the cohesion energy (energy gained by a nanotube due to addition of an extra carbon atom) calculated using liquid surface model for nanotubes of different chiralities. Cohesion energy is a measure of the stability of the nanotube. The graphs are plotted for nanotubes of radii 3.8 Å and 10.17 Å. The number near each point corresponds to the value of the chiral index m of the nanotube.

Left plot shows that, of all nanotubes growing on top of a catalyst particle of radius 3.8 Å, the nanotube with n=8 and m=3 has the highest cohesion energy. Here the energy difference between the most stable nanotube and the least stable nanotube corresponds to a temperature of 150 K, which is comparable to the growth temperature of nanotubes in chemical vapor deposition. Plot (b) in Fig. 2 illustrates the fact that for nanotubes growing on top of bigger catalyst particles, the difference in cohesion energy is much less in comparison to those growing on smaller catalyst particles. For a catalyst particle of size 10.17 Å, the nanotube with n=19 and m=11 is the most stable one.



Figure 2: Cohesion energy for nanotubes of radii 3.8 Å (a) and cohesion energy for nanotubes of radii 10.17 Å (b). The numbers near each point corresponds to the value of the chiral index m. The graph is plotted in such a way that the energy of the less favorable nanotube is taken as zero.

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THE MECHANISM OF DNA MECHANICAL MELTING

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The process of DNA double helix unzipping is considered as mechanical melting assisted by external force. The probable pathway of the mechanical strands separation in the course of unzipping is determined. The pathway depends on the structure organization of the double helix, the manner in which external force is applied, and the kinetic parameters of the base pair opening in the double-stranded chain. It is assumed in our model that the base pair unzipping consists of the nucleic bases stretching of the DNA complementary pairs and the base pair rotation [1]. It was also shown that for the interpretation of the temperature dependence of unzipping force one needs accounting for the metastable states being formed in the course of the double strand DNA unzipping.

For the description of the DNA unzipping the two-stage mechanism of the external force action is proposed. It is assumed that during the first stage the force grows up to some critical value but without producing any significant DNA unzipping effect. This stage is relatively quick being characterized by the time intervals typical for the sound propagation in the DNA double helix. The DNA unzipping itself occurs at the second stage and is determined by the conformational transformations of the double helix. This process goes much slower than the first stage. The two-stage mechanism gives an explanation for the cooperative nature of the unzipping process under physiological conditions and the threshold character of external force action.

The nonlinear mechanics of DNA unzipping is described in the frame of the two-component model. It is demonstrated that the boundary between the open and the closed parts of the helix (so called "fork") moves along the chain as a step-like excitation (kink soliton). It is demonstrated that the external force in the course of the DNA unzipping plays the similar role as temperature in the process of DNA melting. It is shown that for the stable unzipping of the double helix it is necessary to allow the rotation of the DNA chain and to keep the velocity of unzipping fork propagation low in comparison with the sound velocity in DNA. It is demonstrated that the fluctuations of the fixed force have the same origin: the heterogeneity of the DNA base pairs and the heat fluctuations [2].

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MECHANISM OF ANOMALOUS DEFORMATION OF BISTABLE DNA SITES

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DNA structure is strongly conditioned by heterogeneity of base pairs (b.p.) sequence, the solution components, and interactions with proteins or ligands. Certain DNA fragments can have some energy-wise equivalent conformations. In many cases such sites undergo anomalous large scale deformations of the double helix. For example TATA-box 2 nm long can have bistable so called heteronomous conformation with coexisting of different sugar-ring forms (C2'-endo, C3endo) in the nucleotides pair of double helix monomer link. The fragment in the complex with proteins bends on roughly 80° and unwinds on 110° (see [1] and cited therein).

We suggest that bistability plays key role in anomalous deformability of small site length of DNA. We have developed nonlinear models [2-4] in the frame of phenomenological approach allowing studying the influence of the conformational transformations of DNA on the shape of the double helix chain (intrinsically induced mechanism of DNA deformation). In the term of two component nonlinear model of intrinsically induced DNA deformation, it is argued, that the significant bending of short fragments of confluent bistable strand may be realized with energy greatly smaller than energy analogous deformation estimated according Worm Like Chain (WLC) model, on the assumption of realizing of boundary conditions (on the ends of fragment present different conformational states) and decrease of the resistance of DNA to bending approx in 3 times in comparison with that predicted by the WLC.

The evolution of our approach of intrinsically induced deformation is presented in this work. Besides to internal conformational component and induced with it bending deformation, elastic twist and its correlation with bend have been taken into account. Twist-bending coupling itself leads to effective softening of double helix rigidity, but it is insufficient for explanation of anomalous deformation of short DNA site as TATA-box. From the other hand twist-bending coupling provide circumstance realization of intrinsically induced mechanism. Quantitative estimation in the frame of our theoretical model agrees with experimental ones obtained for the anomalous deformation of the TATA-box DNA fragment. That testifies about key role of conformational component in anomalous DNA bends. So mechanism of the intrinsically induced deformation may explain the observed anomalous deformations of bistable DNA fragments.

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HIERACHY OF CHROMATIN ORGANIZATION IN INTERPHASE CELL NUCLEI OF EUKARYOTES BY SANS

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Eukaryotic cells have solved packing problem by folding their DNA into a highly compacted chromatin structure. It is becoming increasingly clear that chromatin in cell nuclei is a labile dynamic structure playing a crucial role in many aspects of gene regulation [1]. Investigation of chromatin arrangement over a broad range of scales requires a method that would allow to gather information of the general principles of chromatin organization in cell nuclei under native or nearly native conditions. One of such methods is small angle neutron scattering (SANS), which yields not only information on structure of chromatin as a whole, but also allows to deduce organization of its protein and DNA components by using contrast variation technique. SANS/USANS measurement of chromatin arrangement were performed for the nuclei of chicken erythrocytes, bovine white blood cells and rat leukocytes. The results [2] show the higher-order structure of chromatin in cell nuclei can be described in terms of fractal geometry and exhibits different characteristics in cells with different functional state.

The relations between nucleosome structure dynamics and regulation of such cell function as DNA transcription, replication and repair, has become one of intensively studied problems in the field of molecular and cell biology. Nucleosome dynamics involves both modification of hystone core proteins by acylation, methylation and phosphorylation and nucleosome movement along DNA by remodeling proteins. The current models view this dynamics on the local level, describing the changes in the nucleosome structure up to core dissociation to tetramers H3 – H4 and dimers H2A – H2B tied to the activity of transcription and replication molecular machineries [3]. One could suppose that in anomalously proliferating cells the fraction of the nucleosomes whose structure has been modified in such a way might be fairly high.

We have compared the spectra of small angle neutron scattering (SANS) on nucleosomes in the native nuclei of chicken erythrocytes, lymphocytes from rat spleen, and the nuclei of HeLa human and A238 chinese hamster cell lines. SANS data were acquired on D11 spectrometer (ILL, Grenoble, France) with the preparation procedures described in [2]. As seen in Fig. 1, for HeLa and A238 cell nuclei the scattering intensity in the region that correspond to the nucleosome structure (Q ~ 0.06 Å⁻¹, [3]) was 3 to 5 times lower when compared to rat lymphocyte and chicken ervthrocvte



nuclei. The distance distribution function for the latter two cell types was bimodal, which is characteristic for nucleosome structure [4]. The data suggest wide-spread modification of the structure of the nucleosome core in the nuclei of anomalously proliferating cells.

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CANALIZATION OF GENE EXPRESSION IN THE DROSOPHILA BLASTODERM

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Developing embryos exhibit a robust capability to reduce phenotypic variations which occur naturally or as a result of experimental manipulation. This reduction in variation occurs by an epigenetic mechanism called canalization, a phenomenon which has resisted understanding because of a lack of necessary molecular data and of appropriate gene regulation models. In recent years, quantitative gene expression data have become available for the segment determination process in the *Drosophila* blastoderm. At the same time, predictive theoretical models for gene regulation have been developed. Together these advances make it possible to precisely characterize the epigenetic mechanism of canalization by means of dynamical systems theory supported by quantitative gene expression data.

Acquisition and processing of quantitative data was performed as previously described [1]. The numerical implementation of the gene circuit equations is as described [2] with the addition of time varying external inputs.

We have detected that extensive variation in early segmentation gene expression patterns is markedly reduced by the time gastrulation begins [1], and that in the gap gene system this reduction in variation is the result of cross regulation. We demonstrate the validity of this explanation by showing that variation is increased in embryos doubly mutant for *Kr* and *kni*, disproving competing proposals that canalization is due to an undiscovered morphogen, or that it does not take place at all. We further show that canalization can be understood in terms of dynamical systems theory. In the anterior half of the embryo, variation reduction occurs because the system's qualitative dynamics are controlled by point attractors, but in the posterior variation reduction is governed by an attracting manifold. These results demonstrate that a complex multigenic phenomenon can be understood at a quantitative and predictive level by the application of dynamical systems theory.

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MODELING THE ORGANIZATION OF THE *EVEN-SKIPPED* PROXIMAL 1.7 KB UPSTREAM REGULATOGY REGION IN TERMS OF BINDING SITES

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A central problem in modern molecular genetics is that of understanding how DNA regulatory sequences control gene expression. Metazoan regulatory regions are extremely complex and qualitatively different from those of prokaryotes. For example, the regulatory regions of genes controlling development in Drosophila are large and consist of groups of binding sites, called cis-regulatory modules (CRMs), each controlling some aspects of gene expression. The goal of our work is to understand the role of proximal 1.7 kb upstream regulatory sequence in the regulation of the Drosophila even-skipped (eve) gene in terms of binding sites.

To achieve this aim we have applied an approach which includes both mathematical modeling and experiment. We 1) quantitatively monitor gene expression at high resolution in space and time; 2) characterize transcription binding sites; 3) use new quantitative and predictive model of transcriptional readout of the proximal 1.7 kb of the Drosophila even-skipped gene to calculate the effect of a set of transcription factors bound to a large group of binding sites.

As a starting point we consider the 34-site model that includes binding sites for repressors: Kruppel (Kr), Giant (Gt), Knirps (Kni) and Tailless (Tll) and activators: Bicoid (Bcd), Hunchback (Hb) and Caudal (Cad). This model was published in [1]. We propose that Hb can act as activator only if it is bound to the site located close to the binding site of Bcd, otherwise Hb acts as a repressor. To check this hypothesis we modify the 34-site model by considering that Hb bound to hb1 site acts as a repressor. This modification improves the quality of fits. The rms of a new model was 8.66 and the features of experimental data were more accurately reproduced.

Next we consider the participation of Sloppy-paired 1 (Slp1) protein in the transcriptional regulation of *eve 2* stripe. Slp1 is expressed in a gap gene-like domain anterior to *eve* stripe 2. *In silico* addition of the Slp1 binding site (position from -1221 to -1205) to the 34-site model further decreases the rms value (rms=8.48) and improves the quality of patterns.

Our results clarify the organization and regulation of the *eve* upstream region. The *in silico* modeling of transcription provides new insights into the mechanisms of gene regulation and allows to thoroughly analyze gene regulatory regions.

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STABLE BIOLOGICAL PATTERN FORMATION IN VARIABLE ENVIRONMENT: A MODEL OF SEGMENTATION GENE EXPRESSION IN *DROSOPHILA*

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The development of multicellular organisms such as *Drosophila* is both precise and reproducible. We can distinguish two basic concepts of how this precise and reproducible behavior occurs in development and in other biological processes [1]. The first one can be called the 'noisy input, robust output' concept. It claims that each of the individual steps involved in the process is noisy and variable, and this biological variability is suppressed only through averaging over many elements or through some collective property of the whole network of elements. The second concept presents the 'precisionist' viewpoint, in which each step in the process has been tuned to enhance its reliability, so that the output noise range stays in the tolerance limits of the next input at each step where the information transmission occurs.

We consider the segment formation process in the early development of the Drosophila embryo and present some mathematical results in favor of the 'noisy input, robust output' concept. The segment formation in *Drosophila* is controlled by expression of maternal genes and zygotic segmentation genes. In the classical model, the borders of expression domains of some segmentation genes, including gap gene hb, get formed as a threshold dependent response to the maternal protein Bcd. A serious problem in this model arises from the fact that Bcd concentration exhibits high embryo to embryo variability, which essentially exceeds that of the hb domain border [2]. A candidate for mechanisms stabilizing the expression of gap genes under variable Bcd is the cross regulation between gap genes. We explore this hypothesis by studying a mathematical model of gap gene expression formulated in [3]. Under simplifying assumptions of stationarity and sharp sigmoid regulation function in model equations, the expression patterns in the model can be analytically derived as superpositions of local interfaces. We obtain analytical formulas for variations of these interfaces as functions of Bcd variation. One also links the pattern variation in the model to the variation of basins of attraction for different attractors in different cells. By using this approach, we demonstrate that the mechanism of mutual regulation in the segmentation gene network is able to provide the experimentally observed stability rate of segmentation gene expression. Therefore, the stability of pattern formation appears as an intrinsic property of the whole gene network.

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Author index

Aguado A	<i>Th-III-3</i>
Aguilar A	We-I-1
Alekhin O. S	PS-19
Becker U.	PS-17
Belyaev A. K.	PS-18, We-II-1
Benrezzak S	<i>Tu-III-1</i>
Berenyi Z	We-III-2
Bernigaud V.	<i>Th-IV-2</i>
Boltalina O. V.	PS-16
Bonačić-Koutecký V	<i>Th-IV-1</i>
Böyükata M	PS-10
Brabec T	We-I-3
Bréchignac C	<i>Tu-III-1</i>
Broyer M.	Fr- <i>I-2</i>
Bryzgalov V. V.	PS-16
Bykov N. Y.	PS-02
Cahuzac Ph	Tu-III-1
Calvo F	Th-III-2
Campbell E. E. B.	PS-06
Cederquist H7	h-IV-2, We-III-2
Concina B	We-II-4
de Souza Cruz F. F	<i>Tu-II-2</i>
Dedkov Yu. S	PS-15
Demin O. V.	<i>Fr-IV-3</i>
Denifl S.	We-III-3
Döppner T	
Drozdov S. V	PS-08. PS-07
Dubov D. Yu.	PS-08, PS-07
Dugourd Ph.	<i>Th-III-2</i>
Dunsch L. F	
Esteves D	We-I-1
Fennel T.	We-I-3
Ferreira da Silva F	We-III-3
Figge M. T.	<i>Fr-III-3</i>
Filatov M. V.	PS-24
Galichin V. A.	PS-08. PS-07
Geng J.	<i>Tu-II-1</i>
Gerasimov V. I	PS-19
Gherghescu R. APS-10	, Tu-IV-2, Tu-I-3
Gianturco F. A	
Gigilio E	PS-04
Glazunov E	<i>Fr-IV-2</i>
Gol'dt I. V.	PS-16
Gordeev Yu. S	PS-16, PS-15
Greiner C	PS-01
Greiner W.PS-10, PS-03. Fi	r-III-2, Fr-III-1.
Fr-II-2, Th-IV-3, Th-III-1.	Th-I-3, Tu-IV-2.
Tu-III-3, Tu-I-3	, ,

Gursky V. V	PS-27, Fr-IV-1
Güvenç Z. B	PS-10
Haag N	<i>Th-IV-2</i> , <i>We-III-2</i>
Haberland H	<i>Th-III-3</i>
Habibi M	We-I-1
Hampe O	We-II-4
Hempel M.	Th-II-2
Hentges R	PS-17
Hervieux PA	PS-05, PS-04
Hock C	<i>Th-III-3</i>
Huber B. A	<i>Th-IV-2</i>
Hussien A	Th-IV-3, Tu-III-3
Hvelplund P	<i>Th-IV-2</i>
Ionides J. M. C	PS-26
Isaev-Ivanov V	PS-24, Fr-IV-2
Islamov A	PS-24, Fr-IV-2
Itkis M. G.	<i>Th-I-2</i>
Ivanov V. K <i>PS</i> -	18, PS-13, PS-12, Tu-1-2
Jellinek J.	<i>Tu-I-1</i>
Johansson H.	<i>Th-IV-2</i>
Johnson B. F. G	
Kalabushkin A. E	PS-19
Kanevska P. P	PS-23
Kappes M. M.	
Karelov D	Fr-IV-2
Kedalli N	10-111-1 ער סת
Kentzniger E	PS-24 Wo I 1
Kilcoylie A. L. D	DC 12 Tu 12
Kondow T	
Konkov O I	
Korica S	PS-17
Korol A V	PS-03 We-II-3 We-II-2
Kostvuk A	<i>PS-03. Fr-II-2</i>
Kozlov K. N.	
Kresin V. V	We-III-1
Kuklin A.	PS-24, Fr-IV-2
Langer B.	
Lanzov V.	Fr-IV-2
Lauter H.	PS-24
Lebedev D	PS-24, Fr-IV-2
Leshchev D. V	PS-02
Li Z	<i>Tu-IV-1</i>
Lo S	We-II-3
Lui B	<i>Th-IV-2</i>
Lyalin A	<i>Tu-III-3</i>
Mafuné F	Fr-II-3
Manil B.	<i>Th-IV-2</i>

Manu.	PS-25
Märk T. D	We-III-3
Massaouti M	We-II-4
Masson A.	Tu-III-1
Mathew M.	PS-21
Matveeva A. D.	PS-26
Maurat E	<i>PS-05</i> , <i>PS-04</i>
Meiwes-Broer KH.	We-I-3
Meyer-Hermann M.	<i>Fr-III-3</i>
Michler F	PS-01
Mikoushkin V. M.	<i>PS-16</i> , <i>PS-15</i>
Mishustin I. N Fr-III-2, I	Fr-II-2, Th-II-1
Molodsov S. L.	<i>PS-16</i> , <i>PS-15</i>
Morozov A. N.	PS-14
Nakajima A	<i>Tu-III-2</i>
Nakamura M.	PS-09
Nesterenko V. O	<i>Tu-II-2</i>
Neumaier M.	We-II-4
Nieslen S. B.	<i>Th-IV-2</i>
Nikonov S. Yu	PS-15
Nikonov Yu. A	PS-19
Oganessian Yu. Ts.	<i>Th-I-1</i>
Pantina R. A.	PS-24
Petukhov M.	<i>Fr-IV-2</i>
Phaneuf R. A.	We-I-1
Poenaru D. N <i>PS-10</i> , 7	<i>[u-IV-2, Tu-I-3]</i>
Polozkov R. G <i>PS-18</i> , <i>PS-13</i> ,	, PS-12, Tu-I-2
Popok V.N	PS-06
Prikhodko A. V	PS-20
Pschenichnov IF	r-III-2, Fr-II-2
Rabinovitch R.	We-III-1
Radulescu O.	PS-27
Ramunno L	We-1-3
Rangama J.	<i>Th-IV-2</i>
Reinhard PG	<i>Tu-II-2</i>
Reinitz J <i>PS</i> -26, 1	PS-25, Fr-IV-1
Reinköster A.	PS-17
Rudnev V. S.	<i>PS-08</i> , <i>PS-07</i>
Saaimann U	
Samsonov A. M	PS-27, Fr-IV-1
Samsonova M. G.	<i>PS-20</i> , <i>PS-25</i>
Schaffner-Bielich J	<i>Th-II-2</i>
Scheler P.	We-111-3

Schenke B.	PS-01
Schippers S.	We-I-1
Schlathölter T	Fr-II-1
Schmidt H. T Th-I	V-2, We-III-2
Schmidt M Th-I	III-3, Tu-III-1
Schöbel H	We-III-3
Scifoni EFr-	-III-2, Fr-II-2
Shaginyan V. R	<i>Th-II-3</i>
Shnitov V. V.	PS-16
Solov'yov A. V.PS-22, PS-21, F	PS-18, PS-13,
PS-12, PS-10, PS-03, Fr-III-2	, Fr-II-2, Th-
IV-3, Th-III-1, We-II-3, We-I	<i>I-2</i> , <i>Tu-IV-2</i> ,
Tu-III-3, Tu-I-3, Tu-I-2	
Solov'yov I. APS-21, Fr-I	III-1, Th-III-1
Sominski G. G.	PS-14
Straβburg S.	Th-III-3
Surdutovich EFr-	-III-2, Fr-II-2
Surkova S	PS-25
Svetlov I. A.	PS-14
Takeda Y	Fr-II-3
Tiggesbäumker J	We-I-3
Titovets Yu. F.	PS-19
Tiukanov A. S	PS-18
Toennies J.	<i>Tu-II-3</i>
Toperverg B. P	<i>PS-24</i>
Toropkin A. I.	PS-18
Tumareva T. A	PS-14
Vakulenko S. A	<i>PS-27</i>
Verkhovtsev A. V.	<i>PS-12</i> , <i>Tu-I-2</i>
Volkov S. N <i>PS-23</i> , <i>PS</i> -23, <i>P</i>	PS-22, Fr-I-3
von Issendorff B.	<i>Th-III-3</i>
Vostrikov A. A	<i>PS-08</i> , <i>PS-07</i>
Vučković S	PS-06
Vyalikh D. V	PS-16
Wang J. C	We-I-1
Xia C	We-III-1
Yakubovich A Th-I	V-3, Th-III-1
Yang S.	We-I-1
Yatsyshin P. I	PS-13
Zappa F	We-III-3
Zelenskij Yu. N	PS-19
Zettergren H Th-I	<i>V-2</i> , <i>We-III-2</i>