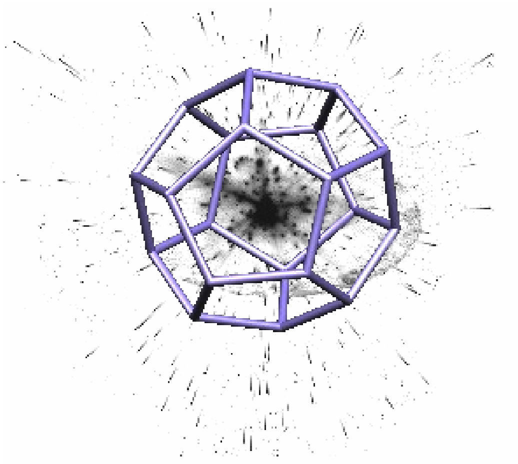

ISACC 2003

International **S**ymposium
"**A**tomic **C**luster **C**ollisions:
fission, fusion, electron, ion and photon impact"

Saint-Petersburg (Russia), July 18-21, 2003

Editor: Andrey V. Solov'yov
Technical Editor: Ilia A. Solov'yov

Abstracts

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Preface

The International Symposium "Atomic Cluster Collisions: fission, fusion, electron, ion and photon impact" (ISACC 2003) is a satellite meeting of the XXIII International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC 2003, Stockholm, Sweden). This Symposium was recognized by the European Physical Society (EPS) as **Europhysics Conference**. The ISACC 2003 will be held on **July 18 - 21, 2003 in Saint Petersburg, Russia**, at the former Palace of Grand-Duke Vladimir (nowadays used as the House of Scientists) located in the heart of St. Petersburg, near the Hermitage Museum.

This international symposium will promote the growth and exchange of scientific information on structure and properties of atomic cluster systems studied by means of photonic, electronic and atomic collisions. Particular attention during the symposium will be devoted to dynamical phenomena, many-body effects taking place in cluster systems, which include problems of fusion and fission, fragmentation, collective electron excitations, phase transitions and many more. Both experimental and theoretical aspects of atomic cluster physics, uniquely placed between atomic and molecular physics on the one hand and solid state physics on the other, will be discussed at the symposium.

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Conference program

Friday 18 July, 2003

8:45 - 9:00		**ISACC-2003 Opening**
9:00 – 11:00		**Structure and properties of atomic clusters, part I**
	Fr-I-1	**J.-P. Connerade** – *Confined atoms*
	Fr-I-2	**M. Manninen** – *Simulations of melting and ionization potential of metal clusters*
	Fr-I-3	**V. Shaginyan** – *New approach to density functional theory in nuclear and atomic cluster physics*
	Fr-I-4	**Il. Solov'yov** – *Ab initio calculations and modelling of atomic clusters: structure and photo-processes*
11:00 – 11:30		**Coffee break**
11:30 – 13:30		**Structure and properties of atomic clusters, part II**
	Fr-I-5	**V. Nesterenko** - *Electric and magnetic orbital plasmons in spherical and deformed clusters*
	Fr-I-6	**J. Jellinek -** *Metal clusters and the transition to metallicity*
	Fr-I-7	**M. Broyer** – *Electric dipole and charge transfer in mixed clusters*
	Fr-I-8	**L. Schweikhard** – *Cluster studies in ion traps*
13:30 – 15:00		**Lunch**
15:00 – 17:00		**Photoabsorption and photoionization of clusters**
	Fr-II-1	**H. Haberland** – *Phase transitions in sodium clusters*
	Fr-II-2	**S. Manson** – *Photoionization of confined atoms*
	Fr-II-3	**U. Becker** – *Imaging delocalized electron clouds: photoionization of fullerenes in Fourier reciprocal space*
	Fr-II-4	**R. Polozkov** – *Jellium model for photoionization of fullerenes and metal clusters*
17:00 – 18:30	**PS**	**Poster session** *(coffee and snacks are provided during the poster session)*

Saturday July 19, 2003

9:00 - 10:30		**Fission and fusion dynamics of clusters, part I**
	Sa-I-1	**C. Brechignac** – *Stability and fragmentation at nano-scale*
	Sa-I-2	**W. Greiner** – *Exotic fission processes in nuclear physics*
	Sa-I-3	**C. Guet** – *Fission of clusters and microdroplets*
10:30 - 11:00		**Coffee break**
11:00 - 13:00		**Fission and fusion dynamics of clusters, part II**
	Sa-I-4	**F. Sebastianelli** – *Ionic nucleation dynamics in He and Ne clusters*
	Sa-I-5	**A. Lyalin** – *Metal cluster fission: deformed jellium model and molecular dynamics simulations*
	Sa-I-6	**H. Stöcker** – *Multifragmentation, clustering, and coalescence in nuclear collisions*
	Sa-I-7	**I. Mishustin** – *Multifragmentation phase transition in atomic nuclei*
13:00 - 14:00		**Lunch**
14:00 - 16:00		**Electron scattering on clusters**
	Sa-II-1	**I. Fabrikant** – *Low-energy electron attachment to Van der Waals clusters*
	Sa-II-2	**T. Märk** – *Electron interactions with atomic an molecular clusters: excitation, ionization, and dissociation*
	Sa-II-3	**A. Solov'yov** – *Plasmon excitations in electron and photon collisions with metal clusters and fullerenes*
	Sa-II-4	**V. Kresin** – *Capture of slow electrons by metal clusters and fullerenes*
16:00 - 16:30		**Coffee break**
16:30 - 18:30		**Clusters in laser fields, part I**
	Sa-III-1	**R. Schmidt** – *Collision and laser induced dynamics of molecules and clusters*
	Sa-III-2	**A.W. Castleman** – *Probing the dynamics of cluster ionization processes with femtosecond lasers*
	Sa-III-3	**K.-H. Meiwes-Broer** – *Metal clusters in intense laser fields*
	Sa-III-4	**M. Rost** – *Rare gas clusters in intense laser fields*

Sunday July 20, 2003

Free day: *Excursions to the **Hermitage** museum and former Russian Tzar residence **"Peterhof"***
(see guided tour program for more details)

Monday July 21, 2003

9:00 - 10:30		**Clusters in laser fields, part II**
	Mo-I-1	**L. Wöste** – *Learning about clusters by teaching lasers to control them*
	Mo-I-2	**B. v. Issendorff** – *Cooling of the hot electron gas in free sodium clusters*
	Mo-I-3	**Y. Sato -** *Attosecond phase control of vibrational wavepackets in the HgAr vdW complex*
10:30 - 11:00		**Coffee break**
11:00 - 13:00		**Ion-cluster collisions, part I**
	Mo-II-1	**M. Ichihashi** and **T. Kondow** – *Collision of metal clusters with simple molecules: adsorption and reaction*
	Mo-II-2	**B. Huber** – *Collisions of highly charged ions with cold fullerenes and with clusters of fullerenes*
	Mo-II-3	**E. Campbell** – *Fullerene collision dynamics*
	Mo-II-4	**N. Kabachnik** and **H. Lutz** – *Multiple ionization and fragmentation of C_{60} in collisions with fast ions*
13:00 - 14:00		**Lunch**
14:00 - 15:30		**Ion-cluster collisions, part II**
	Mo-II-5	**K. Wohrer** and **M. Chabot** – *Cluster excitation and ionization in high velocity collisions: the atomic approach*
	Mo-II-6	**F. Martin** – *Charge transfer and fragmentation in atomic collisions with metal clusters and the fullerene C_{60}*
	Mo-II-7	**E. Salzborn** – *Electron and ion impact on fullerene ions*
15:30 - 16:00		**Coffee break**
16:00 – 18:00		**Clusters on a surface**
	Mo-III-1	**A. Nakajima, M. Ohara, M. Mitsui, K. Kaya** – *Soft-landing of vanadium-benzene sandwich clusters onto self- assembled monolayer (SAM)*

	Mo-III-2	**V. Mikoushkin** – *Collisions of electrons and photons with supported atoms, supported clusters and solids: transformation of electronic properties*
	Mo-III-3	**H. Yasumatsu, T. Hayakawa, S. Koizumi and T. Kondow** – *Physical and chemical properties of size-selected clusters landed on solid surface by cluster impact.*
	Mo-III-4	**A. Masson** – *Ag(n)OxHy clusters deposition on Graphite*
18:00 – 18:10		**ISACC Closure**

Overview of Abstracts

Structure and properties of atomic clusters

Photoabsorption and photoionization of clusters

Fission and fusion dynamics of clusters

Electron scattering on clusters

Clusters in laser fields

Ion-cluster collisions

Clusters on a surface

Posters

Invited Speakers

Structure and properties of atomic clusters

Fr-I-1

CONFINED ATOMS

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The concept of “quantum confinement” will be traced back to early papers on the subject, and the recent revival of the subject of confined atoms will be described. Examples will be given of quantum confinement, ranging from atoms under pressure (both physical and chemical) through atoms in bubbles and dots or impurities in clusters through to endohedral atoms, and references to recent work will be given. Various ways of modelling confined atoms will be described, based on Hartree-Fock, Dirac-Fock and RPAE methods with modified boundary conditions. Examples of the outcome of such calculations will be given. The filling of shells in atoms under pressure will be described, together with a discussion of the triggering or controlling of atomic orbital collapse, and the practical importance of including relativistic interactions will be stressed. A universal scheme for representing the non-linear part of the atomic compressibility will be presented. Examples of its application will include the case of compressed “eberlonium”. Extensions of the model to endohedral fullerenes will be considered, and shown to result in new types of avoided crossings. The different types of resonances in endohedral metallofullerenes will be classified. Finally, problems specific to the imposition of relativistic boundary conditions will be discussed.

Fr-I-2

SIMULATION OF MELTING AND IONIZATION POTENTIAL OF METAL CLUSTERS

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We have used classical and ab initio molecular dynamics to study the melting of sodium clusters[1,2] in order to see the effects of the geometric and electronic magic numbers on the melting temperature as a function of the cluster size. It seems that classical many-atom interactions can not explain the experimentally observed size-dependence of the melting temperature[3]. The results suggest that the electronic shell structure plays an important role in determining the melting temperature. We are using ab initio molecular dynamics for selected cluster sizes for studying the effects of the electronic structure.

The effect of the melting transition on the ionization potential was studied for sodium clusters with 40, 55, 142, and 147 atoms. The results reveal no correlation between the vertical ionization potential and the degree of surface disorder, melting, or the total energy of the cluster obtained with the ab initio method.

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NEW APPROACH TO DENSITY FUNCTIONAL THEORY IN NUCLEAR AND ATOMIC CLUSTER PHYSICS

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Clusters and fullerenes are new and unusual objects of scientific research and technology applications for design of new materials. They can be considered as located on the border between atoms and solid bodies, possessing the features of both solids and atoms or atomic nuclei. The accumulated experience in the field of nuclear physics is of great importance for a basic research in cluster physics. That is why both atomic clusters and atomic nuclei should be considered within the same approach.

We develop a self-consistent theoretical investigation of clusters and atomic nuclei based on the density functional approach. It is known, that the both of these objects have pronounced shell structure that determines important features of their behavior in the ground state and in the excited states. We concentrate on the mostly fundamental processes, taking place in clusters, such as collective plasmon-like excitations and single-particle excitations, which manifest itself in photoabsorption and photoionization, electron elastic and inelastic scattering, and etc. In the case of atomic nuclei, the main uncertainties when constructing the density functional of a nucleus are related with the contributions coming from the Coulomb interaction and the equation of state of a uniform neutron matter.

The self consistent version of the density functional theory is presented, which allows to calculate the ground state and dynamic properties of finite multi-electron systems and atomic nuclei. An exact functional equation for the effective interaction, using which one can construct the action functional, density functional, the response functions, and excitation spectra of the considered systems, is presented [1]. These results can be represented by using a special diagram technique. An analytical expression for the effective exchange interaction in a homogeneous electron system is derived. In case of atomic clusters, crude analytical expressions for the effective interaction are given. This effective interaction is of finite radius and density dependent. An analytical expression is also derived for the effective single particle potential and an equation is presented for the linear response function of the considered system. Thus it is demonstrated that the dynamic and ground state properties of clusters can be calculated by solving a complete system of integral and differential equations.

The density functional determining the Coulomb energy of nuclei is calculated to the first order in e^2 [2]. It is shown that the Coulomb energy includes three terms: the Hartree energy; the Fock energy; and the correlation Coulomb energy (CCE), which contributes considerably to the surface energy, the mass difference between mirror nuclei, and the single-particle spectrum. A CCE-based mechanism of a systematic shift of the single-particle spectrum is proposed. A dominant contribution to the CCE is shown to come from the surface region of nuclei. The CCE effect on the calculated proton drip line is examined, and the maximum charge Z of nuclei near this line is found to decrease by 2 or 3 units. The effect of Coulomb interaction on the effective proton mass is analyzed.

A homogeneous neutron system with a model pair interaction potential is considered [3]. It was shown that if the scattering length a is negative and sufficiently large the neutron matter becomes a strongly correlated system at the densities $\rho \sim |a|^{-3}$. The qualitative consideration gives strong evidences that the point ρ_{c1} at which the incompressibility vanishes is defined by $\rho_{c1} \sim |a|^{-3}$ provided the scattering length is the dominant parameter of the problem. It means that we consider $|a|$ to be much bigger then the radius of the interaction or any other relevant parameter of the system. Since the bare neutron-neutron potential is sufficiently strong to make a be both negative and the dominant parameter, neutron matter possesses the equilibrium density and energy. This result is in good agreement with recent experimental data [4]. An impact of these properties of a neutron matter on neutron rich nuclei is considered.

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Fr-I-4

AB INITIO CALCULATIONS AND MODELLING OF ATOMIC CLUSTERS: STRUCTURE AND PHOTO-PROCESSES

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Using *ab initio* theoretical framework based on the all-electron Hartree-Fock (HF) approximation and the post-HF perturbation theory on many-electron correlation interaction we have performed a systematic calculation and investigated structure and properties of neutral and singly charged sodium and magnesium clusters consisting of up to $N=20$ atoms. Alternatively, we have performed this calculation with the use of the density functional theory (DFT).

We have calculated optimized geometries of neutral and singly-charged *Na* [1] and *Mg* [2] clusters, their multipole moments, static polarizabilities, binding energies per atom, ionization potentials and frequencies of normal vibration modes.

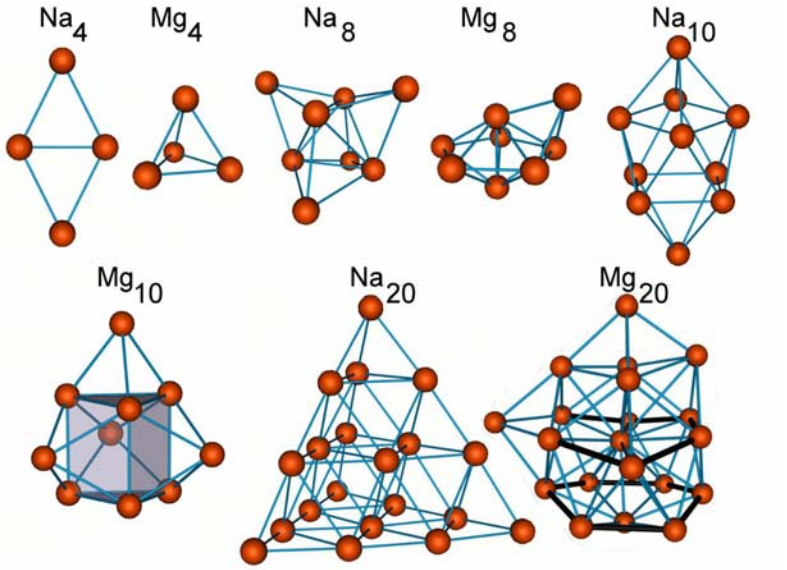

Figure 1: Magic sodium and magnesium clusters

In figure 1, we compare the geometries for the most stable *Na* and *Mg* clusters with N=4,8,10,20 atoms. According to the spherical jellium model, the magic clusters correspond to the shell closings of delocalized electrons, $1s^21p^61d^{10}2s^21f^{14}2p^6$, and possess the higher stability than their neighbours. Thus, Na_8 and Na_{20} are the magic sodium clusters, while Mg_4, Mg_{10} and Mg_{20} are the magic magnesium clusters. Note that often the point symmetry group of magic clusters is relatively high as compared with that for non-magic clusters. However, the Mg_{20} cluster possesses relatively low point symmetry group (C_S) due to the appearance of the two deformed hexagonal rings in the cluster structure. The hexagonal ring of atoms is the basic element of the hexagonal closest-packing (*hcp*) lattice, influencing the cluster symmetry and stability. Here, we do not present all the cluster geometries which have been calculated and analysed. For details, we refer to the papers [1-2].

Fr-I-4

For *Na* and *Mg* clusters and their singly charged ions in the cluster size range considered, we have calculated photoabsorption spectra using *ab initio* framework based on the random phase approximation and DFT. In our work, for the first time, we have performed theoretical investigation of the photoabsorption spectra of *Mg* clusters. In order to test our approach, we have calculated within the same model the photoabsorption spectra for a number of neutral and singly charged *Na* clusters and compared our results with the available experimental data and other calculations (see [3] and references therein).

In figure 2, we present the oscillator strengths for optically allowed transitions calculated for the most stable isomers of Mg_2, Mg_4 and Mg_{10}. The photoabsorption spectrum for the Mg_4 cluster has a prominent peak at the energy about 4 eV, which can be identified as a Mie plasmon resonance. For the Mg_{10} cluster, the plasmon peak is splitted due to the cluster axial quadrupole deformation. Note that the splitting of the plasmon peak in Mg_4 arises due to the axial octupole deformation. For the Mg_2 cluster, the plasmon peak is hard to identify in the distribution of oscillator strengths, which means that the number of delocalized electrons in Mg_2 turns out to be insufficient for the formation of the plasmon resonance in this system.

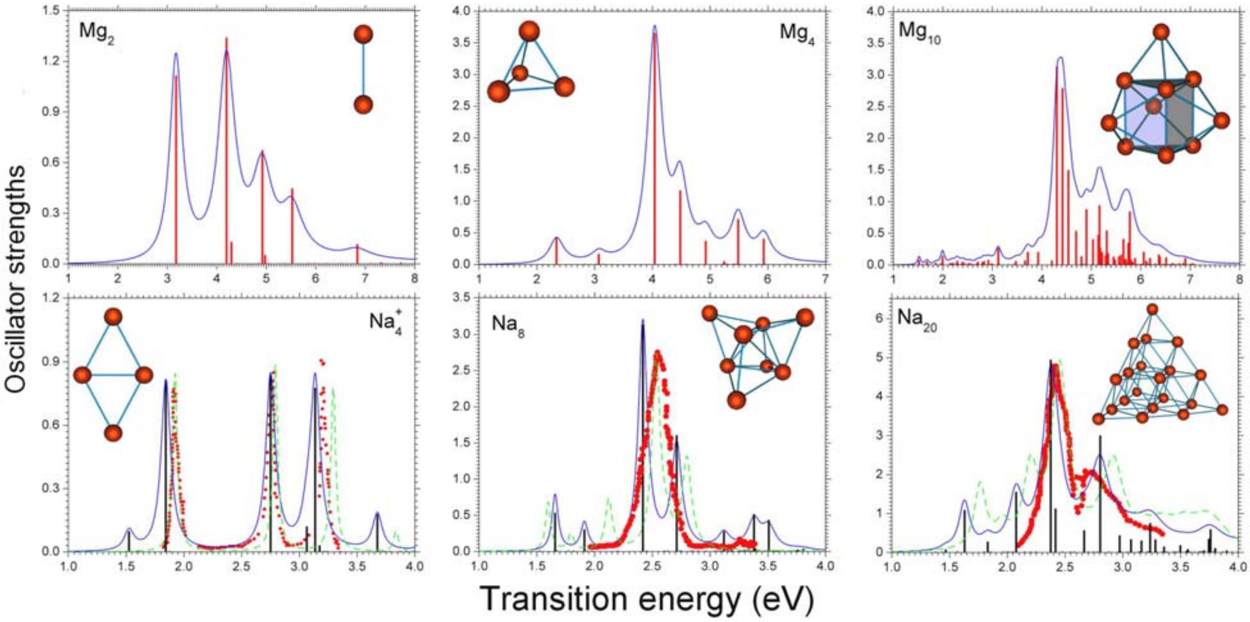

Figure2: Oscillator strengths for the optically allowed transitions in *Na* and *Mg* clusters

We also present the experimentally measured photoabsorption spectra for the Na_4^+, Na_8 and Na_{20} clusters (dots). We compare them with our results (solid lines) and with the earlier reported theoretical data [3] (dashed lines). This comparison demonstrates that our approach is in a good agreement with the results of other theories and experiment [3]. Our calculations demonstrate that for the formation of a surface plasmon it is sufficient to have 8 delocalized electrons in a system (see figure for Mg_4 and Na_8). Note that the smallest sodium cluster, for which the plasmon peak can be identified, is Na_7. It possesses 7 delocalized electrons.

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Fr-I-5

ELECTRIC AND MAGNETIC ORBITAL PLASMONS IN SPHERICAL AND DEFORMED CLUSTERS

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Electric (E1, E2, E3) and magnetic orbital (M1) plasmons in sodium clusters are studied within a self-consistent random-phase-approximation (RPA) method [1] based on the Kohn-Sham LDA functional.

The experimental data [2] on the E1 plasmon in axial sodium clusters are analyzed [1,3]. The calculations show that, while in light clusters plasmon properties (gross structure and width) are determined mainly by deformation splitting, in medium clusters with $N > 50$ the Landau fragmentation becomes decisive. Moreover, shape isomers come into play with contributions to the plasmon spectrum comparable to the ground state one.

The magnetic orbital low-energy (0.3-1.0 eV) M1 scissors mode (SM) in deformed clusters is discussed [4-6]. This mode appears in any *deformed* two-component finite quantum system. It was already observed or predicted in atomic nuclei, quantum dots, diluted gases of Bose and Fermi atoms. In clusters, SM determines the Van-Vleck paramagnetism and leads to a strong anisotropy of the magnetic susceptibility (dia-para anisotropy in Na_{27}^+) [5]. Detailed ionic structure destroys the local spherical symmetry and causes a finite M1 response even in clusters with zero global deformation [6].

Perspectives to observe E2, E3, and M1 plasmons in photoabsorption and inelastic electron scattering are discussed in detail.

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Fr-I-6

METAL CLUSTERS AND THE TRANSITION TO METALLICITY*

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One of the most intriguing manifestations of the size-dependence in properties of cluster systems is that small atomic clusters of elements that are metals in bulk quantities may not possess metallic attributes. These attributes then emerge as the clusters grow in size. The emphasis in the talk will be on the size-induced transition to metallicity as exhibited in magnesium clusters [1-3].

Data on structural and electronic properties of neutral and anionic magnesium clusters obtained using density functional theory (DFT) will be presented and analyzed [1-4]. These will include isomer-specific spectra of electron binding energies computed using a new general and accurate scheme for conversion of the Kohn-Sham eigenenergies of DFT into binding energies of electrons [5]. The principal elements of the scheme will be described.

The computed results will be compared with the data obtained in photoelectron spectroscopy (PES) experiments. We will illustrate and emphasize the important role of the charge state, in addition to the size-dependence, in the proper interpretation of these data. We will also show that the computed isomer-specific spectra of electron binding energies can be used to identify the structural forms of the clusters generated/measured in PES experiments.

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Fr-I-7

ELECTRIC DIPOLE AND CHARGE TRANSFER IN MIXED CLUSTERS

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The electric dipole moment of mixed clusters may be measured by beam deviation in a strong inhomogeneous electric field. For rigid clusters the dipole moment leads to a broadening of the beam. The dipole value may be deduced from theoretical simulation of this broadening. For non rigid clusters, the dipole may be statistically oriented along the electric field. This phenomenon of paraelectricity results in a global deviation of the beam. The measured electric susceptibility follows the Curie law and also allows us to determine the electric dipole. Various mixed clusters may been studied by this technique. Selected examples will be discussed to illustrate the main results and the importance of dynamical effects.

The metal-fullerene clusters M-C_{60} represent a model system. At low temperature, the molecule is rigid and the electric dipole may be deduced from the broadening of the molecular beam. When the temperature increases, the metallic atom becomes mobile on the fullerene cage, and the measured susceptibility leads to the determination of the electric dipole through the Curie law, in agreement with the results obtained at low temperature. These electric dipole values are obtained for alkali metals and transition metals. Results are compared to ab initio calculations and allow us to deduce the charge transfer between the metal and the fullerene.

The transition metal-benzene complexes are also investigated for a row of the periodic table. The dipole measurements allow us to compare experimental results with ab initio calculations and to discuss the chemical bonding in these complexes. In sandwiches M-$(C_6H_6)_2$, symmetric and asymmetric structures are found depending on the number of d electron of the transition metal atom.

The small alkali-halide clusters with one excess electron (M_nX_{n-1}) have cuboid structures and offer a striking example of the influence of the structure on the electric dipole moment . For given sizes (for example $M_{18}X_{17}$) strong electric dipoles are measured, while for other sizes, the dipole is ten times smaller. This may be easily related to the cuboid structure, as well as to the localization or delocalization of the excess electron.

Finally, the importance of dynamical aspects is illustrated in two selected examples. In the $(PABA)_2$ molecule, we show that the dipole moment induced by the vibration may give a significant contribution to the electric susceptibility. In sodium-coated C_{60} clusters, the observed electric dipole is discussed taking into account the motion of metallic atoms on the fullerene surface as well as the wetting-non wetting transition.

Fr-I-8

CLUSTER STUDIES IN ION TRAPS

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Atomic clusters may be captured in ion traps for extended storage. While trapped they can be treated repeatedly by various interactions and their reaction can be monitored for extended periods of time. The use of Penning traps (Ion Cyclotron Resonance traps) adds mass spectrometric methods for the isolation of the particular cluster species of interest as well as various techniques for mass analysis of the reaction products. Thus an apparatus like the Cluster Trap [1] (Fig. 1) provides the means for a number of interesting investigations, such as the following two examples:

(a) While most cluster sources produce only neutral and singly charged species, the trapped clusters can be further charged during their storage in the trap. Most notably, not only multiply charged cations, but also polyanions have been produced and prepared for further investigations [2]. From the many decay pathways that are in principle available for an excited dianionic metal cluster, neutral monomer evaporation end electron detachment have been observed. Large dianionic metal clusters tend to evaporate atoms, while smaller ones emit electrons. In addition, the detachment of two electron seems to be a competing pathway in spite of the observation of monomer evaporation for singly charged anionic clusters of the same size.

(b) Another development is concerned with the precision measurement of dissociation energies [3]. To this end, a new experimental technique has been introduced which instead of relying on the modeling of decay rates makes use of a combination of the results of direct and sequential decay measurements. Thus, most systematic uncertainties due to further assumptions on the decay mechanisms cancel out. In contrast, the new results may now serve as benchmarks for simulations of the dissociations.

The contribution will include a short introduction to cluster ion trapping and an overview of the investigations mentioned above.

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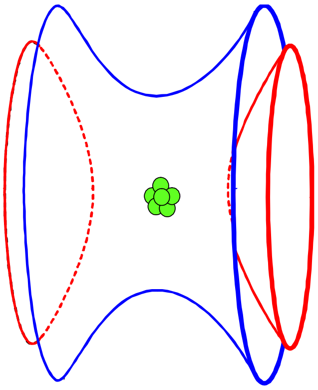

Fig. 1: Schematic representation of the Cluster Trap.

Photoabsorption and photoionization of clusters

Fr-II-1

PHASE TRANSITIONS IN SODIUM CLUSTERS

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The solid to liquid transition in sodium clusters has been studied in detail [1,2]. The experiment prepares a positively charged sodium cluster of a specified size, e.g. Na_{100}^+, and known temperature T. The energy E of the cluster is measured in a photo–fragmentation nano–calorimetry experiment. Thus, for a free cluster in vacuum, one can construct the caloric curve $E = E(T)$, from which the melting point and the latent heat of fusion can be read off. The observed large fluctuations have not been understood theoretically so far. The ideas have been extended to the liquid to gas transition. An experiment will finally be presented, which allows to generalize the experimental method to other atoms and molecules.

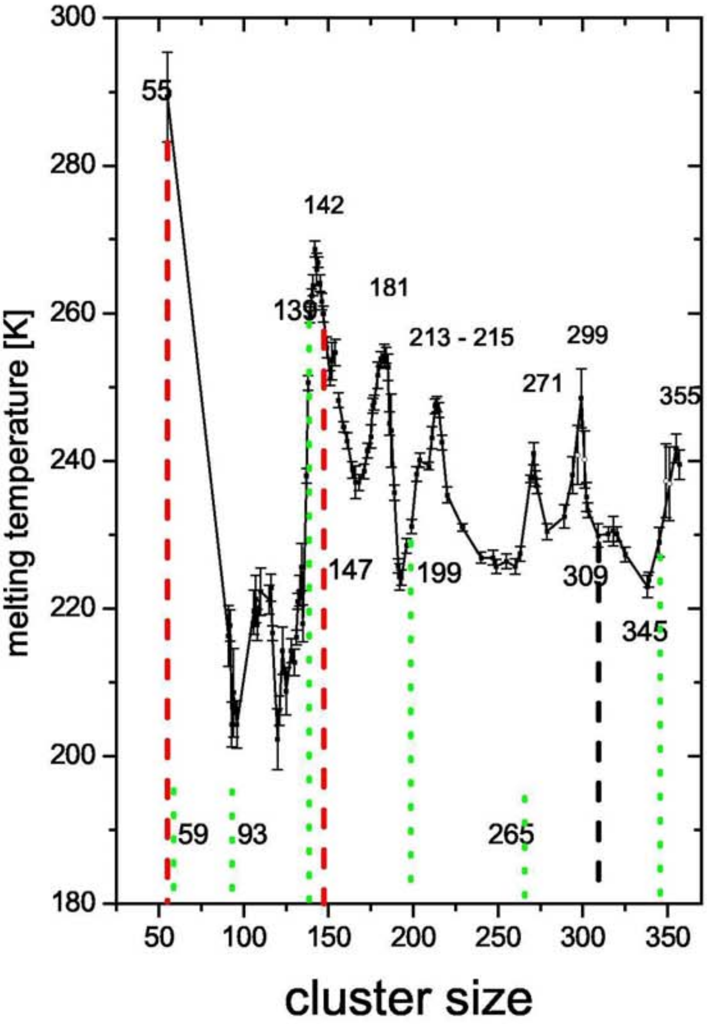

Figure 1: The measured melting temperatures of sodium clusters are plotted against the number N of atoms in the cluster. Some N values are indicated in the figure. The data points are connected by straight lines, in order to guide the eye. Note, that the melting temperatures do not seem to converge to their bulk value (371 K) in this size range. The dotted and dashed vertical lines indicate electronic and geometrical shell closings, respectively. No correlation of the extrema with any shell closings can be seen. The latent heats and entropy changes upon melting show similar oscillations[1,2].

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Fr-II-2

PHOTOIONIZATION OF CONFINED ATOMS

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Atoms or atomic ions trapped in a fullerene cage like C_{60} are of interest for a variety of reasons. Aside from the intrinsic interest of how the oscillator strength distribution is altered by the presence of the confining potential, the confining an atom opens the possibility of creating new materials with properties designed for specific purposes. To study this, a program of theoretical studies of the photoionization of confined atoms and ions has been initiated. In this report, an overview of these studies is presented.

A variety of theoretical methodologies have been used in the studies. To get a qualitative picture of the effects of confinement, simple spherical potentials have been employed to model the action of the confining cage. These studies have revealed significant insight into the photoionization of confined atoms. In addition to the modification of extant atomic properties, we have uncovered the existence of new kinds of resonances termed *confinement resonances* which arise from the interference between the electron wave emerging directly, and one that scatters off the confining potential [1], a phenomenon much like EXAFS but considerably stronger. These resonances appear not only in the integrated subshell cross section, but in dipole and nondipole contributions to the photoelectron angular distribution as well. In connection with the nondipole effects, the existence of these confinement resonances can increase the nondipole angular distribution parameter γ at tens of eV by several orders of magnitude [2].

A theoretical methodology has also been developed to treat the problem more exactly. The method treats each carbon atom of the C_{60} cage surrounding an atom A, A@C60, individually, thereby introducing explicitly the non-spherical nature of the confining potential [3]. Using this more sophisticated theory, many of the aspects the photoionization of endohedral A@C60 found with a spherical potential have been confirmed. Complex photoelectron angular distribution patterns are observed for photoionization of fixed-in-space endohedral atoms. In addition, it has been found that, contrary to the conventional wisdom, if the confined atom or ion is not at the center of the cage, the photoionization cross section and photoelectron angular distribution are changed dramatically as a function of the displacement from the center and the direction of the displacement.

The work reported herein was performed in collaboration with A. S. Baltenkov, J.-P. Connerade, and V. K. Dolmatov. The research was supported by CRDF, NASA and NSF.

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Fr-II-3

IMAGING DELOCALIZED ELECTRON CLOUDS: PHOTOIONIZATION OF FULLERENES IN FOURIER RECIPROCAL SPACE

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Photoelectron spectroscopy is a versatile tool for structural studies exploiting the diffraction properties of core electron emission. However, the information on the properties of electron distributions from where they are emitted, that valence electrons carry, have been exploited only since very recently. The reason for this is the fact that valence electrons are not sensitive to scattering centers but to rapid changes of the potential energy causing their binding. In a sense, both localized centers and delocalized electron clouds may be imaged by valence electron emission if the system is spherically symmetric. This condition is fulfilled by a whole class of systems, clusters and more specifically fullerenes. Particularly clusters which are well described within the jellium model are perfectly suited for such size dependent studies. Moreover, because the production of mass selected clusters is still a very difficult task, fullerenes offer an attractive alternative for the exploitation of the potential of valence photoemission measurements to extract structural information from cross section behavior.

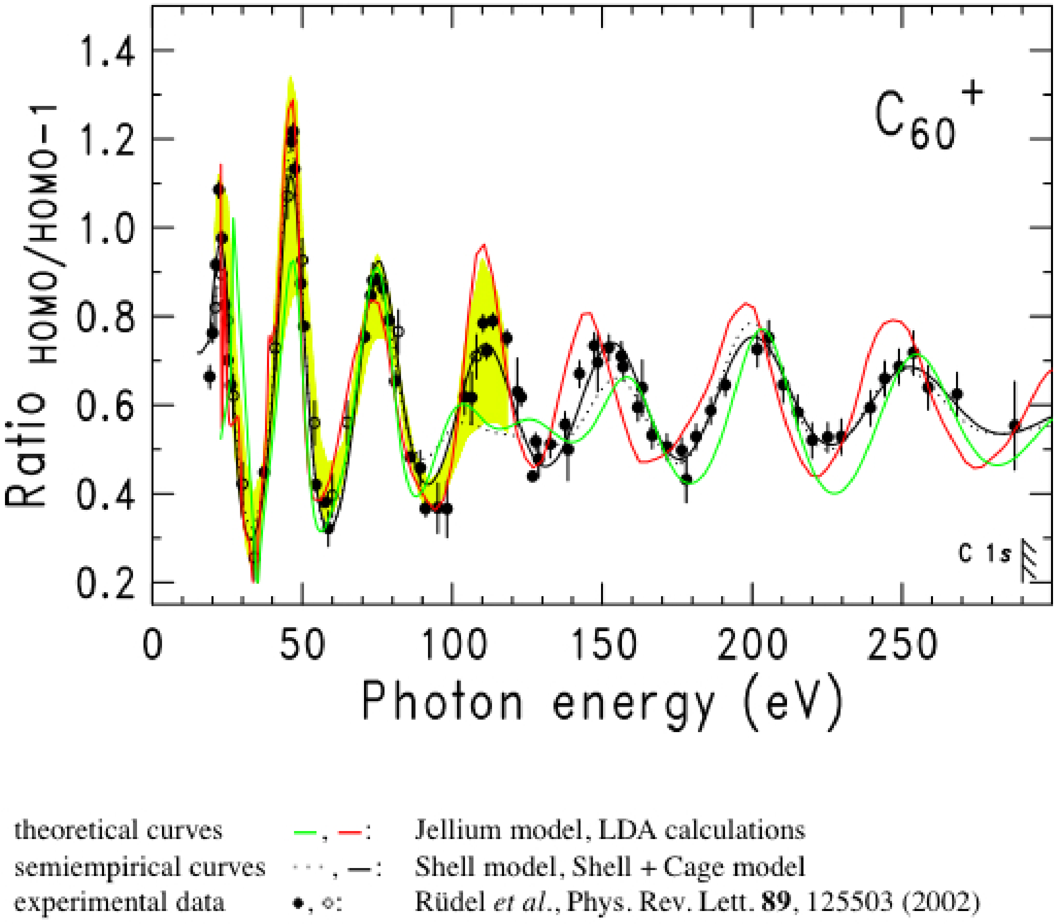

Fig. 1. Branching ratio HOMO/HOMO-1 from near threshold up to the carbon K-edge. The figure contains differnt experimental data sets and theoretical calculations [1, 2].

Fr-II-3

Such studies have been successfully performed during the last years on C_{60} and in part on C_{70}. The characteristic cross section behavior which exhibits the structural information on the fullerenes is the intensity modulations of the various valence photoelectron lines, in particular the HOMO and HOMO-1 lines across excitation energy. These energy dependent modulations reflect directly the carbon cage and conducting shell structure of C_{60} and C_{70}. The oscillations are alternating in phase with the angular momentum and symmetry of the final state of the outgoing electron giving rise to distinct oscillation in the branching ratio between the valence lines of different symmetry. Fig. 1 shows these oscillations in the branching ratio between the two outermost molecular orbitals of C_{60} together with different theoretical curves. Recent refinements of the partial cross section data over a large energy region made it possible to analyze the observed oscillations in terms of the desired structural information. Fourier transformed cross section data directly display the radius of the fullerene and the thickness of the delocalized electron cloud [1]. New measurements for both gas phase and solid state show almost identical behavior of the branching ratio and will be presented and discussed in terms of the weakness of the binding in solid C_{60} [3].

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Fr-II-4

JELLIUM MODEL FOR PHOTOIONIZATION OF FULLERENES AND METAL CLUSTERS

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In this report I present the results of calculation for the structure and photoionization of the fullerenes and metal clusters within jellium model. These results were obtained by theoretical atomic physics groups of St.Petersburg Physical-Technical Institute and St.Petersburg State Politechnical University.

Being the unique hollow cage structure the fullerenes have attached considerable interest over the years. The first-principle calculations have been performed on the subject, in particular for the most famous extremely stable fullerene C_{60}. These sophisticated approaches treated properly the high icosahedral symmetry of the molecule. However, the basic features of photoprocesses can be understood in the scope of a spherical model. In our earlier work [1] we have used this framework to describe the photoionization process involving fullerenes. We considered the fullerene as a spherical shell and employed the jellium model. The local density approximation (LDA) has been used for calculating initial state wavefunctions. Cross sections for the photoionization process have been calculated using the self-consistent many-body theory based on LDA and the random phase approximation (RPA). The method was successfully tested in its application to the well-studied plasmon resonance of fullerene C_{60} and then the photoionization of the smallest C_{20} fullerene has been theoretically described for the first time. The calculations revealed two resonant structures: (i) the near-threshold resonance and (ii) the plasmon-type resonance.

Within the RPA based on LDA approach we calculate the partial cross section for the photoionization of the highest occupied molecular orbital (HOMO) and the next lower-lying HOMO–1 orbital of the fullerene C_{60} at the high energy region. The partial photoionization cross sections for gas phase C_{60} obtained by means of photoelectron spectroscopy exhibit prominent oscillations [2]. In [3], this behaviour was interpreted in terms of intramolecular interference of incoming and outgoing waves. The calculated spectrum demonstrates strong oscillatory behaviour because photoelectron might form a spherical standing waves inside the hollow structure of the fullerene [4]. The influence of the form of the potential well on the photoionization cross section is investigated [4]. For this purpose, we have introduced some parametric modification of the model.

Presenting these results, we hope that our findings could lend impetus to further experimental investigations. Our approach allow us to reveal physical nature of the cross section peculiarities: near-threshold resonance, plasmon peak, oscillatory structures. The interpretation of these phenomena are given in the context of influence of collective many-electron effects and the hollow molecular structure specific to fullerenes.

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Fission and fusion dynamics of clusters

Sa-I-1

STABILITY AND FRAGMENTATION AT NANO SCALE

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Control of matter on the nano-scale already plays in important role in scientific disciplines as diverse as physics, chemistry, materials science, biology. However, the first fundamental question, which rises following the preparation of nano-objects is: Are these objects stable?

Studying their fragmentation is one of the keys to understand their stability. Even though quite general concept can effectively describe various aspects of fragmentation processes at different length-scale, at the nano-scale the instabilities leading to fragmentation may considerably influence the morphology of the nano-objects. Moreover, the fascinating capability that a nano-object has to modify its shape in order to minimize its free energy leads to shape modification, evaporation or fragmentation that may be easily observed in a reasonable time scale.

This issue will be discussed in the light of several examples: cluster evaporation, fission, nano-wire fragmentation…

Sa-I-2

EXOTIC AND FUSION PROCESSES IN NUCLEAR PHYSICS

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Nuclei undergo symmetric, asymmetric, superasymmetric fission, all of them from very cold to very hot processes. We shall discuss the theoretical predictions as well as experimental verification. Furthermore, cluster radioactivity, theoretically predicted by Poenaru, Sandulescu and myself [1,2] is observed for a wide range of emitted clusters. It is a process between fission and α-decay.

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Sa-I-3

FISSION OF CLUSTERS AND MICRODROPLETS

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Finite size droplets with an electrical charge being greater than some critical value are unstable, since cohesive forces no longer can resist the repulsive Coulomb forces. Nuclear fission provides the most dramatic example of Coulomb dissociation. The nuclear liquid drop undergoes fission through a sequence of large deformations that lead to a binary symmetric fragmentation. The nuclear quantum mechanical effects break this symmetry and explain the observed mass distribution of fission fragments. Multi-charged atomic clusters and microdroplets can also undergo Coulomb dissociation, but surprisingly enough, little is known on the details of fission in this case.

Ab-initio molecular dynamics is a useful tool to investigate fission of highly charged metal clusters[1]. Although these calculations remain limited to small systems, they show that cluster fission is very asymmetric. Asymmetric fission is expected from liquid drop considerations. Micrometer sized droplets do also fission asymmetrically, although there is so far, no direct measurement of the fragment size distribution. However, the onset of instability is today well understood. Recent experiments have indeed confirmed for the first time the Rayleigh theory [2]. Note that the features of fission as wall as the conditions for the onset of instability are altered by external electric fields as shown by recent classical calculations [3].

When an atomic cluster is suddenly brought to a very a high charged state, it undergoes Coulomb explosion. However the charging process (either strong femtosecond laser irradiation or multiple ionization in collisions with multi-charged ions) is usually accompanied by heating of electrons. The coupled dynamics of electrons and ions plays an essential role in the interplay between Coulomb forces and kinetic pressure and affects the conditions for explosion [4].

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Sa-I-4

DYNAMICAL EVOLUTION OF CORE FORMATION IN SMALL RARE GAS CLUSTERS WITH IONIC IMPURITIES

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Clusters formed by large aggregates of rare gases (Rg) have been studied for a long time because of both their intrinsic interest at the fundamental level and of the possibilities they offer to taylor special materials containing specific, additional atoms or molecules as dopants (1).

The chief observational tool for detecting structural features of such Rg clusters has been that of ionizing the initial aggregate, following then its fragmentation kinetics (2). The ionization process, on the other hand, profoundly modifies the chemical makeup of the clusters and introduces strong perturbations in the structure of their bonding network with respect to the initially neutral species. It therefore follows that it acquires crucial importance to be able to understand and describe, at the molecular level, the effects induced in the clusters by the formation, growth and developments of stable, ionized cores (negative and positive ions) within larger, initially neutral Rg clusters.

The structure and dynamics of such cluster core evolution, their actual chemical compositions and their effects on cluster stabilities have been of interest to our research group in Rome for sometime (3-12), where we have endeavoured to analyse from first principles the structures of the ionized Neon clusters (4,7), that of the corresponding ${}^4He_n^+$ clusters (8,11), the effects of H^- impurities in ${}^4He$ clusters (5,12) and the time evolution of a quantum wavepacket describing the Rg cores after the initial ionization process (9,10).

Recent results on metal impurities inserted in ${}^4He$ clusters (eg. Li and Na atoms), on the cationic impurity of H^- in 4Hen and Ne_n, and on the structures of such clusters as n increases, will be presented at the meeting and discussed in detail in terms of their effects on the final stability of the (cluster + dopant core) complex as a function of its size.

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METAL CLUSTER FISSION: DEFORMED JELLIUM MODEL AND MOLECULAR DYNAMICS SIMULATIONS

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We report new results of *ab-initio* all-electrons MD simulations as well as the jellium model calculations of fission barriers for sodium clusters. The following symmetric ($Na_{10}^{2+} \to 2Na_5^+$ and $Na_{18}^{2+} \to 2Na_9^+$), as well as asymmetric ($Na_{10}^{2+} \to Na_7^+ + Na_3^+$ and $Na_{18}^{2+} \to Na_{15}^+ + Na_3^+$) fission channels are considered.

The jellium results are obtained with the use of the two-center deformed jellium model [1–3]. The importance of cluster deformation effects in the fission process is elucidated with the use of the overlapping-spheroids shape parametrization allowing one an independent variation of deformations in the parent and daughter clusters [4, 5]. We investigate the role of the exchange and correlation effects in metal-cluster fission process on the basis of both the open-shell two-center deformed jellium Hartree-Fock method and local-density approximation (LDA) [4, 5]. Comparison of results of the two approaches allows us to illustrate the importance of the exchange component of the many-electron interaction in the fission process and make important conclusion about the relative role of the two different channels of the reaction. The role of the exact exchange and many-body correlation effects in metal clusters fission is analysed. It is demonstrated that the influence of many-electron correlation effects on the height of the fission barrier is more profound if the barrier arises nearby or beyond the scission point.

The MD calculations are performed with the use of the Gaussian 98 software package [6]. We utilize the $6-311G(d)$ basis set of primitive Gaussian functions to expand the cluster orbitals and the density-functional theory based on the hybrid Becke-type three-parameter exchange functional paired with the gradient-corrected Lee, Yang and Parr correlation functional ($B3LYP$) [6].

We investigate the isomer dependence of the fission barriers as well as the barriers for transition between different cluster isomer forms. For this purpose, we consider three different isomers of the parent doubly-charged Na_{10}^{2+} cluster having the ionic structure of distorted tetrahedron (lowest energy state), or characterized by the C_{4v} and D_{4d} point symmetry groups.

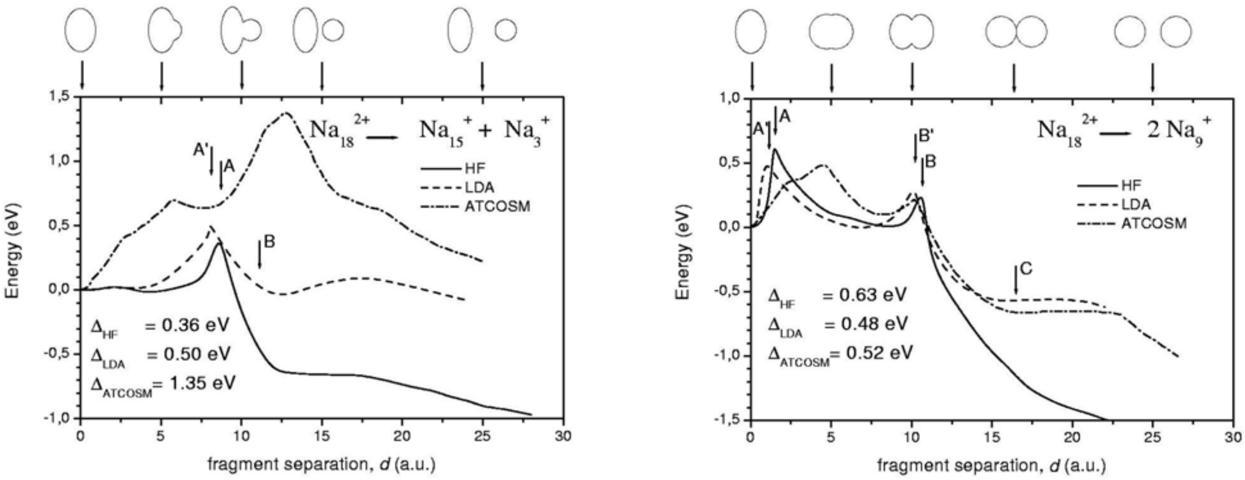

Figure 1: Fission barriers in the two-center deformed jellium Hartree-Fock (solid lines) and LDA (dashed lines) approaches calculated in this work for the asymmetric $Na_{18}^{2+} \rightarrow Na_{15}^{+} + Na_{3}^{+}$ and symmetric $Na_{18}^{2+} \rightarrow 2Na_{9}^{+}$ as a function of fragments separation distance d. Deformations of the parent and daughter clusters are taken into account. The zero of energy put at $d = 0$. The evolution of cluster shape during the fission process is shown on top of figures. We compare our results with those derived in ATCOSM (dash-dotted line) [7]. Vertical arrows show the alterations of the electronic configuration.

The described models form the basis for further systematic development of the more advanced *ab initio* many-body theories for the process of metal clusters fission.

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Sa-I-6

Multifragmentation, Clustering, and Coalescence in Nuclear Collisions

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Nuclear collisions at intermediate, relativistic, and ultra-relativistic energies offer unique opportunities to study in detail manifold fragmentiation and clustering phenomena in dense nuclear matter.

At intermediate energies, the well known processes of nuclear multifragmentiation – the disintegration of bulk nuclear matter in clusters of a wide range of sizes and masses – allow the study of the critical point of the equation of state of nuclear matter. On the other hand, ultra-relativistic heavy-ion collisions offer a glimpse at the substructure of hadronic matter by crossing the phase boundary to the quark-gluon plasma. The hadronization of the quark-gluon plasma created in the fireball of a ultra-relativistic heavy-ion collision is, again, a clustering process. We will present to models which allow the simulation of nuclear multifragmentation [1] and the hadronization via the formation of clusters [2] in an interacting gas of quarks.

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Sa-I-7

MULTIFRAGMENTATION PHASE TRANSITION IN ATOMIC NUCLEI

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Multiple production of nuclear fragments in nuclear reactions at intermediate energies is well established phenomenon. Mass and charge distributions of these fragments vary with excitation energy in the way which would be expected for a liquid-gas phase transition. In particular, a power-law mass distributions are observed at certain conditions which correspond to the critical point of this transition. In this talk I will describe recent theoretical developments aiming to give a realistic description of these phenomena on the basis of statistical and dynamical models. In particular, I will demonstrate that the Statistical Multifragmentation Model (SMM) gives very good description of data in situations when the emitting source is close to thermal and chemical equilibrium. I will mention drawbacks of the Fisher's droplet model and show how it can be modified in order to include the finite-size effects. Molecular-dynamics simulations of nuclear disintegration in explosion-like processes will also be presented.

Electron scattering on clusters

Sa-II-1

LOW-ENERGY ELECTRON ATTACHMENT TO VAN DER WAALS CLUSTERS

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Electron attachment to molecular Van der Waals clusters is often strongly affected by vibrational Feshbach resonances (VFR) corresponding to the temporary vibrational excitation of an individual molecule in the cluster with the simultaneous capture of the electron by the long-range field of the cluster. Two very different types of VFRs were detected by the experimental group at the University of Kaiserslautern. The first type, observed in electron attachment to methyl iodide dimers and trimers [1], has its origin in dissociative attachment to the monomer. With increasing number of monomers in clusters, the energy of VFR is rapidly shifting away from the vibrational excitation threshold and the resonance width is rapidly growing. Essentially no structure is left in the attachment spectrum for $(CH_3I)_2{\cdot}I^-$. This phenomenon was explained by the effects of solvation and increased electron-target long-range polarization interaction in dissociative attachment.

In contrast, the VFRs observed in electron attachment to $(CO_2)_N$ clusters [2,3] and $(N_2O)_N$ clusters [4] remain sharp with increasing N. Another interesting feature associated with this second type of resonances is that corresponding monomers (CO_2 and N_2O) do not attach electrons in the low-energy region. The position of VFRs in these systems can be explained by simple model calculations for the binding energy of the captured electron in the VFR state relative to the energy of the neutral cluster which carries the same amount of intramolecular vibrational energy. We assume that the binding energy is simply due to the combined effects of the long-range attraction between the electron and the cluster and the short-range interaction U_0 at distances smaller than the cluster radius R_N. We only take into account the polarization attraction neglecting, in the average over the cluster, the effects associated with a possible dipole moment (for example, in N_2O molecules) and the quadrupole moment.

In view of the success in application of this model to explanation of the observed red shifts in positions of VFRs [2-4], we have developed it further by incorporating a coupling between the vibrational excitation channels and nondissociative attachment channel. The latter channel is due to electron attachment to the extended affinity states with the following redistribution of the excess energy among the phonon modes [5]. The coupling between the vibrational states of the neutral molecule and vibrational states of the corresponding anion is included by using the displaced harmonic oscillator model [6] with appropriate choice of parameters allowing us to describe vibrational excitation of monomers. The electron-phonon coupling for the case of CO_2 clusters was estimated from the results for the capture width [5].

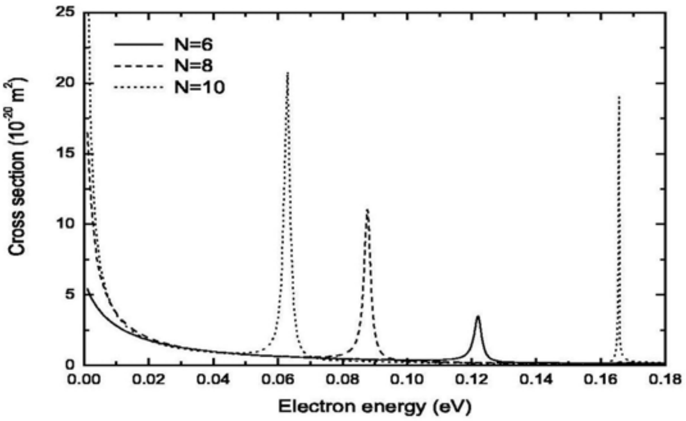

Fig. 1. Cross sections for electron attachment to CO_2 clusters for different number of monomers N.

In Fig. 1 we present cross sections for electron attachment to $(CO_2)_N$ clusters for $N = 6$, 8, and 10. The model incorporates vibrational excitation of the Fermi-coupled pair of the bending overtone and the symmetric stretch mode (020)/(100) with the average energy 166 meV. The position of the VFR is red-shifted with N, in accordance with observation and theoretical model of Ref. [2]. The width of VFR does not change significantly with N. The resonance amplitude is growing with N, however. Moreover, a second resonance appears at $N = 10$. At energies below 40 meV attachment is dominated by the zero-energy peak which grows as $1/E^{1/2}$ with decreasing energy. On the other hand, strong zero energy peaks are observed in experiment [2,3] only when a VFR overlaps zero energy.

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Sa-II-2

ELECTRON INTERACTIONS WITH ATOMIC AND MOLECULAR CLUSTERS: EXCITATION, IONIZATION AND DISSOCIATION

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Fragmentation of finite size systems is a wide spread phenomenon in nature, including such diverse phenomena as the break-up of sub-microscopic objects or collisions between asteroids. The study of fragmentation of systems like nuclei, molecules and clusters has attracted much interest recently and one intriguing result is the recognition that the general features of this phenomenon (e.g. fragmentation patterns) are rather independent of the actual system studied and its corresponding interaction forces. It is well known that highly excited finite atomic systems will relax by either emitting electrons, neutral particles (dissociation), or a continuous spectrum of photons. These reactions are the molecular analogues to thermionic electron emission, evaporation, and black body radiation in solid state physics. Moreover, multiply charged systems may decay via fission reactions ejecting charged rather than neutral fragments analogous to nuclear fission. It is thus not surprising that one important field in cluster science (attracting recently growing interest) is the study of the fragmentation behaviour of excited cluster ions $X_n^{z+,*} \rightarrow \sum X_p^{q+}$ produced by such means as photon, electron and ion impact (including charge transfer reactions), collision induced dissociation (CID) or surface induced dissociation (SID) reactions.

Mass spectrometric studies of spontaneous (metastable) decay reactions and of (prompt) dissociative reactions of mass-selected cluster ions induced by photons, electrons, heavy particles (CID) or surface collisions have provided a wealth of information about structure, stability and energetics of these species and the dynamics of the corresponding decay reactions. Surprisingly few studies, however, have been reported measurements concerning the kinetic energy release distribution (KERD) for the decay of such excited cluster ions. The most common mechanism that drives the unimolecular, metastable decay of atomic cluster ions is vibrational predissociation in which the excess energy is statistically distributed over all energetically accessible degrees of freedom. However, unimolecular dissociation may also be driven by mechanisms that involve non-statistical, localized storage of excess energy.

Using a high resolution two sector field mass spectrometer of reversed geometry (BE) we have measured in the past years metastable fractions and mass-analyzed ion kinetic energy (MIKE) peaks for metastable (spontaneous) and electron-induced decay reactions involving monomer evaporation and fission reactions of atomic and molecular cluster and fullerene ions. Both, average kinetic energy release, <KER>, data derived from the peak shapes and the time dependence of the metastable fractions show a characteristic dependence on cluster size yielding immediate information on the metastable fragmentation mechanism. Moreover, these <KER> data contain information about the transition state temperature and thus one can use finite heat bath theory to calculate the corresponding binding energies of the decaying cluster ions. The recent addition of (i) a third sector field to this two sector machine (resulting in a BE1E2 field configuration) and of (ii) a high performance electron gun has enabled us now to study in great detail the time dependence of the kinetic energy release distribution (KERD) over a relatively wide range of ion lifetimes. Moreover, using a recently developed high resolution electron/molecular beams apparatus we are also able to study the energetics/dynamics of the cluster ions produced by electron impact ionization (i.e. by comparing measured appearance energy as a function of cluster size with values calculated by *ab initio* methods)).

Results obtained recently include for instance high precision KERD measurements for the decay of rare gas dimer ions in conjunction with model calculations (using recently calculated potential energy curves for the rare gas dimer ions of Ne, Ar, Kr and Xe) allowing us to obtain information on the dynamics and the mechanisms of the underlying spontaneous decay reactions $Rg_2^{+*} \rightarrow Rg^+ + Rg$, i.e. leading to the conclusions that these metastable dissociations are not due to the well known mechanisms for small molecular ions such as electronic predissociation and/or due to tunneling, but are of the exotic type where dipole allowed spontaneous radiative decay initiates the molecular dissociations. Using this newly constructed device we are also studying currently for the first time KERDs and BEs of isotopically resolved cluster ions, e.g., of large rare gas cluster ions (an upper size limit in earlier studies arose from the fact that different naturally occurring isotopes will contribute to a chosen metastable peak when *n* exceeds a certain value, e.g. for neon above n =13) and in addition of fullerene ions smaller and larger than C_{60} (also here new insight can be gained by these high resolution measurements).

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Sa-II-3

PLASMON EXCITATIONS IN ELECTRON AND PHOTON COLLISIONS WITH METAL CLUSTERS AND FULLERENES

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This work gives a survey of physical phenomena, manifesting themselves in electron and photon collisions with atomic clusters, in which collective electron excitations (plasmon excitations) play an important role [1]. The main emphasis is made on electron scattering on fullerenes and metal clusters, however some results are general and well applicable to other types of clusters. This work is addressed to theoretical aspects of electronic and photonic collisions with atomic clusters, but relevant experimental results are also discussed.

It is demonstrated that the electron diffraction plays an important role in the formation of both elastic and inelastic electron scattering cross sections [1]. Diffraction phenomena are also found to be important in the photoionization process of fullerenes [2].

It is elucidated the essential role of the multipole surface and volume plasmon excitations in the formation of electron energy loss spectra on clusters (differential and total, above and below ionization potential) and the total inelastic scattering cross sections [1]. The inelastic scattering of fast electrons on metal clusters is treated in the range of transferred energies above the ionization threshold. It had been demonstrated that in this energy range many-electron collective excitations, namely, the volume plasmons, provide dominating contribution to the differential cross section resulting in its resonance behaviour.

Attention is paid to the elucidation of the role of the polarization interaction in low energy electron-cluster collisions [1]. This problem is considered for electron attachment to metallic clusters and the plasmon enhanced photon emission.

The multiphoton regime for multipole plasmon excitations in metal clusters is discussed. It is demonstrated that, in addition to dipole plasmon excitations, multipole plasmons (quadrupole, octupole, etc) are excited in a metallic cluster by multiphoton absorption processes, resulting in a significant difference between plasmon resonance profiles in multiphoton and single-photon absorption [3].

Mechanisms of electron excitation widths formation and relaxation of electron excitations in metal clusters and fullerenes are discussed [1].

Some attention is paid to the applicability of the jellium model for the description of metal clusters and fullerenes properties [4-6] and the cross sections of the collision processes involving atomic clusters [7].

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Sa-II-4

ATTACHING AND DETACHING METAL CLUSTER ELECTRONS

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Slow electron capture and near-threshold photoionization of free alkali-metal clusters and nanoparticles will be discussed.

In a series of experiments [1-3], we demonstrated that metal clusters are very efficient at capturing low-energy (sub-*eV*) electrons. The large capture cross sections can be quantitatively explained by the Langevin picture in which a passing electron feels long-range polarization attraction from the cluster and spirals into the center of force. The sticking coefficient of such an infalling electron is close to unity, implying that inelastic electron-metal cluster collisions offer adequate energy relaxation channels and no significant symmetry restrictions. This is different from electron-fullerene attachment whose cross section is also large due to the polarization attraction, but is much more structured [4,5]. At higher electron energies, direct impact-induced fragmentation appears to set in [6].

The observations give rise to important further questions involving the relaxation channels of the captured electrons and the associated time scales. We plan to obtain further insight by monitoring mass-resolved anions born of electron-cluster collisions; an update will be presented.

We also have investigated the photoionization behavior of nanoscale alkali particles in a beam [7,8]. Photoionization yield curves were measured as a function of temperature. Near the ionization threshold, they can be fitted very well by finite-temperature Fowler plots, originally derived for bulk surfaces. The $T \rightarrow 0$ thresholds extracted from the data precisely match the literature work function values, and the temperature shifts of the work functions are in agreement with the predictions of semi-empirical models. The accuracy of the measurement attests to the fact that the study of free nanoclusters in beams offers a very accurate complement to traditional surface spectroscopy. Further above threshold, the yield functions display maxima whose origin is unclear at the moment, but which are suggestive of inelastic scattering involving surface plasmon excitation.

Finally, we demonstrate that the aforementioned Fowler photoemission curves turn out to work well even for much smaller clusters (e.g., $K_{30\text{-}101}$ [9]). Both the ionization potentials and the internal cluster temperatures can be successfully extracted from such a fit [10]. This result raises interesting questions about the limits of applicability of bulk-derived models and highlights the need for the development of a general analytical theory of metal cluster photoionization.

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Clusters in laser fields

Sa-III-1

COLLISION AND LASER INDUCED DYNAMICS OF MOLECULES AND CLUSTERS

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Collisions and laser induced dynamics in atomic systems are investigated within the framework of the so-called Nonadiabatic Quantum Molecular Dynamics (NA-QMD) developed [1] and extended [2,3] recently. The theory treats the nuclear dynamics and electronic excitations as well as their coupling by combining time-dependent density functional theory with classical molecular dynamics. The newly developed method to combine a LCAO basis with grid basis functions [3] for the Kohn-Sham orbitals allows to treat the electrons with very different spatial extensions (core, valence and ionized electrons). The theory is applied to collisions with clusters (metal clusters, fullerenes) and the laser interaction with molecules.

In the first case, it is shown, that the excitation mechanism is basically different in metal clusters [4] and fullerenes [5]. In the second case, we present for the first time full three-dimensional calculations of molecules in a laser field [6]. Dramatic differences in the alignment between H_2^+ and H_2 were found. As an outlook we present also first calculations of collisions under the influence of a laser field with the aim to control the mechanism (e.g. the charge transfer).

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Sa-III-2

PROBING THE DYNAMICS OF IONIZATION PROCESSES IN CLUSTERS

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Phenomena associated with the electronic excitation, relaxation and ionization of clusters can span a wide range of time scales. In the case of weakly bound systems with high ionization potentials, processes in the femtosecond time scale dominate, while in the case of strongly bound clusters with low ionization potentials, delayed ionization extending to microseconds and beyond can be operative. Additionally, electron excitation in clusters arising from short laser pulses can contribute to the formation of highly charged species. Examples of each of these potentially important processes will be discussed, with attention focused on quantifying the cluster properties and laser excitation responsible for their dominance.

In particular, three classes of systems will be discussed. 1) The influence of laser fluence, wavelength, and pulse duration will be presented for the case of van der Waals clusters, showing the effects on the formation of high charge states. The possibility of using ensuing coulomb explosion as a way of arresting intermediates in fast reactions will be discussed. 2) The formation of ion-pairs and concomitant rearrangement of solvent molecules around the ions will be presented for the case of acid solvation phenomena. 3) Met-Cars, unique early transition metal-carbon clusters of composition M8C12, display both fast excitiation and relaxation dynamics and competitive delayed ionization are operative that depend on the laser excitation characteristics.

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Sa-III-3

METAL CLUSTERS IN INTENSE LASER FIELDS

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The interaction of metal clusters with intense laser light fields leads to a giant up–charging and a subsequent Coulomb explosion. Most interestingly, it has been shown that for free metal clusters the highest charge states of the ionic fragments are not produced with the shortest laser pulses (and hence the highest intensity of $1.5*10^{16}$ W/cm^2) but with pulses having a width of 600 fs to1000 fs [1,2]. This phenomenon we currently attribute to plasmon enhanced ionization.

Recently the observed charging dynamics has been reproduced using the pump-probe technique which gives a much higher time resolution and simplifies the interpretation. Applying this technique to free clusters and those which are embedded in superfluid helium droplets, yields shorter reaction times for the embedded clusters [3].

The ionization dynamics in the helium environment is more complex and additional effects can be observed: E.g., using moderate intensities (10^{12}-10^{13} W/cm^2), the transient cluster signal changes on a picosecond time scale. After passing through a minimum at 10 ps to 20 ps it recovers and reaches the initial value at about 100 ps. This might be the first real time observation of cluster reassembling which is enabled by the surrounding helium droplet.

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Sa-III-4

INTERACTION OF SMALL RARE GAS CLUSTERS WITH INTENSE LASER PULSES: THE DIFFERENCE BETWEEN eV AND keV PHOTONS

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We elucidate the mechanism of energy absorption from a short laser pulse of eV photons in small rare gas clusters [1,2] and show that it is akin to enhanced ionization first discovered in diatomic molecules [3]. Emphasis is put on the relation between energy absorption by the cluster and laser pulse length [4].

In the second part of the talk we compare the dynamics under eV photon pulses with those under keV photon pulses which will be available from the X-ray free electron laser. We investigate the same small rare gas clusters as before and find a strikingly different behavior, namely a suppressed energy absorption compared to the isolated atom to be compared to the enhanced energy absorption under eV photon pulses [5].

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Mo-I-1

LEARNING ABOUT CLUSTERS BY TEACHING LASERS TO CONTROL THEM

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Metal clusters are good model systems for investigating elementary processes of photoinduced molecular dynamics by means of femtosecond pump&probe spectroscopy. In this regard the complexity of photochemical systems is a most important parameter with regard to coherent control scenarios, in which active modes should independently be addressable from the bath. The investigation of metal clusters allows progressly to inclease the number of active and passive modes. Transient two- and multiphoton ionization spectroscopy on clusters of a selected size is a powerful tool to probe wave packet dynamics, structural reorientations, charge transfers and dissociative events in their different vibrationally excited electronic states and their ground state. When, however, the pulse shapes of the irradiated fs are changed, quite distinct processes may be observed. We employed this phenomenon to optimize individual reactive channels in fragmentative pathways of photo-excited clusters. The optimum pulse shapes, as we obtained them by means of self-learning, evolutionary algoritms, reflect well instrinsic properties of the particles involved. Future applications of the approach will be discussed.

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Mo-I-2

COOLING OF THE HOT ELECTRON GAS IN FREE SODIUM CLUSTERS

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Recently we have shown that the electron gas in a free sodium cluster can be heated by a single fs-laser pulse to temperatures high enough for thermal electron emission to occur [1]. This emission can be described by a simple model: the laser excites the collective motion of the electrons (the plasmon), which after a very short time (a few fs) decays into single electron-hole excitations. Due to the strong electron-electron interaction within a short time this nonthermal energy distribution of the electrons is transformed into a thermal one. Typical temperatures achieved with laser intensities of a few 10^9 W/cm^2 are 5000 K to 10000 K. The electron gas then cools by electron-phonon coupling, that is by energy transfer to the vibrational modes of the lattice. As the electron emission rate is a strongly nonlinear function of the electron gas temperature, it can be used to monitor this cooling process.

Time-resolved pump-probe photoelectron and photofragmentation spectra of free size selected sodium clusters Na_n^+ with n between 16 and 250 are presented. The results show the time dependence of the electron gas cooling, which allows one to determine the electron phonon coupling constant of this system.

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Mo-I-3

ATTOSECOND PHASE CONTROL OF VIBRATIONAL WAVRPACKETS IN THE HgAr vdW COMPLEX

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The wave-packet (WP) control using a pair of temporally separated, identical femtosecond (fs) laser pulses is one of the fundamental schemes of WP control [1]. The double-pulse scheme has been developed as the Ramsey interferomery or the bound-state interferometry to probe the time evolution of Rydberg WPs in atoms [2-5] and the vibrational WPs in diatomic molecules [6, 7].

I discuss here the double-pulse control to manipulate nuclear WPs created on the *A* state of HgAr van der Waals dimer [8, 9]. The first laser pulse (center wavelength 254.4 nm, time duration 300fs) induces the $(A\ ^30^+,\ v)\leftarrow(X\ ^10^+,\ v=0)$ transition and a WP is generated on the *A* state. The WP is a linear superposition of the vibrational eigenfunctions $u_v(R)$ (v=3, 4 and 5) of the *A* state and can be written as

$$\psi_A(R,t)=\sum_{v=3,4,5} a_v(t)\,u_v(R)\exp\left(-i\omega_{X,0}^{A,v}\,t\right)$$

where $\omega_{X,0}^{A,v}$ is the angular frequency for the $(A\ ^30^+,\ v)-(X\ ^10^+,\ v=0)$ transition, and a_v is a time-dependent complex coefficient. The WP follows a quasi-classical vibrational motion with a period $T_{VIB}\approx 1\text{ps}$ as shown in Fig. 1.

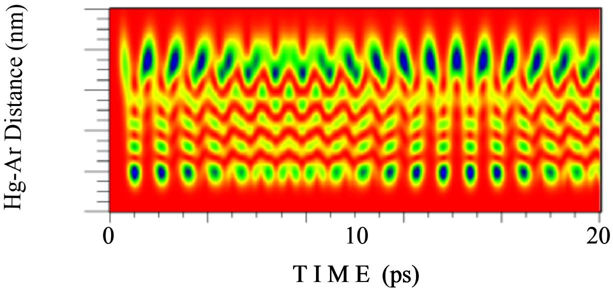

Fig. 1. Simulation of the vibrational wave-packet generated by a single shot of the 300fs-laser-pulse on the *A*-state of HgAr. The absolute square $|\psi_A(R,t)|^2$ of the wave-packet is contour-plotted.

After finishing the laser pulse, the coefficient a_v is independent of time. Within the first order perturbation approximation, a_v is proportional to product of the *A*-*X* dipole transition moment, the $(A,\ v)-(X,\ v=0)$ Franck-Condon overlap integral and the Fourier transform of the time-dependent coherent laser field [5, 7].

Two WPs generated by a pair of pulses interact constructively or destructively depending on the phase difference given by the inter-pulse-delay τ. This results in a modulation of the *A* state population as a function of the time delay τ. We have achieved 10 attoseconds (as) or higher resolution in tuning τ for the laser field with a center optical cycle $2\pi/\omega_L = 2\pi c/\lambda_L$ about 848 as and observed almost 100% fringe contrast by probing the *A* state vibrational populations [10].

The WP interaction is characterized by the laser optical cycle $T_{LASER} = 2\pi/\omega_L$ and the quasi-classical vibrational recurrence time $T_{VIB} = 2\pi/(\omega_{v+1}-\omega_v)$, $(\omega_v \equiv \omega_{X,0}^{A,v} \approx \omega_L)$. The phase difference between two adjacent levels develops by $\Delta\phi = (\omega_{v+1} - \omega_v)\tau$ in a delay time τ. If τ is set equal to an integer *n* or a half-integer (*n* + 0.5) times T_{VIB}, the phase difference develops by $\Delta\phi = 2n\pi = 0$ or $\Delta\phi = (2n+1)\pi = \pi$ in τ. The WP simulations show clear distinction of the WP space and time modes for these distinct delay times.

As long as the first order perturbation is valid, the double-pulse control can be viewed as optical interference probed by a molecular spectral filter. When the time-dependent double-pulse field with an inter-pulse delay τ is Fourier-transformed into the frequency domain, the energy spectrum (or the power spectrum) of the field forms a deeply modulated spectral profile. The modulated spectrum has several peaks within the energy-spread of the single pulse and the peaks appear with spacing $2\pi/\tau$. If τ is set equal to nT_{VIB}, then the spacing, which is equal to $(\omega_{v+1} - \omega_v)/n$, can be matched to the spacing of the optical (*A, v*)—(*X, v*=0) transition frequencies of HgAr.

Calculations of the τ dependent populations at each of the vibrational levels are shown in Fig. 2 for delay time regions (a) $\tau \approx 1.5T_{VIB}$ and (b) $\tau \approx 2T_{VIB}$. For $\tau \approx 1.5T_{VIB}$, two WPs crosses with relatively weak interaction, and the population is modulated with the phase difference by π between the states *v*=3 and *v*=4. For the delays $\tau \approx 2T_{VIB}$, two WPs overlaps well and interfere significantly each other to results in asymmetric Beutlar-Fano type profiles due to a second order effect of the laser-cluster interaction. This is a time-domain version of inter-channel interaction.

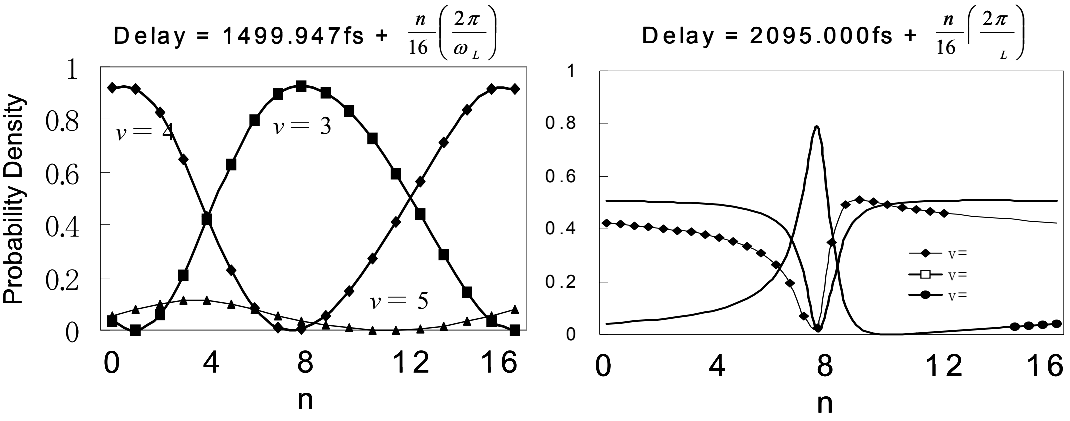

Fig. 2 Calculations of the vibrational population control by the inter-pulse-delay tuned with attoseconds accuracy. (Left): $\tau \approx 1.5T_{VIB}$, (Right): $\tau \approx 2T_{VIB}$.

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Ion-cluster collisions

Mo-II-1

COLLISION OF METAL CLUSTERS WITH SINGLE MOLECULES: ADSORPTION AND REACTION

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Low-energy collision of a metal cluster with a molecule is closely related to catalytic processes involving the molecule on the metal surface. When the molecule collides with the metal cluster ion, the molecule is weakly trapped by the metal cluster ion due to an electrostatic interaction (physisorption), and then chemisorbs and reacts. The product ions are observed experimentally. In this relation, we have investigated the collisional processes of cluster ions of Ni, Co, Pt, Cr and Cu with simple molecules (methane, ethylene, benzene, methanol, *etc.*) at the collision energies less than 1 eV, and have found that the product ions changes drastically with the cluster size.

In the collision between a metal cluster ion (Ni_n^+) and a methanol molecule (CH_3OH), demethanation ($Ni_n^+ + CH_3OH \rightarrow Ni_nO^+ + CH_4$) proceeds particularly at the size of 4, the chemisorption at the size of 6, and carbide formation ($Ni_n^+ + CH_3OH \rightarrow Ni_{n-1}C^+ + NiO + 2H_2$) at the sizes of 7 and 8. The size-specificity of the chemisorption and the reactions is related to the electronic and geometric structures of the cluster ions. In the chemisorption of CH_3OH on Ni_n^+, the cross section is anti-correlated with the HOMO-LUMO gap of Ni_n^+. This finding indicates that the formation of the chemisorption bond accompanies electron promotion from HOMO to LUMO. Similar results are obtained in the chemisorption of benzene to Ni_n^+. In the chemisorption of CH_3OH on Cu_n^+, a similar anti-correlation is obtained in general, but the concept of the HOMO-LUMO gap is not applicable in the size range around the size of 9 probably because of the structural change in this size range (see Fig. 1). It seems that the structural change reflects on the formation of different reaction products; $Cu_{n-1}^+(H)(OH)$ at the sizes of 4 and 5, Cu_nO^+ at the sizes of 6-8, and $Cu_n^+(CH_3OH)$ at the sizes larger than 9. The structure change in the vicinity of the size of 9 is explained by calculation.

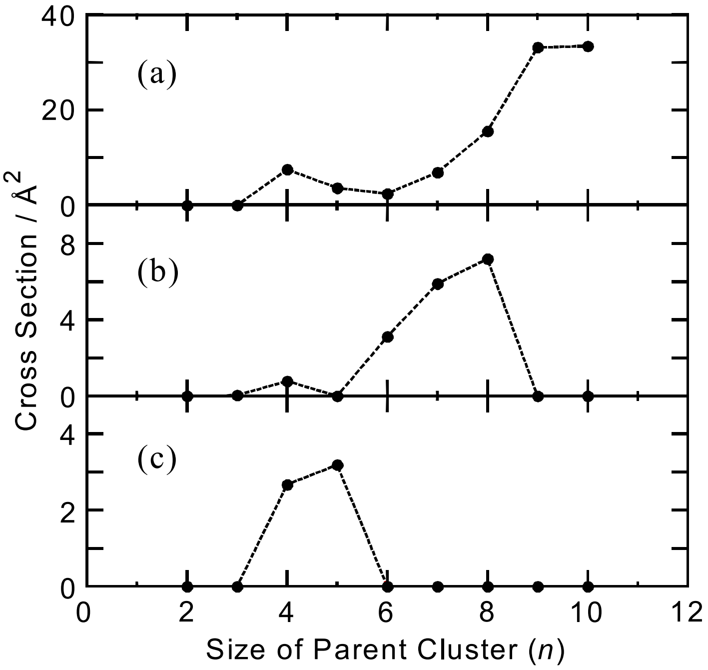

Figure 1: Cross sections for the production of $Cu_n^+(CH_3OH)$ [panel (a)], Cu_nO^+ [panel (b)] and $Cu_{n-1}^+(H)(OH)$ [panel (c)] as a function of the cluster size. The collision energy is 0.2 eV.

Mo-II-2

COLLISIONS OF HIGHLY CHARGED IONS WITH CLUSTERS OF FULLERENES

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Multiply charged clusters of fullerenes are interesting objects as different types of bindings are active. As already shown in first experiments by T.P. Martin's group [1] studying singly and doubly charged C_{60} clusters, the intermolecular binding is very weak (of Van der Waals type) compared to the strong covalent binding prevailing in individual fullerenes. It is the aim of this project to extend the investigations to higher charge states and to analyse the charge mobility in these loosely bound systems.

In the experiment neutral fullerene clusters which are produced in a gas aggregation source are (multi-) ionised in collisions with highly charged Xe-ions (Xe^{z+}, z=20-30). The reaction products (intact clusters and fragments) are studied with high-resolution time-of-flight mass spectrometry; they are detected with a multi-hit system working in an event-by-event acquisition mode.

A typical time-of-flight mass spectrum (see Figure 1) shows singly and multiply charged fullerene monomers and clusters with charges up to q=4 and containing up to ~30 fullerene molecules. The extracted appearance size increases from n=4 to n=21 when the charge increases from q=2 to q=4. The fragment distributions, the multi-stop spectra (several charged fragments are observed per event.) and the kinetic energy releases have been analysed and will be discussed in terms of the mobility of the excess charge and possible structures.

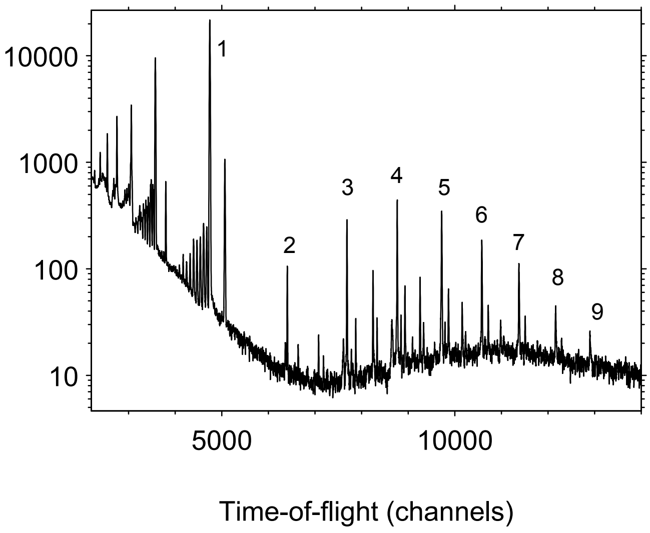

Figure 1: Time-of-flight spectrum of fullerene clusters. The numbers give the fullerenes per cluster (q=1).

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Mo-II-3

FULLERENE COLLISION AND IONISATION DYNAMICS

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Fullerenes have proven to be fascinating model systems for probing and understanding the complex dynamical behaviour of highly excited molecules and clusters. Many experimental investigations, using both collisional and photon excitation, have been carried out to probe the fragmentation and ionisation mechanisms. In this talk I will present two quite different kinds of experiments that provide information on the dynamics of highly excited fullerenes: one involves the fusion and fragmentation of fullerenes in fullerene ion - neutral fullerene collisions and the other involves ultrashort pulse (fs) multi-photon excitation, ionisation and fragmentation.

The molecular fusion reaction between two colliding fullerenes has been studied in some detail [1]. It differs from fusion of heavy ion collisions or from theoretical predictions for colliding metal clusters in some important ways. A simple intuitive line-of-centres or absorbing sphere model has been successfully applied to interpret fusion cross sections in heavy ion collisions and has also been invoked to interpret the fullerene-fullerene cross sections. However, there are three major discrepancies between the experimental fullerene fusion cross sections and the predictions of the simple model: (1) The absolute magnitude of the experimentally determined cross section is much smaller than the simple model prediction, (2) the threshold behaviour has a different energy dependence and (3) the cross section drops off significantly more rapidly than predicted at high energy. We discuss the experimental results and present a theoretical interpretation for the deviation of the experimental results from the simple line-of-centres or absorbing sphere picture. We also take a closer look at the fragmentation behaviour after fusion and compare the experimentally determined collision energy dependence of the fragmentation patterns with a simple maximum entropy model.

The energy transferred in fullerene-fullerene collisions, at the energies discussed here is predominantly vibrational. The comparison of experiment with theory suggests that this energy is rapidly thermalised and that subsequent fragmentation processes can be described in an entirely statistical manner. The situation is different with ultrashort pulse laser excitation. Here, energy is absorbed by the electrons. We have shown that the subsequent ionisation behaviour depends on the timescale: < 50 fs we see predominantly direct multiphoton ionisation; for times in the range $50<t<300$ fs we see statistical (thermal) electron emission from a hot electron bath but with vibrationally cold molecules and for $t > 300$ fs we start to see the statistical thermionic electron emission from a system with equilibrised electronic and vibrational temperatures [2]. The development of the equilibration of the molecules can be nicely followed using a combination of pump-probe techniques, mass spectrometry and photoelectron spectroscopy. The intermediate time regime has been quantitatively explained within the context of a simple statistical model, This model can not only satisfactorily predict the measured electron kinetic energy distributions but also quantitatively reproduces the charge dependence of the ion yields and is able to provide information on the absorption cross section and level densities [3]. The only genuinely free parameter in the model is the electronic-vibrational coupling time that is found to be approximately 240 fs, in agreement with recent, unpublished results from pump-probe experiments. The model can also explain the results of Penning ionisation experiments [4].

Mo-II-3

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MULTIPLE IONIZATION AND FRAGMENTATION OF C_{60} IN COLLISIONS WITH FAST IONS

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A short overview of recent experimental and theoretical results on multiple ionization and fragmentation of C_{60} in collisions with singly and multiply charged ions will be presented. Experimentally, the reaction fragments (electrons and positively charged ions) have been detected and mass analyzed using a time- and position-sensitive multi-particle detector. The projectile ions ranged from H^+ to Ar^{z+} ($z = 1$-3) with velocities of about 1 au [1,2].

The fragmentation pattern is very complicated and consists of several groups of fragments: multiply charged fullerenes, fullerene-like ions produced by successive evaporation of C_2-fragments from excited fullerene ions, and small charged fragments C_n^+ resulting from complete break-up of a fullerene cage (multi-fragmentation). The fragmentation pattern and the relative strength of the groups strongly depend on the projectile charge and collision energy. We have studied these dependencies with a special attention devoted to the multi-fragmentation process. Using a coincidence technique we have observed up to seven correlated small C_n^+ fragments. The multi-fragmentation pattern is different for fast and slow projectile ions clearly indicating different mechanisms of fragmentation.

The experimental results are compared with some theoretical calculations and estimations based mainly on the idea that ionization and fragmentation of fullerene is determined predominantly by the energy transferred by the charged projectile to the electronic degrees of freedom of the fullerene. For fast ions the statistical energy deposition model explains successfully the multiple ionization [3]. For slower collisions the velocity dependence of the multi-fragmentation agrees well with the calculations in the non-adiabatic quantum molecular dynamic model [4]. In spite of these successes, serious theoretical work is still necessary to understand the mechanism of ion-fullerene collisions and of the following processes of redistribution of energy leading to multi-fragmentation.

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Mo-II-5

CHARGE TRANSFER AND FRAGMENTATION IN ATOMIC COLLISIONS WITH METAL CLUSTERS AND THE FULLERENE C_{60}

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In the last few years we have developed and applied various theoretical tools to evaluate charge transfer, excitation and evaporation cross sections in collisions of metal clusters (neutral and positively charged) with atoms (neutral and positively charged). The collisions are studied using a molecular close coupling formalism and a postcollisional rate-equation model [1]. The method benefits from the different time scales associated with the collision and the internal motion of the cluster nuclei. The collision description includes the many-electron aspect of the problem and makes use of a realistic cluster potential obtained with density-functional theory and a spherical jellium model. The evaporation model takes into accounts the non-harmonic effects of the ionic motion and describes sequential evaporation to any order within the framework of the microcanonical statistical model of Weisskopf.

In this talk we will present results for Na_9^+ +Cs, Li_{31}^{2+} + Cs and He_2^+ + C_{60} collisions. In all cases the relative abundance of the different fragments depends critically on the cluster temperature and the spectrometer time of flight window. Good agreement with recent experimental results [2,3] has been found for alkali clusters. In addition, we have evaluated dissociation energies [4] for evaporation of carbon dimers from C_{60}^{q+} ions (q = 0,1,2) formed in single and double charge transfer reactions [5]. These dissociation energies are necessary to understand the fragmentation patterns observed experimentally.

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Mo-II-6

Cluster excitation and ionization in high velocity collisions : the atomic approach

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In medium and high velocity collisions ($v \geq 1$ a.u) between clusters and atoms, ionization and electronic excitation dominate. The treatment of these single and multiple electron processes will be presented in its simpler form, namely, in the independent atom and electron collisional model [1]. The underlying approximations will be discussed and missing effects (sharing of electrons, interferences) quantified when possible. Qualitative predictions of the model (alignment effect, sensitivity of multi-electron processes to the cluster shape) will be discussed. Confrontation to experiment for (multi)-ionization and excitation of C_n^+ clusters in medium velocity collisions with atoms will be presented.

In a second part, we will discuss electron capture and fragmentation in C_n^+->He, Ne, Ar systems ($v=2.6$ au, $n \leq 9$). Information on the energy deposited into C_n neutral clusters will be derived from measurements of non dissociative and dissociative branching ratios [2] and application of statistical theories [3].

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Mo-II-7

ELECTRON AND ION IMPACT ON FULLERENE IONS

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Fullerenes have been the subject of intense research within the last decade. The interaction of these molecules with various projectiles, e.g. photons, electrons, ions and atoms, has been investigated extensively. In general, **neutral** fullerenes have been used as targets.

Employing the crossed-beams technique [1], [2], we have studied the interaction of electrons and ions, respectively, with fullerene **ions**.

For electron impact on the positively-charged fullerene ions C_{60}^{q+} (q = 1,2,3), we have measured the cross sections for single ionization as well as for C_2 fragmentation at electron energies up to 1000 eV. The ionization cross sections show some unusual features in shape and charge state dependence. The cross sections for the loss of a C_2 fragment indicate the presence of two different mechanisms.

For electron impact on the negatively-charged fullerene ions C_m^- (m = 60,70,84), the cross sections for multiple ionization and fragmentation into product ions C_{m-n}^{q+} (q = 1,2,3 and n = 0,2,4) have been measured. The data indicate that different mechanisms account for the detachment of the extra electron from the negatively-charged fullerene and the formation of a positively-charged ion, respectively.

In the first ever ion-ion crossed-beams experiments involving fullerene ions, we have studied electron transfer in the systems $He^{2+} + C_{60}^+$ and $C_{60}^{2+} + C_{60}^+$, respectively, at keV- collision energies. The experimental data are compared to very recent theoretical cross section calculations.

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Clusters on Surface

Mo-III-1

SOFT-LANDING OF VANADIUM-BENZENE SANDWICH CLUSTERS ONTO SELF-ASSEMBLED MONOLAYER (SAM)

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Vanadium (V) – benzene cluster ions, produced by laser vaporization with reaction toward benzene vapor, were size-selected and deposited onto self-assembled monolayer (SAM) with deposition energy of 20eV. Infrared (IR) spectra of $V_n(\text{benzene})_{n+1}$ (n=1 and 2) on SAM were measured at a substrate temperature of about 20 K. The spectrum of $V_1(\text{benzene})_2$ was in agreement with both the reported spectrum and the theoretical calculation, showing that $V_1(\text{benzene})_2$ forming a sandwich structure was soft-landed onto SAM without fragmentation. IR spectrum of $V_2(\text{benzene})_3$ shows that $V_2(\text{benzene})_3$, prepared in gas phase reaction, forms double-decker sandwich structure and was soft-landed successfully on/in SAM. These results show that SAM can be used as a useful shock absorber (buffer) in soft-landing experiment.

From IR spectrum of soft-landed $V_1(\text{benzene})_2$, temperature programmed desorption (TPD) spectrum of it, x-ray photoelectron (XP) spectrum of SAM substrate and atomic force microscope (AFM) image of it, it was expected that the $V_1(\text{benzene})_2$ clusters migrate on/in SAM at a substrate temperature of about 250K. This migration leads to dissociation of soft-landed clusters, resulting that V nanoclusters are produced on/in SAM.

Mo-III-2

COLLISIONS OF ELECTRONS AND PHOTONS WITH SUPPORTED ATOMS, SUPPORTED CLUSTERS AND SOLIDS: TRANSFORMATION OF ELECTRONIC PROPERTIES

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Photoionization, electron scattering and excitation of supported atoms, supported clusters and solids have been studied to clarify the question: how the electronic properties of matter are formed as isolated atoms join into clusters and as the clusters are transformed into solids? A complex of electron spectroscopy methods - XPS/AES, e-AES and EELS has been applied to the study. The transition “supported atom - supported cluster - solid” has been studied for silver and copper supported by an quasi-inert substrates (graphite, Si), for copper and arsenic in dielectric matrixes (SiO_2 , GaAs). As a result of the study, the way of definition of average number of atoms in supported clusters has been suggested. “Know how” to grow quasiisolated supported clusters with definite average number of atoms and with low size- dispersion has been accumulated. Regularities of transformation of electronic properties of matter in the transition “supported atom - supported cluster - solid” have been established [1]. It was revealed for clusters supported by surfaces that the electron binding energies drastically decrease due to promotion of quasimolecular orbitals at the beginning of the cluster formation. Then, electron structure of matter is mainly transformed due to increasing extra-atomic relaxation energy at the next stages of cluster growth. The increase of the relaxation energy is the main reason for shifts of pfotoelectron and Auger lines at these stages. Enormous pfotoelectron and Auger line-shifts have been revealed in the transition "supported atom - supported cluster" in bulk matrix. It has been shown that electron core levels drastically go down in this transition contrary to the case of supporting surface. This effect has been explained by the compression of valence orbitals. Evidence has been obtained that the electron structure of supported clusters is characterized by the shell structure. This structure manifests itself as stepwise peculiarities in the dependences of relaxation energy and Auger-lines on cluster size. Fig.1 shows that the positions of the steps coincide with the magic numbers. The conclusion has been made that the shell electron structure of supported flat clusters is formed according to the same regularities as that of the spherical free ones. Effect of nonmonotonous variation of spin-orbital interaction in varying cluster size has been revealed which can be qualitatively explained by the variation cluster-surface interaction (polarization). The local surface plasmon generation in supported clusters consisting of only a few atoms has been revealed. The size related "red" shift of cluster plasmon energy due to excitation of low energy modes was also revealed. The general conclusion was made that electron energy structure of supported clusters with diameters of more than 10 A is very close to that of the bulk.

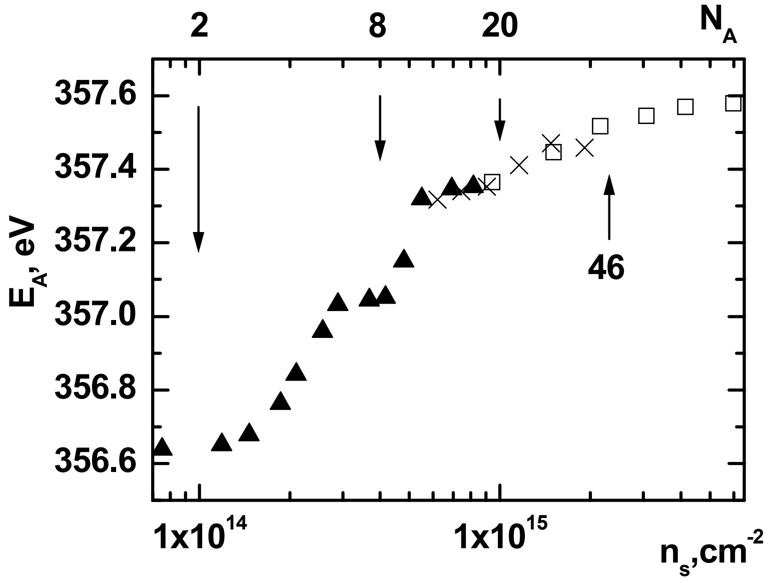

Fig.1: The dependence of Ag $M_{4,5}V^2$ Auger electron energy on the average number of atoms in silver clusters supported by graphite surface. The positions of "magic" numbers are indicated by arrows.

Transition “cluster – solid” has been studied for fullerenes C_{60} when these carbon clusters condense into van der Waals crystal and when condensed fullerenes decay under electron or synchrotron radiation and are transformed into amorphous carbon. The conclusion has been made that electron properties of aggregated fullerenes are practically the same as that of free fullerenes because fullerene molecules in such an aggregated state are weakly bound by van der Waals couplings. The transformation of fullerenes into amorphous carbon is accompanied by the decrease of electron binding energies and radical increase of the relaxation energy as in the case of metal clusters. The research was partly supported by INTAS grant № 2136, and NWO grant № 047.009.012.

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Mo-III-3

PHYSICAL AND CHEMICAL PROPERTIES OF SIZE-SELECTED CLUSTERS LANDED ON SOLID SURFACE BY CLUSTER IMPACT

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The fundamental properties of a cluster deposited on a solid surface depend critically on the cluster size, the site at which the cluster resides, etc. [1]. In order to elucidate the properties, it is necessary to observe it as a single cluster level. In this relation, we deposited metal clusters on a surface of a single crystal and observed the individual metal clusters by means of a scanning-tunneling microscope (STM) and scanning-tunneling spectroscopy (STS). In this paper, we particularly reported a study on a single platinum cluster on a silicon (111) 7x7 surface, by landing size-selected cluster-ions on the surface.

The apparatus consists of a cluster-ion source, a quadrupole mass-filter, a landing stage and an STM [2]. Platinum cluster ions with the size range of 1-45 were produced in a magnetron sputtering-source [3], size-selected in the mass filter, and allowed to collide onto a Si(111) 7x7 surface maintained at the temperature of 300 K at a collision energy, E_{col}, of 0.5-3 eV per platinum atom. A typical electric current of $(\mathrm{Pt})_{10}^{+}$ was 1 nA. The clusters deposited on the surface were observed by the STM at a pressure less than $5\mathrm{x}10^{-9}$ Pa and at the temperature of 77 or 300 K.

Figure 1 shows a typical STM image of $(\mathrm{Pt})_5$ deposited at E_{col}=3 eV, which was obtained by scanning with a tungsten tip in a constant current mode (topographic image) at a bias voltage, V_{s}, of -2.00 V, the tunneling current, I, of 500 pA and at the temperature of 300 K. An atomically resolved STM image of the silicon surface is observed, although the image of the clusters is not atomically resolved. The STM image shows that the clusters are dispersed homogeneously and are not influenced by repeating STM scans. Figure 2 shows the apparent-height profile of $(\mathrm{Pt})_5$ along the solid line indicated in Figure 1; the height is calibrated against the known step height of the silicon surface. The wide peak superimposed on the corrugated profile (attributed to silicon atoms) originates from $(\mathrm{Pt})_5$. The cluster has the apparent diameter and the height of 4.5 and 0.8 nm, respectively. Figure 3 shows STS spectra measured on $(\mathrm{Pt})_{35}$ and $(\mathrm{Pt})_{20}$ at the temperature of 77 K. Peaks are discernible at V_{s}=1.2 and 1.4 eV for $(\mathrm{Pt})_{35}$ and $(\mathrm{Pt})_{20}$, respectively.

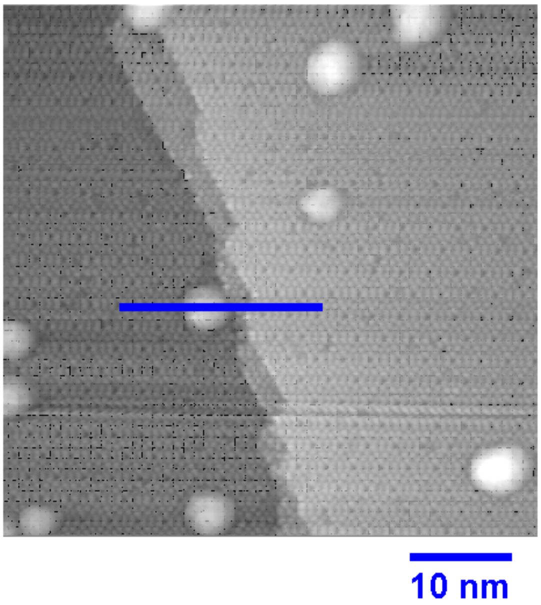

Figure 1: STM image of $(\mathrm{Pt})_5$ deposited on a silicon (111) 7x7 surface at the collision energy of 3 eV per platinum atom. Along the solid line shown in the image, a height profile was measured (see Figure 2).

The clusters are not movable on the surface because they are not collected to the step sites, and stick so firmly to the surface that they do not move by the repeating STM scans. It is likely that

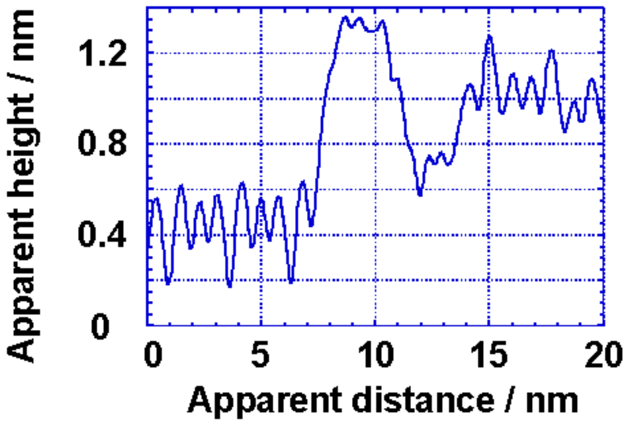

Figure 2: Apparent-height profile of $(Pt)_5$ deposited on a silicon (111) 7x7 surface along a line indicated in Figure 1.

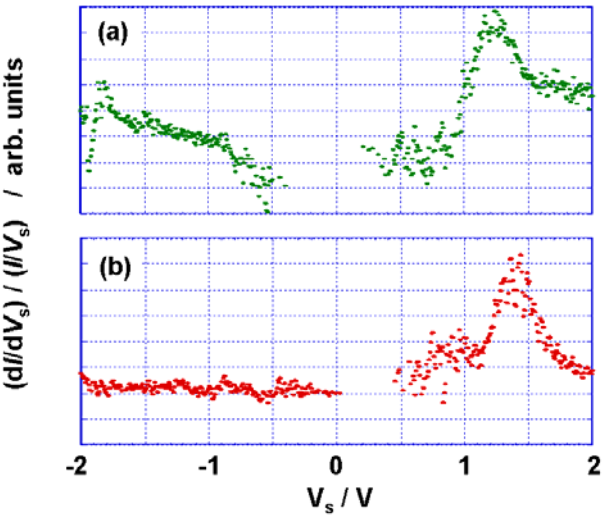

Figure 3: Scanning-tunneling spectra for $(Pt)_{35}$ (panel a) and $(Pt)_{20}$ (panel b) on a Si(111) 7x7 surface at a temperature of 77 K. The differential signal, $(dI/dV_s)/(I/V_s)$, of the tunneling current, I, is shown as a function of the bias voltage, V_s. The clusters were deposited at the collision energy of 0.5 eV per platinum atom.

the cluster-impact heating [4] causes the cluster to form chemical bonds between the clusters and the surface. Seemingly, the clusters are neither dissociated nor aggregated on the surface, because the number density of the clusters on the surface measured by the STM is comparable to that calculated from the total charge of the cluster ions arriving at the surface. The apparent diameters of $(Pt)_5$ are ranged from 3 to 5 nm. The values are much larger than that of $(Pt)_5$ in the gas phase (~0.5 nm) because of a finite radius of the STM tip and a finite tunneling distance. The real diameter of $(Pt)_5$ on the surface turns out to be 1-2 nm by taking the above-mentioned factors into consideration. The clusters are deposited intact on the surface in the entire E_{col} range studied because the height profile did not change with E_{col}. Electronically excited states of the cluster located at an energy of 1.2-1.4 eV contribute to the peak observed in each STS spectrum.

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Mo-III-4

EVOLUTION AND STABILITY OF NANO STRURES OF SILVER OBTAINED BY SOFT LANDING OF CLUSTERS ON GRAPHITE (OOOI) SURFACE

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Low impact energies avoid the destruction of clusters during the deposition on graphite surface,hence the clusters diffuse and aggregate In previous studies we have shown how the morphology of the resulting nanostructures can be controlled by the size of the impinging clusters and the defects of the surface (1).In contrast of previous experiments which investigated the pure metal or semiconductor clusters deposition ,we have performed experiment in which the islands are grown by preformed cluster deposition carrying oxygen/hydroxide molecules by introducing oxygene and water in the cluster nucleation region.

The dynamics of the cluster diffusion as well as the relaxation of non-equilibrium island morphology resulting from cluster deposition, strongly depends on the cluster chemical composition.

Few oxide/hydroxide molecules in some incidentt silver clusters used to grow island on the graphite surface,does not change the cluster diffusion on graphite but considerably enhances the surface-self-diffusion of silver atoms on the surface of silver island. Even if the mechanism is not still undrestood we can deduce from such a result that incorporating of atomic oxygen in silver particle increases their coarsening and may decrease their melting temperature.(2)

By contrast, the complete oxydation or hydroxylation of the deposited clusters slow down their mobility giving rise to a dense nano-phase of particles agglomerated in chain -like structures.

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Posters

PS-01

DIFFRACTION OF SLOW PHOTOELECTRONS BY C_{60} CAGE

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Within the approximation of representing the potential of the C_{60} molecule as a cluster of non-overlapping atomic potentials [1], the phenomenon of the diffraction of slow electrons emitted in the process of the near-threshold 1*s* photoionization of the Li atom located far from the C_{60} cage has been considered.

The evolution of the shape of the photoelectron angular distribution has been studied as a function of the distance of the Li atom from the C_{60}. It is found that, as in the case of the atom located inside the C_{60}, the photoelectron angular distribution is significantly distorted (as compared with a free atom) by the process of electron scattering by the carbon atoms forming the C_{60} cage. This distortion is especially pronounced when the polarization vector of the radiation is directed along the line connecting the nucleus of the ionized atom with the geometrical center of the cage. In this case, the photoelectrons emitted mainly into a solid angle directed to the C_{60} molecule, and multiply re-scattered by the carbon atoms, generate a diffraction pattern with a well-defined geometrical shadow created by the C_{60} fullerene. The diffraction effects in the photoelectron angular distribution proved to be observable even for distances of the order of ~200 atomic units between the nucleus of the ionized Li atom and the center of the cage. Since there is nothing particularly special about Li 1*s* with respect to photoionization, the diffraction effects presented here should be qualitatively typical for virtually all *ns*-photoionization spectra of any atom located far from C_{60} fullerene cage.

This work was supported by the US Civilian Research & Development Foundation for Independent States of the Former Soviet Union (CRDF), award No ZP1-2449-TA-02, NASA and NSF. The visit of A. S. B. to CTSPS at the Clark Atlanta University was supported by NSF.

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PS-02

MICROSCOPIC STUDY OF SODIUM CLUSTER DEPOSITION ON AN INSULATING SURFACE

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We present the microscopic calculations of the low-energy deposition of small sodium clusters on NaCl surface. The time evolution of the cluster electronic system is described using the Time-Dependent Local Density Approximation (TDLDA). We discuss the deposition mechanism for different initial cluster velocities and orientations relative the surface and demonstrate that extremely low velocities are necessary to ensure a cluster deposition without damaging the original cluster. The real-time motion of the electronic system was described using the TDLDA method in full three-dimensional coordinate-space grid, while the ionic motion of the cluster core was treated within the methods of molecular dynamics (MD). Taking into account that the NaCl substrate is only very little affected by the attached cluster [1] and remains essentially inert, the cluster-surface interaction was described using an effective interface potential [2-3] both for ionic and electronic cluster subsystems. The real-time deposition process was numerically simulated for the case of the small neutral Na_6 cluster that tends to have a stable ground-state deposited isomer with axial symmetry [2].

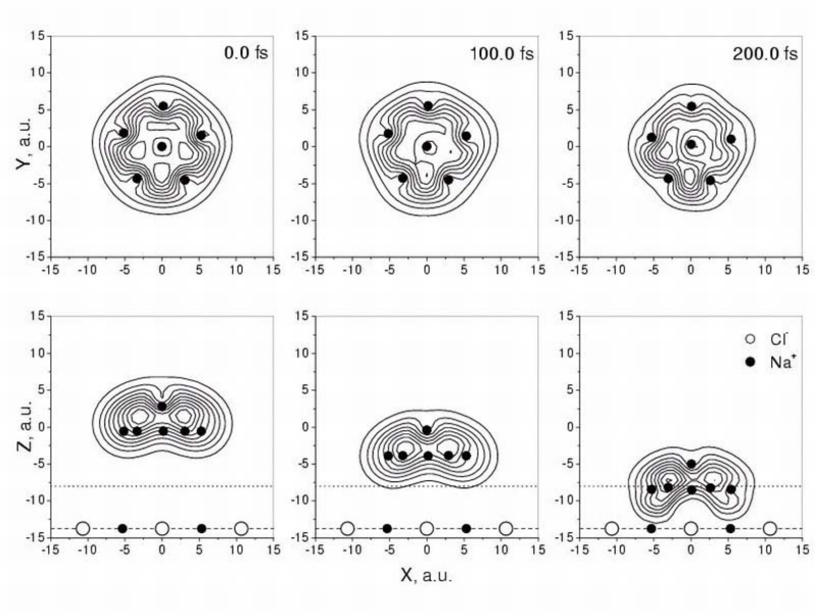

Figure.1 : Electronic charge density and ionic positions during the cluster deposition with initial kinetic energy of 6.9 eV

In Fig.1 we represent the snapshots of the electronic charge density and ionic positions in different time of the cluster deposition with initial kinetic energy of 6.9 eV. The collision leads to the significant cluster deformation, and, as a result, to the transfer of the cluster kinetic energy to its internal degrees of freedom.

PS-02

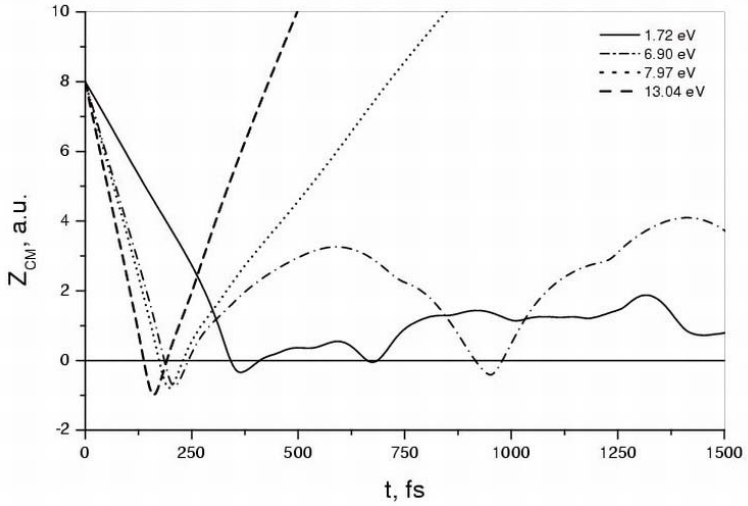

Figure 2: Time evolution of the cluster CM during the deposition.

Fig.2 represents the time evolution of the cluster center of mass (CM) during the deposition with various initial velocities. One can see that there is the deposition energy threshold (i.e. the maximal initial kinetic energy of the cluster that can be attached to the surface), that for the considered Na_6 cluster is about 6.9 eV. For the initial kinetic energies below this value we observe the cluster attachment to the substrate, accompanied by its oscillations in the effective potential well of the surface potential [3]. The detailed study of the deposition process has shown that the deposition threshold is sensitive to the initial cluster orientation with respect to the surface as well as whether the deposition occurs over Cl^- or Na^+ site of the substrate lattice, as far as the kinetic energy loss of the projectile and, as a result, its post-collision behavior depends on the collision conditions. Deposition with kinetic energy above the attachment threshold results in inelastic reflection of the cluster, that leads to its fragmentation due to the excitation of internal ionic degrees of freedom.

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PS-03

SPECTROSCOPIC PROPERTIES OF SODIUM CLUSTERS EMBEDDED IN INSULATING MATRIX

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We present the microscopic study of the optical properties of small sodium clusters embedded into the noble-gas (Ar) matrix. The electronic system of the cluster is described using the Time-Dependent Local Density Approximation (TDLDA) methods. The ionic motion of the cluster core both with the oscillations of the polarizable Ar crystal lattice was treated within the methods of the molecular dynamics (MD). In the real-time numerical simulations of the cluster@matrix optical response the matrix polarization effects [1] were taken into account, in particular the dipole-dipole and the Van-der-Waals interactions.

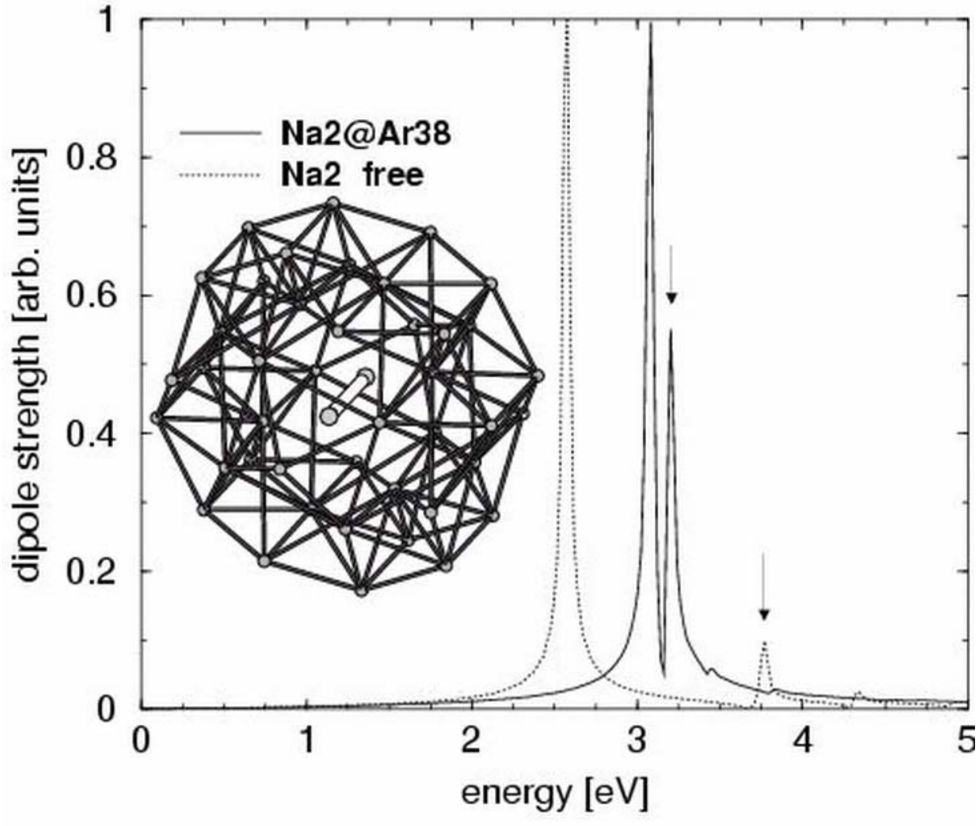

Figure 1: Optimized structure of a matrix-isolated $Na_2@Ar_{38}$ cluster and optical spectra of the embedded system and corresponding free Na_2 dimer.

In Fig.1 we represent the optimized ground state structure of a $Na_2@Ar_{38}$ cluster in a substitutional site of a fcc (face-centered-cubic) Ar lattice containing 38 atoms. The optical spectra, represented in the right-hand side of Fig.1, are calculated both for the free Na_2 dimer and for the case of the $Na_2@Ar_{38}$ system. One can see the significant blueshift and splitting of the dominating peak in the spectrum. The line shift results from the short-range effective repulsive "pressure" of the closest Ar atoms on the embedded cluster, while its interaction with the outer matrix atoms has mainly the more long-range dipole-dipole character and contributes as an extra redshift.

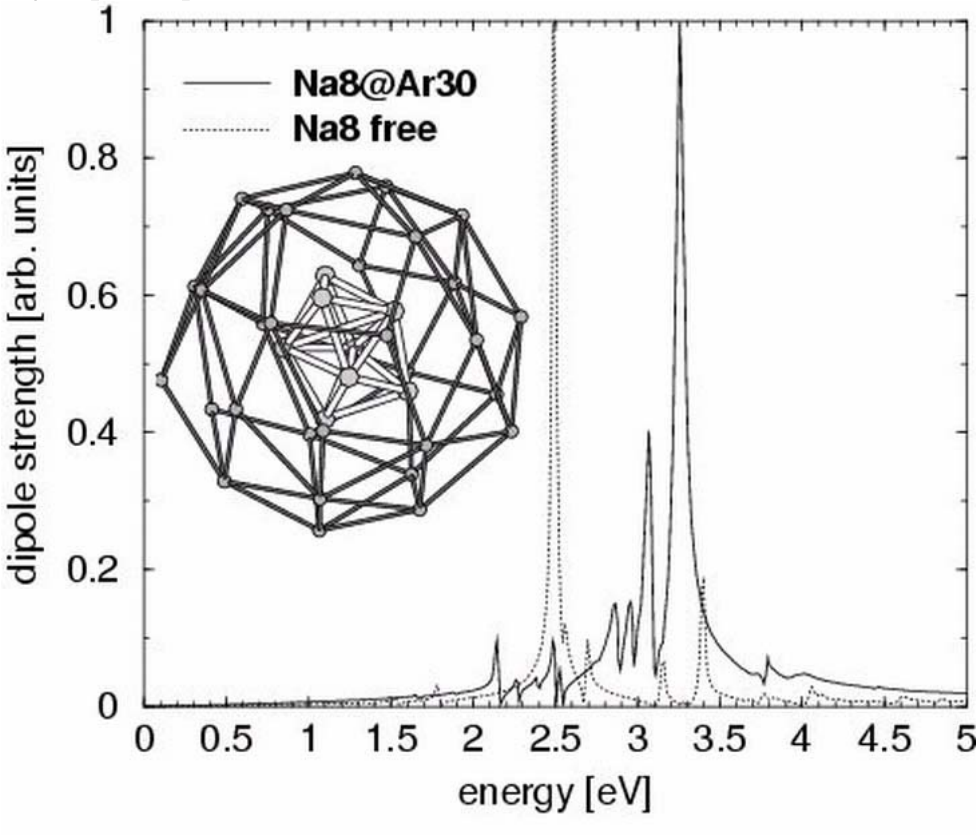

Figure 2 : Optimized structure of a matrix-isolated $Na_8@Ar_{38}$ cluster and optical spectra of the embedded system and corresponding free Na_8 cluster.

In Fig.2 we represent the similar results of the calculations performed for a $Na_8@Ar_{30}$ cluster embedded in the Ar lattice containing 30 atoms. In comparison with Na_2 case we see the growth of the dominant peak linewidth with its attendant fragmentation.

The obtained results are important for a better understanding the physical properties of matrix-isolated atoms and clusters. The model used is suitable to be extended to the larger systems.

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PS-04

Ionization of Metallic Clusters via Double Plasmon Excitation

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We present a theoretical study of ionization of sodium clusters by an intense laser pulse with a photon energy close to the surface plasmon resonance. The proposed model describes the resonance channel of cluster ionization via excitation of a double-plasmon collective electron state that can subsequently decay through a single electron emission. The method of separation of center of mass (CM) coordinate from other electronic degrees of freedom [1] has been employed to take into account the highly excited electronic states. Autoionization decay rate of the two-plasmon excited state together with energy and angular distributions of outgoing electrons has been obtained.

In resent years the rapid development of the laser technologies has leaded to new experimental [2, 3] and theoretical [4, 5] studies of clusters in a strong laser field. It was shown that small clusters irradiated by intense laser pulses exhibit the new features that cannot be described in the traditional framework of the Linear Response Theory. In particular, it became possible to clarify whether the multiplasmon states can be excited. Usually the energy of one plasmon state is lower than the cluster ionization energy, while the two- and higher multi-plasmon levels lie above the ionization threshold and therefore can undergo the ionization decay. That is why one can expect the manifestation of the multi-plasmon states in the cluster ionization [2, 5]. Besides the resonance ionization, there is also the contribution of numerous non-resonant mechanisms that can be adequately described within the thermal emission model [3]. The main goal of our study is to find out under what conditions the resonant mechanism can compete with thermal emission and, therefore, the manifestation of the double-plasmon state can be experimentally observed.

Our study is based on the selfconsistent treatment of the multiplasmon states [1]. For this purpose we separate intrinsic and CM motions of cluster valence electrons. Using the smallness of the CM oscillation amplitude in comparison with the cluster radius we can represent the Hamiltonian of the cluster electrons as a sum of the Hamiltonians of the CM, $\mathcal{H}$, and the intrinsic ,H', motions and the coupling term, W:

$$H = H' + \mathcal{H} + W$$

Hamiltonian $\mathcal{H}$ describes the collective plasmon oscil-
lations of the cluster electrons, while Hamiltonian H' describes the intrinsic excitations. The coupling term is responsible for the damping of collective oscillations via numerous intrinsic excitations including the cluster ionization.

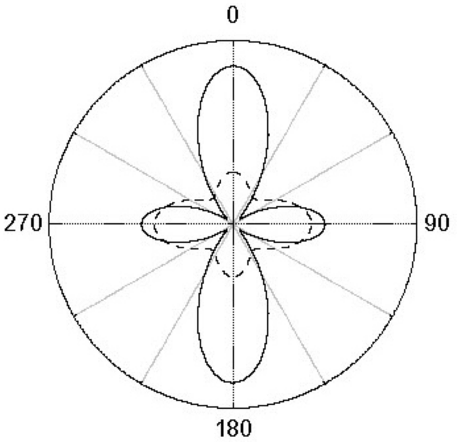

Fig. 1. Angular distribution of electron emission resulting from the decay of the double plasmon state in Na_{41}^{+} (solid line) and Na_{93}^{+} (dashed line) clusters.

We consider the ionization in the plasmon resonance region as a multistep non-linear process, in which the photons are initially absorbed to excite the plasmon oscillations, and then the double- and higher multiplasmon states decay via electron emission. The emission rate for the

PS-04

double plasmon state, i.e. the corresponding autoionization width, has been calculated using the time-dependent perturbation theory:

$$\Gamma_i = 2\pi \sum_h \int |A_h(\mathbf{p_e})| \, \delta\left(\frac{p_e^2}{2m} - I_h - 2\omega_p\right) \frac{d\mathbf{p_e}}{(2\pi)^3},$$

where $A_h(\mathbf{p_e})$ is the ionization amplitude calculated using the wave functions of the CM and the intrinsic electronic motions and the coupling interaction W, $\mathbf{p_e}$ is the momentum of the ejected electron, index h designates the quantum numbers of the ionized valence shell, I_h is the corresponding ionization potential, ω_p is the surface plasmon resonance energy.

We have calculated the double plasmon autoionization width for the Na_{41}^{+} and the Na_{93}^{+} cluster ions and obtained $\Gamma_i = 18meV$ and $\Gamma_i = 19meV$, respectively. In Fig.1 we show the angular distribution of electron emission resulting from the decay of double-plasmon state in these clusters. As far as thermal emission is isotropic, the angular dependence of the electron emission would be the evidence of two-plasmon excitation.

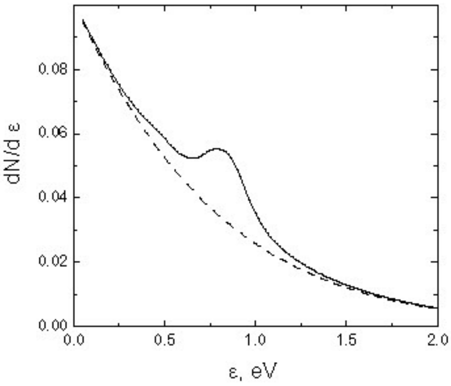

Fig. 2. Energy spectrum of electron emission of Na_{93}^{+} cluster under the laser pulse with intensity $I = 0.22mJ/cm^2$, length $\tau = 235fs$ and frequency $\omega = 2.84eV$. Solid line corresponds to the total ionization spectrum while dashed line shows the non resonance background.

In order to calculate the energy spectrum of the electron emission we replace the delta-function by the Lorentzian profile with the total plasmon resonance width $\Gamma = 0.25eV$ [1]. In Fig.2 we present the emission spectrum containing both the resonance and the thermal emission contributions. For the considered parameters of the laser pulse, the double-plasmon state manifests itself in energy and angular distributions of electron emission. For different laser frequencies, ω, intensities, I, and pulse lengths, τ, the resonant contribution to the cluster ionization significantly changes comparing to the thermal emission. So the contribution of the resonance mechanism might be noticeable only in the plasmon resonance region $\omega_p \pm \Gamma/2$. The dependence of the electron emission on I is also different for the resonant and the thermal emission mechanisms. It is proportional to I^2 for two-plasmon mechanism and has exponential dependence for thermo-ionization. Therefore the high laser intensities are favorable for the latter mechanism. In our work we determine the conditions under that the double-plasmon excitation can be experimentally observed in the cluster ionization irradiated by an intense laser pulse.

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PS-05

Theory of Resonant Photoabsorption of Metallic Cluster in a Strong Laser Field

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We introduce a new approach to describe the resonance photoabsorption of metal clusters in strong laser fields. Our method is based on the separation of the center of mass (CM) and the intrinsic motion of delocalized valence electrons [1]. This allows us to calculate the excitation spectrum of sodium clusters beyond the standard linear response theory, including highly excited states with more than one plasmon. The degree of anharmonicity of dipole plasmon excitations can thus be examined.

In the present theory we separate the collective plasmon mode, that corresponds to a coherent oscillation of the electrons against the ionic background, from all other electronic excitations. Using the smallness of the CM oscillation amplitude we write the Hamiltonian of the delocalized electrons as a sum of a Hamiltonian for the CM motion, $\mathcal{H}$, a Hamiltonian of intrinsic motion, H', and a coupling term, W:

$$H = H' + \mathcal{H} + W.$$

The interaction W is of primary importance for the photoabsorption spectrum. It is responsible of the red shift of the plasmon resonance from the Mie frequency, to a large extent. The additive contribution arising from the spill out effect remains minor. For example, in the case of the Na_{41}^{+} cluster the spill out effect contributes to a $0.2eV$ shift whereas the total red shift is of about $0.7eV$.

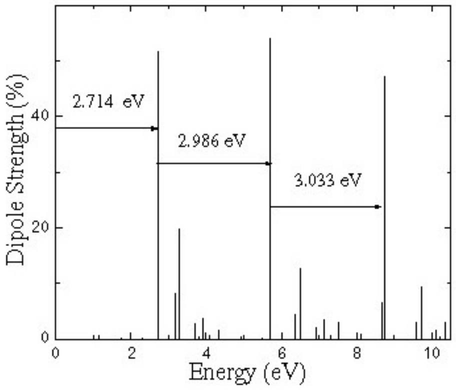

Fig. 1. Excitation energy spectrum including one, two and three plasmon states for Na_{93}^{+} cluster. The height of any line measures its strength as the fraction of pure plasmon excitation

In the linear regime of photoabsorption where only one electron-hole pair can be excited at a moment of time the excitation spectrum calculated within our approach coincides with the results of standard linear response theory. The present theory in the linear regime provides a clear understanding of the plasmon resonance frequency: the red shift results from the repulsion interaction between the collective mode and intrinsic electronic excitations.

An important advantage of this new method is that it allows one to go beyond the linear response. In Fig. 1 we present the excitation spectrum containing the simultaneous excitation of several plasmons in the Na_{41}^{+} cluster. The excited states are grouped according to the number of excited plasmons, n. The most important optical dipole transitions that occur within the sequence of multi-plasmon states are shown by arrows. The corresponding transition energies, i.e. the plasmon frequencies $\omega_n$indicated. Anharmonic effects are readily evidenced by the increase of the plasmon frequency with the number of plasmons. The anharmonic blue shift results from the coupling interaction W.

The predicted non linear blue shift, $\omega_2 - \omega_1 = 0.27eV$, is much smaller than the plasmon frequency $2.7eV$. However it could be observed in a photoabsorption study since it is of the order of the resonance width $\Gamma \simeq 0.25eV$. In Fig. 2 we show the photabsorption spectra of Na_{41}^+ cluster calculated for different intensities of laser field. We find that linear effects are prominent for laser intensities larger than $2 \cdot 10^9 W/cm^2$. As the laser intensity increases, the photoabsorbtion spectrum shifts towards larger energies, as a result of the blue shift of multiplasmon states. Another non-linear effect is the decrease of the maximum photoabsorption with increasing laser intensity. The anharmonic frequency shift breaks the resonance condition and therefore reduces the photoabsorption which proceeds through the sequence of multiplasmon transitions.

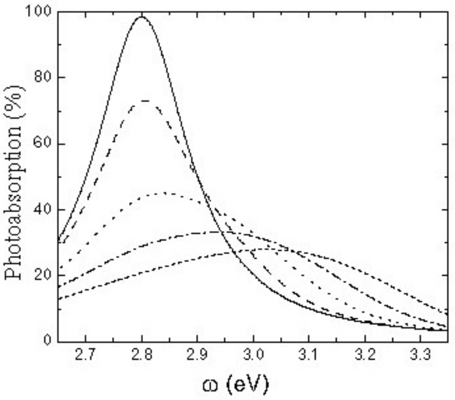

Fig. 2. Photoabsorption spectra of Na_{41}^+ cluster calculated for different intensities of laser field $I = 2 \cdot 10^8, 2 \cdot 10^9, 2 \cdot 10^{10}, 4.5 \cdot 10^{10}, 8 \cdot 10^{10} W/cm^2$ is shown by solid, dashed, dotted, dash-dotted and short dashed lines respectively. The photoabsorption cross section is normalized to maximum of photoabsorption in the linear regime

The present approach can be also applied to study the relaxation of plasmon excitations. The coupling between the plasmon mode and the intrinsic excitations leads to its damping. Our method provides a self-consistent description of the coupling interaction and it can be extended to other damping processes such as electron-phonon interactions [2]

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PS-06

FRAGMENTATION OF RARE GAS CLUSTERS BY ELECTRON IMPACT

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Cluster physics has been developing over several decades now, with rare gas clusters still a fertile area of study. Rare gas clusters provide a firm platform for fundamental investigations, with most studies involving ionization. Applications of rare gas cluster science are also being pursued with possible applications that range from relatively inert, large surface area (per volume) mediums for chemical reactions, to novel light sources. Our group has investigated VUV photon and neutral metastable production from xenon [1], krypton [2], and argon [3,4] clusters using time-of-flight, fragment kinetic energy, photon analysis, and excitation function techniques.

Clusters are supersonically generated using a room-temperature piezo-electric pulsed valve, with a conical nozzle, normally operating at a stagnation pressure of 3.5 atm, a pulse width of 150 μs, and a repetition rate of 65 Hz. A skimmer, with a diameter of 1mm, separates two differentially pumped regions: the expansion and collision chambers. After skimming, the cluster beam enters the collision chamber and is impacted at right angles by an electron pulse (normally 1.6 μs in width).

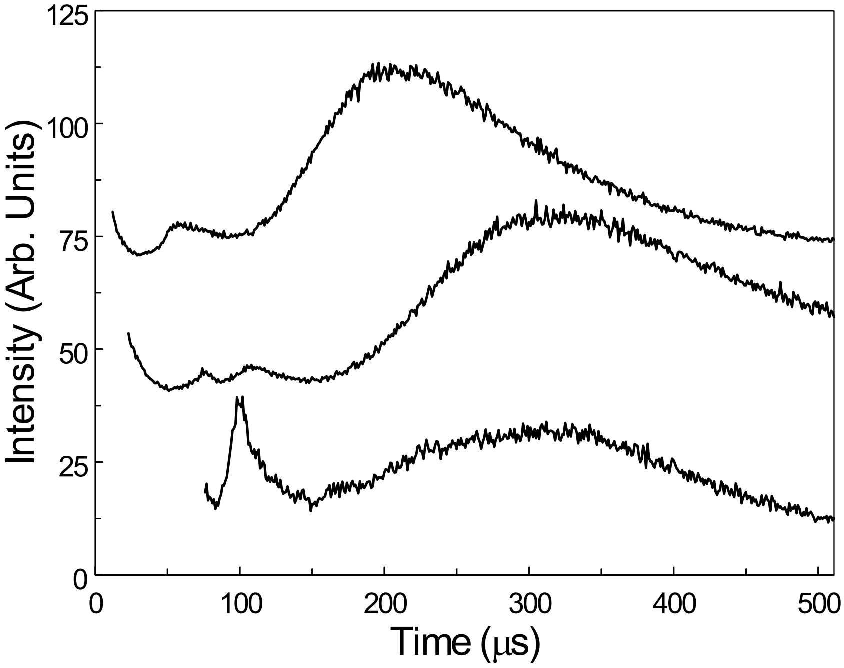

Figure 1: Time-of-flight data for rare gas clusters impacted by 20 eV electrons. The curves are for Xe (bottom), Kr (middle), and Ar (top) clusters. The curves are not normalized and the Ar and Kr data have been shifted upwards for clarity of presentation.

The degree of clustering is probed via an in-line time-of-flight Wiley-McLaren-type mass spectrometer. If necessary, the system could be operated under conditions where negligible clustering occurred. VUV photons or neutral metastable fragments from the collision region were detected with a CsI-coated channel electron multiplier, as shown in [4]. Suitably biased grids were used to exclude charged particles from the detector. The photon and metastable fragment signals were collected at the detector as a function of time. Fragment kinetic energy analysis could be performed on the time-of-flight (TOF) data. Excitation functions were obtained by integrating over a particular time window of the TOF data, corresponding to photons or metastable fragments, and ramping the electron energy. The wavelength range of the VUV photon fluorescence signal could be varied by the use of optical filters placed in front of the channel electron multiplier detector. The particular optical filter provided a lower wavelength cut-off, while the CsI-coating had an upper wavelength cut-off in sensitivity at about 180 nm. A time-to-amplitude converter was used with a multichannel analyzer operating in the pulse height analysis mode to collect the VUV fluorescence, with subsequent lifetime analysis. The energy scale was calibrated using the atomic rare gas singly charged positive ion (i.e., Ar^+, Kr^+, or Xe^+).

Figure 1 shows the collected signal as a function of time for Ar, Kr, and Xe cluster fragmentation by electron-impact. The electron impact energy was 20 eV for all three cases and the nominal start of the electron pulse was at zero time. For convenience of presentation, the photon fluorescence, which coincides in time with the electron beam pulse, has been suppressed. There is a thermal contribution at the longest displayed flight times for each curve. The peaks, seen at intermediate flight times, are due to metastable, neutral, atomic fragments from cluster break-up. The metastable fragment peaks tend to be better separated in time as the mass of the fragment increases (i.e., for Ar to Xe). In all cases, the time-of-flight curves are observed to change significantly with increasing electron impact energy. This indicates that new excitation channels are opening at higher impact energies. The fastest fragments have kinetic energies of approximately 1 eV. A full discussion of this and other features will be presented at the conference.

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PS-07

Lβ_2 SATELLITES SPECTRA EMITTED DUE TO N – SHELL SPECTATOR VACANCY

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The X-ray satellite spectra arising due to $2p_{3/2}^{-1}4x^{-1}$-$4x^{-1}4d^{-1}$ ($x \equiv$ s, p, d) transition array, in the elements Z = 40 to 92, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater (HFS) data on $1s^{-1}$-$2p^{-1}4x^{-1}$ and $2p^{-1}$-$4x^{-1}4d^{-1}$ Auger transition energies and their relative intensities have been estimated by considering cross - sections of singly ionized $2x^{-1}$ ($x \equiv$ s, p) states and then of subsequent Coster-Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in Lβ_2 spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that two satellites observed in the Lβ_2 region of the X-ray spectra of various elements and named β_2^0 and $\beta_2^{(a)}$ in order of increasing energy are mainly emitted by $2p^{-1}4d^{-1}$–$4d^{-2}$ transitions. Considering the relative intensities of these transitions and the mutual closeness in their energies, the most intense one, namely the $^3F_4$-$^3F_4$, and seven others of this array have been associated with the emission of the satellite $\beta_2^{(a)}$, reported in the spectra of elements with Z < 60. In the range Z > 70, the second most intense transition, namely the $^1D_2$-$^1D_2$, and a comparatively weaker transition, namely the $^3D_3$-$^3P_2$ one, deviate from this group. Hence, only six transitions superpose to give rise to this satellite, which has been named as β_2^0, in case of elements with Z > 70, in the literature. In the range Z > 65, this satellite gets an added intensity due to the superposition of some intense transitions $2p^{-1}4f^{-1}$-$4d^{-1}4f^{-1}$ array. This superposition of two arrays in high Z elements justifies the name β_2^0 different from $\beta_2^{(a)}$, given to the analogously placed satellite in the spectra of lower Z elements. Finally, the four closely spaced satellites, reported in the β_2 region of the spectrum $_{46}$Pd have been assigned to suitable $2p^{-1}4x^{-1}$-$4x^{-1}4d^{-1}$ ($x \equiv$ s, p, d) transitions.

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PS-08

GLOBAL ENERGY MINIMUM EVOLUTION IN LENNARD-JONES CLUSTERS GROWING PROCESS

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We present a new theoretical framework for modelling cluster growing process [1]. Starting from the initial tetrahedral cluster configuration, adding new atoms to the system and absorbing its energy at each step, we find cluster growing paths up to the cluster sizes of up to 150 atoms. We demonstrate that in this way all known global energy minimum structures of the Lennard-Jones (LJ) clusters can be found. Our method provides an efficient tool for the calculation and analysis of atomic cluster structure. With its use we justify the magic numbers sequence for the clusters of noble gases atoms and compare it with experimental observations.

Figure 1 demonstrates the striking correspondence of the peaks in the dependence of the second derivative of the binding energy per atom, ΔE_N^2 on cluster size (black squares), calculated for the global energy minimum clusters chain of LJ clusters based on the icosahedral symmetry with the peaks in the abundance mass spectra experimentally measured for *Ar* and *Xe* clusters [2-3]. For the regions, in which the experimentally observed magic numbers do not appear in the ΔE_N^2 for icosahedral global energy minimum cluster structures, we additionally plot the ΔE_N^2 dependence for

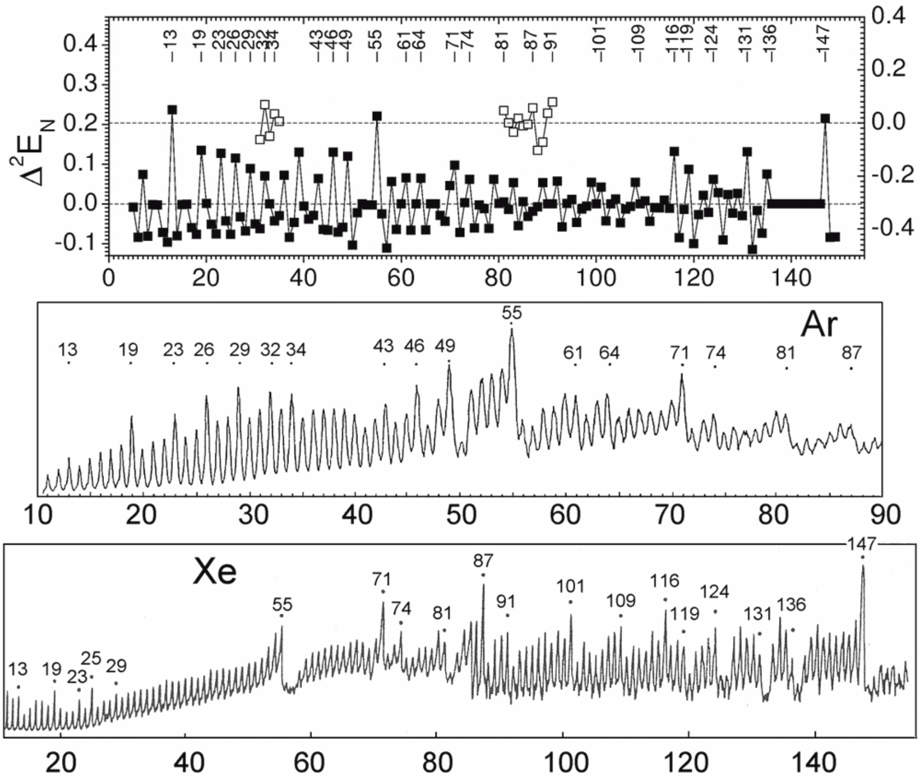

Figure 1: Magic number sequences for *Ar* and *Xe* clusters

energetically unfavourable icosahedral cluster chains, that are energetically very close to the global energy minimum chain, and thus influence the magic number formation (see opened squares in figure 1).

In figure 2, we plot images of the magic clusters up to *N=71*. For *N=32* and *N=34*, we present the icosahedral isomers and the one possessing the global energy minimum. We also plot the image of the octahedral *N=38* cluster, which is found to be more stable than the clusters from the icosahedral chain. Experimentally *N=38* is not found to be the magic cluster, although it is the global energy minimum cluster, being magic for the octahedral cluster chain. This fact can be understood if one takes into account that the cluster chains with different lattice structure are formed independently and the transition of clusters from one chain to another at certain N is completely forbidden or occurs with the low probability.

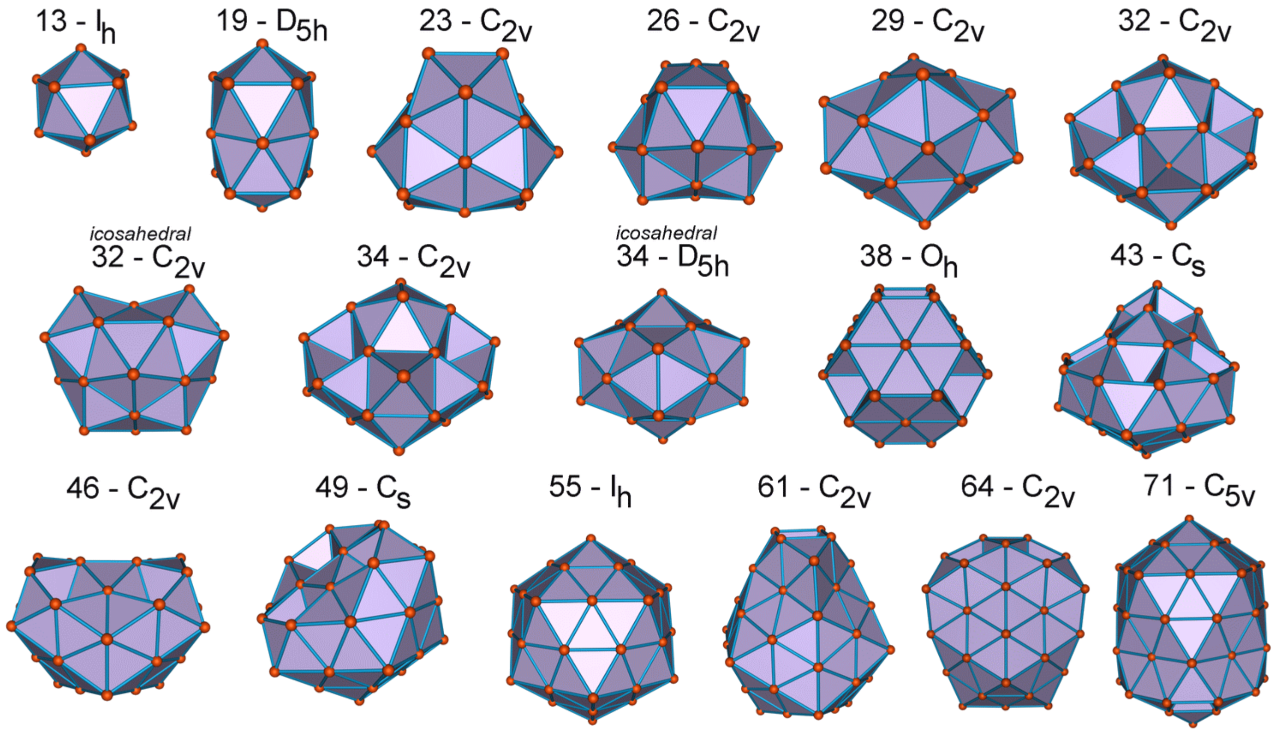

Figure 2: LJ magic clusters geometries

Our method serves an efficient alternative to the global optimization techniques based on the Monte-Carlo simulations (see [4] and references therein) and it can be applied for the solution of a broad variety of problems for which atomic cluster or complex molecular structure is important.

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PS-09

IONIC NUCLEATION IN ^4He CLUSTERS: STRUCTURES AND DYNAMICS OF CHARGED CORES

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The ionization of pure Helium clusters by photon or electron impact causes a great deal of energy to be deposited in these weakly bound aggregates. Experimental [1] and theoretical [2] studies on these clusters suggest the structure of a ionic dimer surrounded by neutral, Van der Waals bound atoms ($\mathrm{He}_n^+ \rightarrow \mathrm{He}_2^+(\mathrm{He})_{n-2}$) - in competition with an ionic trimer core for the smaller clusters. The structure of these aggregates and the relaxation mechanism through which the dimer gets stabilized inside each cluster is the aim of this study. Given these facts, we have carried out accurate calculations (CCSD(T) with aug–cc-pVQZ basis) to obtain a detailed, highly correlated Potential Energy Curve for the isolated core system He_2^+, and then Potential Energy Surface (PES) for the $\mathrm{He}_2^+ + \mathrm{He}$ system. This was firstly analyzed in the rigid rotor approximation, fixing the internuclear ionic dimer distance r to the equilibrium bond length of the isolated molecules He_2^+. This surface has a strong minimum in the linear configuration, and was used by us in a rotational quenching study[4].

Using a Discrete Variable Representation (DVR) [3] approach we found 13 bound states for $\mathrm{He}_2^+(r_{eq})$-He that show a broad delocalization of the third atom when the higher states are populated.

Calculations were performed then for the vibrational extention by scanning several values of r, obtaining a very accurate global 3D He_3^+ PES. Bound state calculations were also carried on a "streched rigid rotor" system to evaluate the differences with the interaction of an excited core [5].

On this three-dimensional surface some model calculations for the time-dependent evolution of the neutral trimer (He_3) photoionization [6] were carried in our group, revealing the production of highly excited He_2^+ ions after the primary process.

Quantum dynamical calculations were then carried out on this system after the evaluation of its vibrational couplings[7]; a series of different approaches with different approximations were tested and finally cross section for the relaxation process from some of the upper states were computed using the Infinite Order Sudden Approximation (IOS) [8]. Their large values found for the relaxation cross sections are a signal of the high probability of the collisional cooling events, even though multiple quantum transitions considering that with this method we obtain an understimation of them (Fig.1).

All the results are indicative of rather fast nucleation in this system and of a very limited charge propagation after the initial ionic monomer is formed as the result of the ionization.

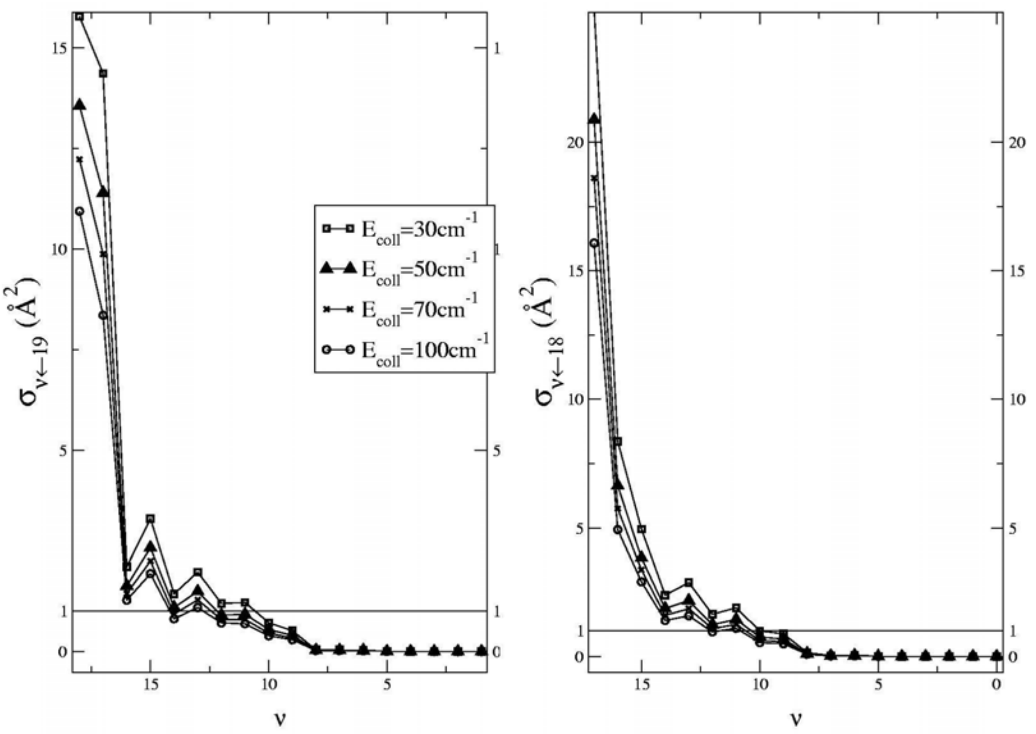

Figure 1: $He_2^+ - He$ computed relaxation cross sections from two of the upper He_2^+ vibrational states ($\nu = 18, 19$, at different energy values) down to all the lower ones.

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PS-10

DYNAMICS AND STRUCTURES OF NEON CLUSTERS WITH CATIONIC AND ANIONIC CORES

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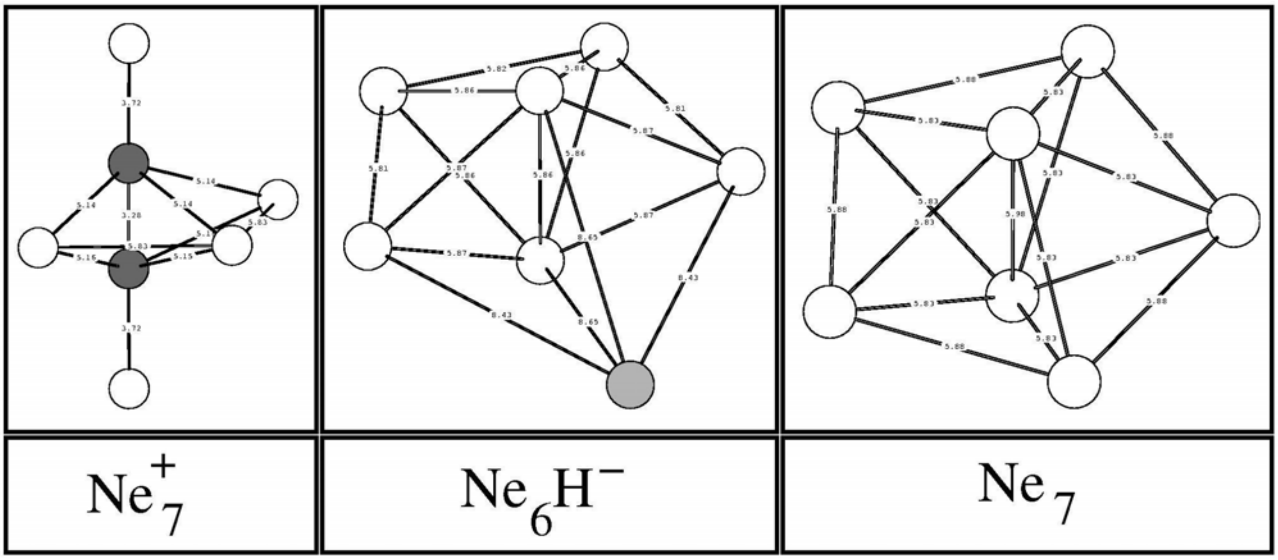
On both theoretical and experimental sides, the interest of chemists and physicists in small ionic clusters involving rare-gas (Rg) atoms has steadily increased in recent years. In particular, experimental findings on the corresponding neutral clusters are usually hard to gather without resorting to ionization. It is therefore very important to understand how the interaction with ions modifies the structure of the original neutral clusters. Experimental studies of charged systems have been performed by injecting atomic or molecular ions into the rare-gas at very low temperature. In our previous work [1, 2] we studied Ne_n^+ clusters both with a DFT approach and with some modeling of the interaction forces within these clusters, finding out that it is possible to describe the overall potential as a sum of pairwise potentials, i.e.

$$V_{TOT} = \sum_{i=3}^{n} V^{(i)}_{(Ne_2^+ - Ne)} + \sum_{\substack{i<j \\ i\geq 3}}^{n} V^{(ij)}_{(Ne-Ne)} \tag{1}$$

in which the first term is the sum of the Ne atoms interactions with the Ne_2^+ system considered as a rigid rotor [2], and the second term is the sum of the interactions between two neutral neon atoms [3]. With this modeling we found good agreement for the structures and the energetics (up to Ne_{25}^+) with previous theoretical [4] and experimental [5] data. These findings are in line with the general view of singly ionized Rg_n^+ for which all the studies so far suggest that these clusters consist of an arrangement of neutral, or almost neutral Rg atoms which are bound by polarization forces and, to a lesser degree, by dispersion forces to a charged central moiety Rg_k^+, the size of which varies with respect to the particular Rg species and to the n values [6]. Much less attention has been devoted to negative clusters containing the H^- ion. Because of the closed shell character of H^- and the absence of short-range bonds between the Rg atoms and the ion, a more regular behaviour can be expected among the different Rg species and the corresponding neutral clusters. We decided therefore the study the structures of the Ne_nH^- systems with different approaches and compare the results so obtained. For the smallest ones of the series (up to Ne_6H^-) we carried out full *ab initio* optimizations finding out that for all of them the negative charge resides on the hydrogen atom, as one could expect from the comparison between the electron affinity of the Ne and the H species (-29 and 72.8 $kJmol^{-1}$, respectively). Given these facts, we decided to study larger systems and model the interaction forces within these clusters as sums of atomic potentials, i.e.

$$V_{TOT}^{atomic} = \sum_{i=2}^{n} V^{(i)}_{(Ne-H^-)} + \sum_{\substack{i<j \\ i\geq 2}}^{n} V^{(ij)}_{(Ne-Ne)} \tag{2}$$



Ne_7^+ Ne_6H^- Ne_7

Figure 1: The 7-particle clusters lowest energy optimized geometries are shown. In the first figure the shadowed atoms represent the Ne_2^+ dimeric core and in the second one the H$^-$. On the right the neutral Ne_7 cluster is shown.

where the first term on the rhs is the interaction potential for isolated $(Ne - H)^-$ [7] and the second one is the same neutral interaction as in the previous equation. The same modeling was used to study the neutral Ne_n clusters and the results obtained show a general agreement with previous work [8]. Finally we employed this global atomic potential for the study of the lowest energy structures of even larger Ne_nH^- systems using an implementation of a genetic algorithm [9]. Comparative results will be presented at the conference.

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PS-11

CONFINEMENT RESONANCES IN PHOTOELECTRON ANGULAR DISTRIBUTIONS FROM ENDOHEDRAL ATOMS

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Angular distribution parameters for 1*s*, 2*s* and 2*p* photoelectrons from the endohedral Ne@C_{60} atom are investigated within the framework of the Dirac bubble potential model. They are found to acquire significant resonances due to the presence of the fullerene shell.

Here we study how the fullerene shell influences the dipole and non-dipole parameters of the photoelectron angular distribution in photoionization of deep subshells of atoms encapsulated inside C_{60}, the so-called endohedral atoms $A@C_{60}$. It is known that C_{60} acts as a resonator resulting in the appearance of *confinement resonances* in the frequency dependence of the total photoionization cross sections of the *A* atom. They show up in the angular distribution as well.

The problem under consideration can be simplified considerably if one takes into account that the geometrical size of a hollow fullerene cage is significantly more than the radii of the internal subshells of the encapsulated atoms. Therefore the wave function of an ionized electron in the initial state can be considered as that of an isolated *A* atom and the surrounding carbon atoms have to be taken into account in describing the molecular continuum only..

For low enough photoelectron energies the C_{60} potential can be presented by a potential of a spherical layer formed by the smeared-on-the-sphere carbon atoms, the so called Dirac bubble potential $V(r) = -V_0\delta(r-R)$, where *R* is the C_{60} radius and V_0 is defined in terms of the affinity energy *I* of the electron to the empty C_{60} molecule. Inside the potential bubble the continuum wave function differs only by a factor, dependent on the photoelectron energy $\varepsilon = k^2/2$, from the regular solution $u_{kl}(r)$ of the Schrödinger equation for a free atom and has the form $\chi_{kl}(r) = \mathrm{T}_l(k)u_{kl}(r)$, with *l* being the electron angular momentum. Outside the sphere the function $\chi_{kl}(r)$ is a linear combination of the regular $u_{kl}(r)$ and irregular $v_{kl}(r)$ solutions of this equation. The coefficients of the linear combination are defined by the matching conditions of the wave functions on the sphere, i.e. at a point $r = R$. The amplitude $\mathrm{T}_l(k)$ and the phase shift $\Delta_l(k)$ of the wave function due to electron scattering by $V(r)$ are defined by the matching conditions at *R*:

$$\mathrm{T}_l(k) = \cos\Delta_l(k)\left[1-\tan[\Delta_l(k)v_{kl}(R)/u_{kl}(R)]\right], \text{ and } \tan\Delta_l(k) = u_{kl}^2(R)\left[u_{kl}(R)v_{kl}(R) - k/\Delta L\right]^{-1}.$$

Here ΔL is the jump of the logarithmic derivative of the wave function at $r = R$.

The angular anisotropy parameters are given by the standard expressions for free atoms, but with the atomic dipole $d_{l\pm1}$ and quadrupole $q_{l\pm2,0}$ matrix elements and phases $\delta_{l\pm1}(k)$, $\delta_{l\pm2,0}(k)$ replaced as follows: $d_{l\pm1} \to \mathrm{T}_{l\pm1}d_{l\pm1}$, $q_{l\pm2,0} \to \mathrm{T}_{l\pm2,0}q_{l\pm2,0}$, $\delta_{l\pm1} \to \delta_{l\pm1} + \Delta_{l\pm1}$, $\delta_{l\pm2,0} \to \delta_{l\pm2,0} + \Delta_{l\pm2,0}$.

The dipole and non-dipole angular anisotropy parameters $\beta_p(\omega)$ and $\gamma_s(\omega)$ are given by:

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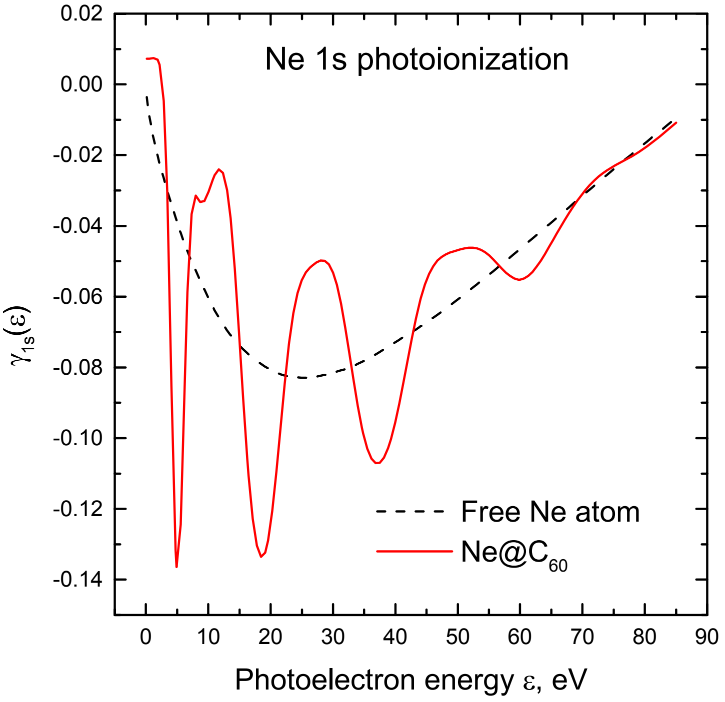
$\beta_p = 2\mathrm{T}_2 d_2[\mathrm{T}_2 d_2 - 2\mathrm{T}_0 d_0 \cos(\Delta_2 + \delta_2 - \Delta_0 - \delta_0)][\mathrm{T}_0^2 d_0^2 + 2\mathrm{T}_2^2 d_2^2]^{-1}$, and
$\gamma_s = 6(\omega q_2 / c d_1)(\mathrm{T}_2 / \mathrm{T}_1)\cos(\Delta_2 + \delta_2 - \Delta_1 - \delta_1)$.
As an example, calculations were performed for *Ne* 1*s*, 2*p*, 2*s* subshells. Figure illustrates the results for γ_s for 1*s,* demonstrating the pronounced resonance structure.



The amplitude of the oscillations rapidly decreases with the growth of ε and almost vanishes starting from about 65 eV.

The resonance behavior of γ_s gives a qualitative explanation of the observed anomalously high values of the non-dipole asymmetry parameters in the two-atom molecule. Let us consider the deep subshell photoionization of the atom *A* in a molecule *AB* with random orientation of the molecular axis in space. The atom *B* is arbitrary located on the sphere with the center at the nucleus of *A* and radius equal to the inter-atomic *AB* distance. The effect of *B* on γ_s of *A* can be taken into consideration by introducing a spherically symmetric potential that imitates the atom *B* smeared on the surface of this sphere. For an isolated atom *A* the ratio q_2 / d_1 is of the order of the radius of the ionized atomic subshell while for the same atom in the molecule this ratio has to be multiplied by $\mathrm{T}_2 / \mathrm{T}_1$ of the amplitudes of the quadruple and dipole parts of the photoelectron wave function at a point of the atom *B* localization.

Oscillations of the angular anisotropy parameters, presented here for *Ne*, are qualitatively typical for any other endohedral atom. The corresponding experimental investigations are recommended and can help to confirm the existence of a rather non-trivial new phenomenon.

PS-12

Description of Dynamic Properties of Finite Many-Electron Systems in the Density Functional Theory

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In a general case, the success of the density functional theory (DFT) is based completely on the availability of reasonable approximations for the exchange-correlation functional F_{xc}, because DFT cannot produce F_{xc} by itself, stating only the existence of this functional [1]. Therefore, DFT needs an external source supplying suitable approximations for the exchange-correlation functional.

Here we solve this problem and present a self consistent version of DFT, which is independent of the approximations and allows to calculate the ground state and dynamic properties of finite multi-electron systems such as atoms, molecules and clusters. The exact functional equation for the effective interaction, using which one can construct the action functional, the exchange-correlation functional, the response functions, and excitation spectra of the considered systems, is presented. Thus, it is possible to convert DFT into a self-consistent theory by constructing the exact equation for the exchange-correlation functional F_{xc}. The proposed version of DFT has another desirable feature: a systematic way to construct successive approximations to F_{xc} is becoming available. We have shown that the functional $F_{xc}[\rho]$ can be used to calculate the response functions. We have also related the eigenvalues of the single-particle Kohn-Sham equations to the real single-particle spectra [2]. Using the fact that the single particle DFT potential $V(r)$ of finite neutral system behaves asymptotically as $V(r \to \infty) - 1/r$ and therefore supports infinite number of discrete levels, we demonstrate that our method is also fit to describe negative charged finite systems such as negative ions or clusters, which have very rich and extremely interesting dynamic properties. In contrast, when dealing with negative ions, the Hartree-Fock method has some drawbacks. Among them there is a well-known consequence of the non-locality of the HF single-particle exchange potential, which leads to the fact that the HF single-particle potential acting on the unoccupied states falls of exponentially. As a result, the HF potential can hardly support unoccupied states, see e.g. [3]. Such a poor situation with the number of states results in strong difficulties in treating negative ions in the pure HF frame.

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PS-13

ELECTRON TRANSFER IN LOW-ENERGY COLLISIONS OF META-STABLE NA$_3^+$ CLUSTER-IONS WITH NA ATOMS

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In these days, there have been some attempts to study charge transfer (CT) reactions in collisions between ions/atoms and clusters both experimentally [1] and theoretically [2]. In most cases, however, the study is limited to the case where the target cluster is in the electronic ground state. To shed light on the difference in the reactivity between the ground state and excited states of clusters, we make a theoretical study on the CT reaction in the collisions of meta-stable triplet state Na$_3^+$ with Na. It is well known that the energetically most stable geometrical configuration of Na$_3^+$ is collinear ($D_{\infty h}$) as for the meta-stable triplet (*a*) state and equilateral triangle (D_{3h}) for the electronic ground singlet (*X*) state. As for the collisions of the ground state Na$_3^+$ with Na (3s,3p), in addition to their experimental work, Roller-Lutz and coworkers [3] has calculated the CT cross section with high accuracy by using the non-adiabatic quantum molecular dynamics.

Here we mainly study on the following CT reaction,

$$Na_3^+(a^3\Sigma^+_u) + Na(^2S) \rightarrow Na_3(X^2\Sigma^+_u) + Na^+(^1S) \qquad (1).$$

In this system, the following 'spin transfer' (ST) reaction is also possible

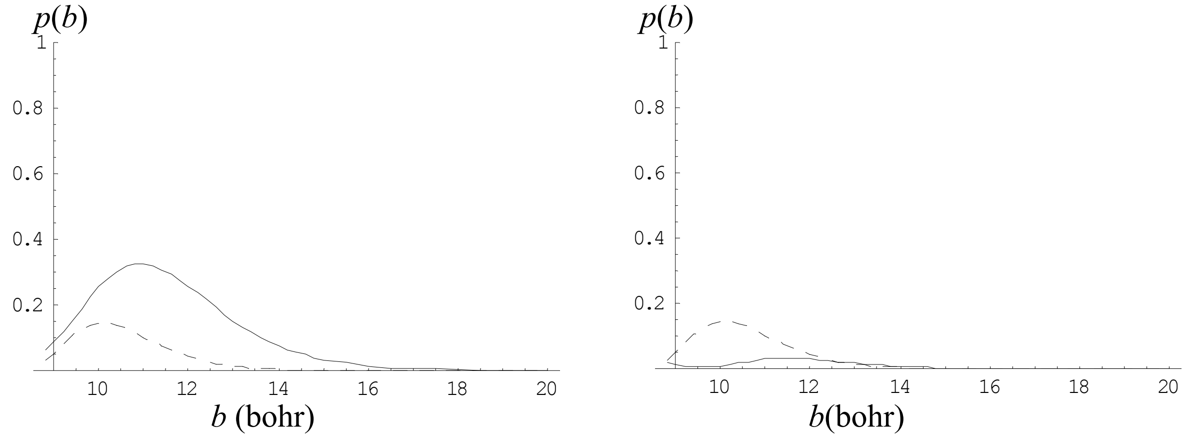
$$Na_3^+(a^3\Sigma^+_u) + Na(^2S) \rightarrow Na_3^+(X^1\Sigma^+_g) + Na(^2S) \qquad (2).$$

The heats of reaction are estimated as –0.5 eV and 0.4 eV for (1) and (2), respectively.

Adiabatic potential energy surfaces and non-adiabatic couplings between two different electronic states are calculated by using semi-empirical diatomics-in-molecules (DIM) method. As for the reaction (1), avoided crossing of two surfaces is seen in the region where the projectile and target have a relatively larger separation (10-15 bohr). On the other hand, the surface crossing for the reaction (2) is seen when the atom approaches the cluster as much as 9 bohr.

Dynamics calculation is carried out within the framework of the perturbed-stationary-state method. Here we assume that the projectile atom moves classically in a linear orbit parallel to the cluster axis. The motion of the atoms in the cluster is frozen during the collision. Figures 1 show the CT (ST) probabilities for collinear Na$_3^+$ cluster as functions of the impact parameter *b* at the collision energy of 6.8 keV in the center-of-mass system. The total CT (ST) cross section is estimated as 87 (24) bohr^2 for the meta-stable triplet *a* state and 11 (24) bohr^2 for the ground *X* state. From this fact, it has been demonstrated that the CT cross section is much enhanced for the case of meta-stable state compared to the case of the ground state. Such a tendency is also reproduced by another calculation using a phenomenological Hubbard model [4].

More detailed report is presented in the article [5].



Figures 1: The charge (solid line) and spin (dashed line) transfer probabilities *p*(*b)* as functions of impact parameter *b* in the collisions of collinear Na_3^+ with Na at the collision energy of 6.8 keV in the center of mass system. The left figure is for meta-stable $a^3\Sigma^+_u$ state and the right one is for the ground $X^1\Sigma^+_g$ state.

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IONIC AND METAL IMPURITIES IN A QUANTUM SOLVENT: H^-, Li, Na AND H IN SMALL ^4He CLUSTERS

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The interactions between H [1] [4], alkali atoms (Na, Li) [4] and ^4He, as well as those between H^- and ^4He, are known to be even weaker than those between two ^4He atoms [2][5][6]. We have employed the Quantum Diffusion Monte Carlo (DMC) method to analyze the $(^4He)_N\,H$, $(^4He)_N\,Li$, $(^4He)_N\,Na$ and $(^4He)_N\,H^-$ (with N=2 [3][8][10][11] or more [9]) systems by constructing the full interaction as a sum of two-body (2-B) potentials chosen among the most recent proposals from literature.

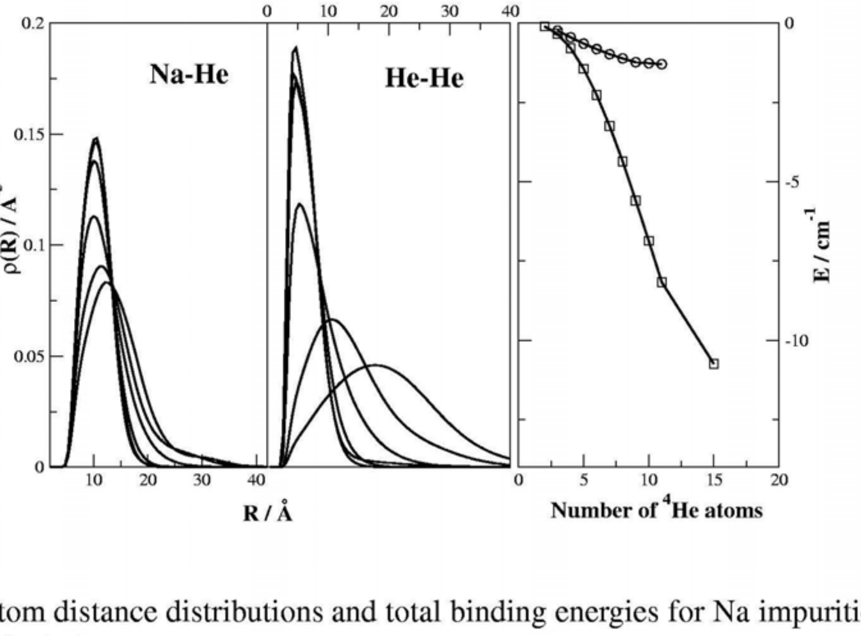

Figure 1: Atom-atom distance distributions and total binding energies for Na impurities in ^{4}He clusters from DMC calculations.

The Diffusion Monte Carlo (DMC) algorithm and stochastic analysis, using the trial function constraint (Importance Sampling [7]) and Metropolis algorithm in short-'time' approximation, are a useful way to study the energetics and structural behavior for such floppy systems.

The total binding energies and the spatial distributions, analysed using several internal coordinates such as atom-atom, atom-geometrical center of system and atom-center of mass distances, have been obtained with the chosen potentials and compared with previous published results, in order to better understand the possible structures of such special systems.

A detailed analysis of our finding on the above systems will be presented at the Meeting.

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PS-15

DISSOCIATIVE EXCITATION OF H_3^+ AND H_2^+ MOLECULES IN THE COLLISIONS WITH He AND O_2 TARGETS

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We have presented results of experimental measurement of the excitation function of hydrogen atomic line $L\alpha$ (λ= 121.6nm) emitted during dissociation of H_3^+ and H_2^+ molecular ions, at collisions with He and O_2 targets in 3-10 keV energy range. H_2^+molecular ions were chose for representing of a prototype case of covalent molecular system, while H_3^+-as a somewhat more complex system.

Knowledge about cross sections of Lyman alpha emission occurring during passing of H_2^+, H_3^+ ions through gases is important in the context of fusion energy research. Such data can be used as basis for diagnostics and determination of plasma parameters in Tokomak devices. Investigation of inelastic processes in the collision of H_3^+, H_2^+ projectiles with different target presents an extra challenge since the molecular nature of H_3^+ and H_2^+ has to be taken into account .Particularly , the revealing factor of orientation of internuclear axis of diatomic H_2^+ or molecular surfaces of three-atomic H_3^+molecules with respect to the velocity of the projectiles will be influenced on probability of the excitation of different inelastic channels [1,2].

The results of measurements for H_2^+, H_3^+ - He, O_2 pairs are presented in figure1.Comparison of a results for H_2^+ - He and H_3^+ - He colliding pairs shows that the value of cross sections of hydrogen atomic line in case of H_2^+ - He is large than for pair H_3^+ - He . The mechanism of these dissociative excitation processes are explained in framework of quasimolecular representations. In the case of H_3^+ - He pair the formation of excited atomic fragments are caused by decay of electronic state ($^1A_2^{//}$) of H_3^+ [2]. Besides strong dependence of probability for formation of excited atomic fragments are observed from the orientation of molecular surface of H_3^+ [2]. From analyze of our experimental results was revealed also that the probability of dissociative excitation sufficiently depends from vibrotional excitation of incident ions H_3^+ .

PS-15

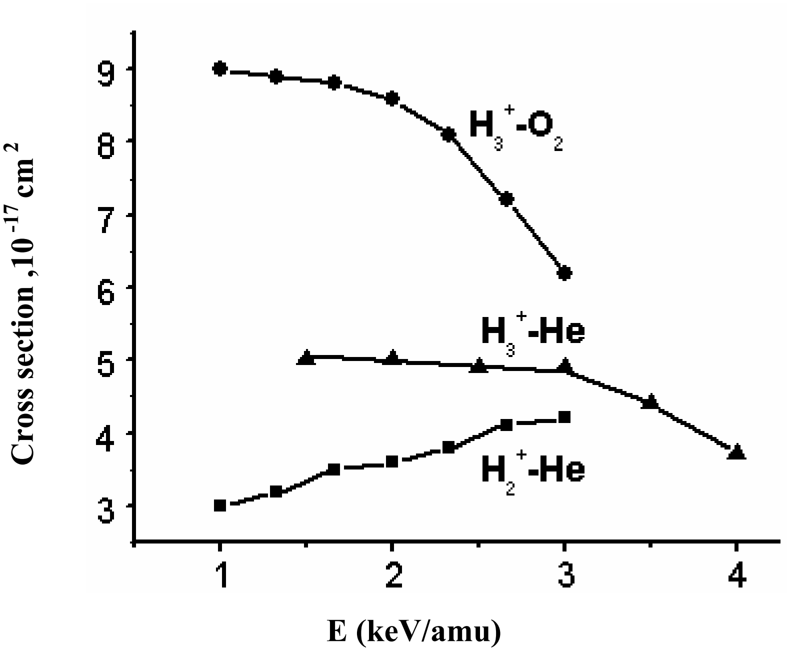

Figure 1: Cross section of Lyman alpha excitation

The superiority of value for cross-section of H_2^+ - He compare to the H_3^+ - He is connected by the fact that the orientation effect of molecular surface reduces the cross-section that is confirmed by our experimental results too. The less contribution of an orientation effect has been expected in case of oxygen target. Moreover in this case, formation of excited fragments of dissociation might be explained not only by primary excitation processes but also by electron capture processes. Perhaps this is the reason for relative high value of cross section for the H_3^+ -O_2 pair. Both statement are confirmed by our experimental results and will be discussed on the conference.

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PS-16

DISSOCIATIVE EXCITATION MECHANISM IN H_2^+ - Ar, He^+ -N_2 AND K^+ - H_2 COLLISIONS

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The aim of presented paper is investigation of mechanism of collision induced dissociation processes. It is known that atomic particles interact with molecule primarily through two basic processes either through collisions with the electronic background (the electronic mechanism) or through close encounter with the atomic cores (the impulse mechanism) [1]. Fragmentation of molecules or clusters is a typical process in which these two basic mechanisms can be well identified. In the present work we have investigated the dissociative excitation processes for the collision of H_2^+ - Ar, He^+ -N_2 and K^+ - H_2 pairs. The investigations were performed by optical spectroscopy method. The measurements were carrying out in the vacuum ultraviolet region (50 - 130 nm) of emitted spectral lines. For the explanation of dissociation mechanism it is necessary to determine the role of orientation effect of molecule in the excitation probability of inelastic channel. Therefore the degree of linear polarization of atomic HeI (388.9 nm) and ionic NII (500.5 nm) lines emitted at He^+ - N_2 collision in moderate energy range 1 - 10 keV have been measured. It is known that high degree of polarization of the radiation of dissociative products is caused by the strong dependence of the excitation probabilities on orientation molecular axis relative to the beam direction[2]. Results of measurements are presented in Figure1. A low degree of polarization (less than 5%) of the radiation of NII (500.5 nm) line obtained in our work suggests that probability of excitation is independent on the molecular orientation and hence the electronic mechanism is valid. This mechanism can be explained in terms of quasidiatomic representation. Analyze of experimental results shows that in the case of H_2^+ - Ar and K^+ - H_2 pairs the investigation of dissociative excitation processes requires a combination of both basic mechanism: a close binary

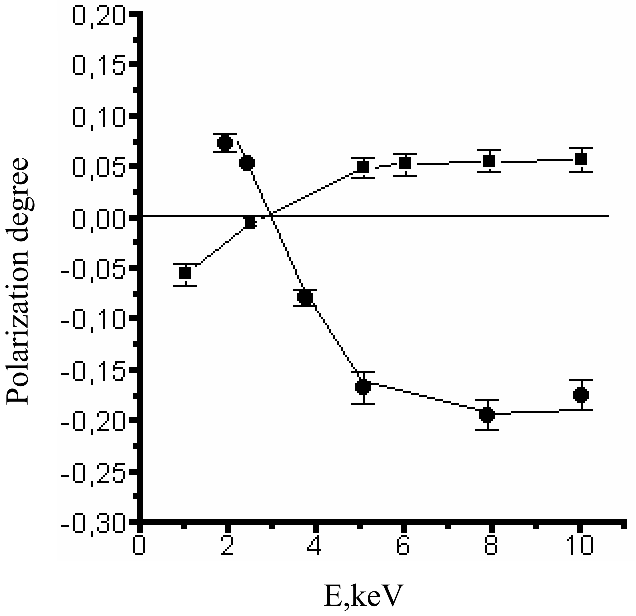

Figure1: Energy dependence of Polarization degree :
- HeI(388.9nm,$3p^3P - 2s^3S$)
- NII(500,5nm,$3d\ ^3F^0 - 3p\ ^3D$)

encounter and an electronic transition. This mechanism can be explained on a term crossing base that successfully is used in case of atom - atom interactions.

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PS-17

THICKNESS DEPENDENT MECHANISM OF ELECTRON EMISSION FROM LiF FILMS BY (e,2e) SPECTROSCOPY

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Secondary electron emission from LiF films of various thicknesses was studied using time-of-flight two-electron coincidence spectroscopy (e,2e). The films deposited on Si(001) surface by thermal evaporation from a Mo crucible, were characterized by Scanning and Transmission Electron Microscopy, Total Current Spectroscopy and Ellipsometry. A very small incident electron current (10^{-13} A) minimized sample surface charging and possible destruction of the film by electron impact.

It was found that the energy distribution of secondary electrons excited from LiF films by 20-50 eV incident electrons depends on the film thickness. Figure 1 presents the two-dimensional energy distributions of correlated electron pairs for thin (c) and thick (d) films together with the scanning electron microscopy images of the films (a,b).

For a thick film (15-17 nm) (Fig.1b) a set of energy distribution curves (EDC) of secondary electrons exhibit emission features at about 7 eV and 11 eV. The energy positions of these maxima do not depend on the incident energy. To reveal the origin of these features, each of the EDCs was spanned in the second dimension E_2 using two-electron coincidence spectroscopy (Fig. 1 c,d). Two-dimensional mapping of the energy sharing between correlated electrons shows that above 25 eV incident energy, one electron of the pair is preferentially emitted with $E_1 = (7.2\pm0.3)$ eV energy and the second one with energy $E_2 = (E_p - 23.3) \pm 0.5$ eV, where E_p is the incident electron energy. At about 30 eV incident energy, a second favoured emission energy of 10.8±0.3 eV is observed.

PS-17

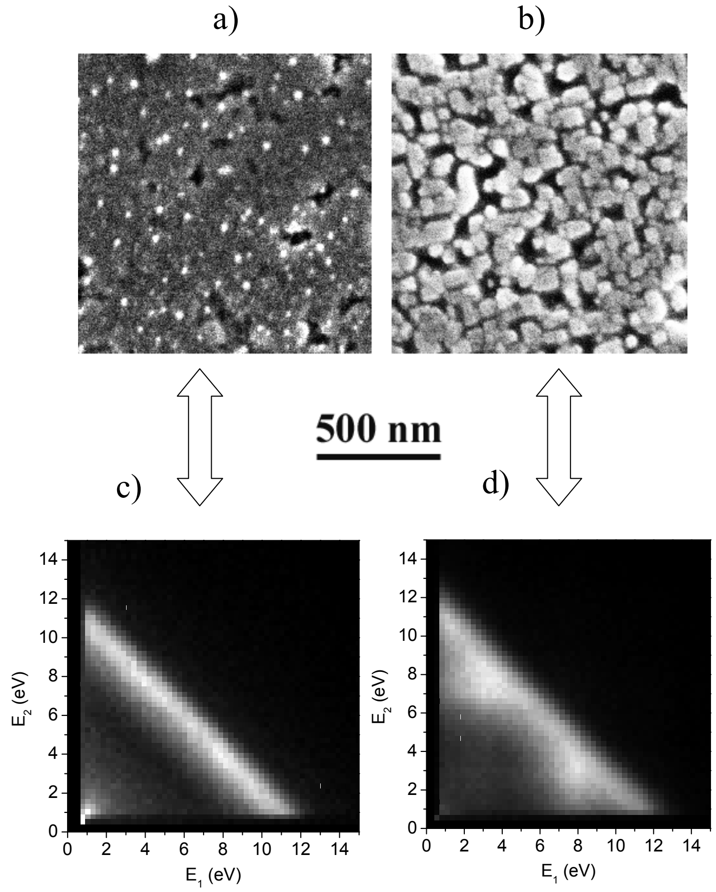

Fig. 1

It is suggested that the mechanism of secondary electron emission from the LiF film includes the excitation of two types of plasmons with subsequent decay via electron ejection. The experimentally determined plasmon energies are $\hbar\omega_1$ = (23.3±0.3) eV and $\hbar\omega_2$ = (26.8±0.4) eV. These energies are consistent with the plasmons model, where one plasmon is associated with interband transition and another one with exciton [1].

For a thin (5-10 nm) (Fig. 1a) LiF film the plasmon-assisted maxima in the (e,2e) spectrum do not appear (Fig. 1c), whereas the binding energy spectrum shows already a dominant contribution from the valence band of LiF.

These results show that the plasmon-assisted mechanism of secondary electron emission from LiF films shows up only at the film thickness above a certain limit.

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PS-18

Projectile induced spin excitations in a spin-polarized cluster: Comparison of calculations using Heisenberg and Hubbard Hamiltonian.

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Within the last few years several papers have been devoted to the experimental study of the interaction between a fast atomic particle with a metallic cluster. Various kinds of non-adiabatic effects have been observed and studied theoretically such as electronic excitation and ionization , charge transfer in cluster atom collision and capture of low-energy electron by Na_n cluster and C_{60}

Other experiments have been performed on spin diffusion in Ferro magnets. Among the main results let us mention the formation of spin-polarized electrons in collisions of multicharged ions with a magnetized iron surface and the spin depolarization of low energy polarized electrons passing through a ferromagnetic film . However, up to now only bulk targets have been used. Similar experiments on finite media or aggregates are missing so fare.

In a previous article we suggested a theoretical description of the spin excitations in a cluster to simulate a surface-atom collision by choosing an adequate cluster size. Our approach is based on a time-dependent Heisenberg Hamiltonian and takes into account only spin excitations and neglects the charge excitations . One of the aims of the present article is to compare results obtained by the Heisenberg Hamiltonian with those obtained using the Hubbard Hamiltonian. This is of interest for spin-dependent surface-atom collisions. The Hubbard Hamiltonian allows the investigation of charge and spin excitations. We study the cases of strong and weak electronic correlations. Due to the basis size of the Hilbert space, comparison between the two models can be carried out only for a small cluster. At the beginning of the collision we assume a spin polarized cluster.

The Heisenberg and Hubbard models are introduced for the spin excitation process. The communication treats the spin and charge excitation dynamics in the target and the projectile during the interaction. The possibility of an electron capture and its effect on the dynamics is described. Finally results for the spin excitations in the target after the target-projectile collision are given.

PS-19

STRONG INFLUENCE OF SIZE QUANTIZATION OF ENERGY SPECTRUM ON EXCITON RELAXATION IN INERT ELEMENT CLUSTERS

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Here the results are reported, which describe the influence produced by dimensional quantization of the energy spectrum of the excitons inside the bands upon the exciton energy relaxation in Ar_N, Kr_N and Xe_N clusters excited by an electron beam. The method used was VUV emission spectroscopy of the clusters formed in supersonic inert gas jets. The VUV luminescence of clusters, namely the RM_n with the intensity maxima 127 nm (Ar_N), 148 nm (Kr_N) and 176 nm (Xe_N) was taken as an indicator (typical for solid inert elements [1]) of the thermal energy relaxation channel for free excitons along their dispersion curve. When the relaxation proceeds along this path, the energy is "discharged" into the lower exciton bands with following, formation of autolocalized excitons of the type of vibrational-relaxed_molecular centers $R_2^*({}^{1,3}\Sigma_u^+)$ (R is the inert element atom) emitting the continuum RM_n. It is shown that this path of exciton relaxation is typical for clusters of large average sizes $\overline{N}$ >150-160 atoms/cluster. But this relaxation channel is suppressed in the critical size region $N_c \propto \Delta E/(3/g)\ h\,\omega_D \sim 100$ atoms/cluster (ΔE is the exciton band width in solids, g is the degeneracy degree of the exciton states, $h\,\omega_D$ is the Debye energy of the phonon). The estimates obtained show that on size energy quantization in the region N_C the energy space between the nearest free-exciton levels in the bands is comparable with or exceeds the Debye energy of a phonon. As a result, the single-phonon process of relaxation typical for large clusters and solid inert elements is replaced with a shower multiphonon process, and the ordinary path of free exciton relaxation is locked. A new possibility arises – exciton autolocalization from the high-energy bands with formation of molecular centers of the type of an excited excimer molecule. The high-excited terms of this molecule are the beginning of the path along which the excited atoms and molecules are desorbed [2]. Therefore, the VUV radiation of the excited atoms R^* (${}^1P_1$, ${}^3P_1$) and excimer molecules R_2^* in the state $C\,0_u^+\left({}^1P_1+{}^1S_0\right)$desorbed from the clusters was used as an indicator of locking the path of free exciton relaxation along the dispersion curve. It is shown spectroscopically that the highest intensity of VUV radiation of the excited particles desorbed from the clusters is achieved just in the size region $\Delta\overline{N}$<150-160 atoms/cluster close to the estimated value $N_C \sim 100$ atoms/cluster.

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PS-20

SIZE EFFECT DESORPTION OF EXCITED PARTICLES FROM INERT ELEMENT CLUSTERS EXCITED BY ELECTRON BEAM

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The VUV cathodoluminescence spectra of Ar_N, Kr_N and Xe_N clusters in the range of mean sizes $10 < \overline{N} < 10^4$ atoms/cluster are described. The clusters were formed in supersonic inert gas jets. The mean cluster size $\overline{N}$ was found by electron diffraction method [1] and was varied with the pressure P_0 and temperature T_0 at the nozzle inlet. For all the inert elements R=Ar, Kr, Xe the following non-trivial emissions were observed: lines of desorbed excited atoms $R^*(^1P_1, {}^3P_1)$; narrow bands displaced by 0.2 nm with respect to the lines towards the red region and ascribed to the desorbed atoms $R^*(^1P_1, {}^3P_1)$ localized near the cluster surface; bands of desorbed excimer molecules in the state $\boldsymbol{C0_u^+(^1P_1+{}^1S_0)}$. The VUV radiation of the excited atoms and molecules desorbed from the clusters was separated from the VUV radiation of the particles in the gas-phase jet applying the law of "corresponding" jets [2], i.e. the maximum of the size dependences of the VUV radiation from the desorbed excited atoms and molecules was obtained in the curve $P_0T_0^{-2.5}$ = const, which corresponds to equal size distributions of the clusters.

The important feature of the above emissions of Ar_N, Kr_N and Xe_N clusters is the fact that they are not present in the VUV spectra of solid inert elements (except for the lines of desorbed atoms $Ar^*(^1P_1, {}^3P_1)$). Besides, the intensity of these emissions increases sharply in the mean size region $\Delta\overline{N}<(150\text{-}160)$ atoms/cluster. These results can be interpreted in terms of the new desorption mechanism operating in a certain size region $\Delta\overline{N}<(150\text{-}160)$ atoms/cluster, which is due to the multiphonon process of exciton relaxation in the clusters caused by size quantization of the energy spectrum inside the exciton bands [3].

The energy diagram of desorption is shown using Ar_{100} clusters as an example. On exciting the Ar_{100} clusters with electrons, high-energy 4p-excitons can appear along with the surface excitons with n=1,1′ и 2, 2′ and the bulk ones with n=1,1′. As the excitons autolocalize from the 4p-band highly excited molecular centers are formed with the dissociation limit Ar^* $(3p^54p)$+Ar $(^1S_0)$. The subsequent transitions to the repulsive terms (with the dissociation limits $^1P_1+{}^1S_0$, $^3P_1+{}^1S_0$ and $^3P_2+{}^1S_0$) lead to dissociation of the highly excited molecules into neutral Ar $(^1S_0)$ and excited $Ar^*(^1P_1, {}^3P_{1,2})$ atoms with high (0.2-0.73 eV) kinetic energies. These energies exceed the highest atomic bond energy in the cluster Ar_N (0.05 eV) that is sufficient for ejection of the atoms from the clusters. Besides, the excimer molecules in the state $\boldsymbol{C0_u^+(^1P_1+{}^1S_0)}$ and in the vibrational-excited states $\boldsymbol{^{1,3}\Sigma_u^{+v}}$ which are formed in the clusters due to collisions of the "hot" excited atoms $Ar^*(^1P_1, {}^3P_{1,2})$ and the ground-state ones also eject from the clusters.

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PS-21

ELECTRON IMPACT IONIZATION OF DIMERS AND CLUSTERS

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The satellite conference ISACC 2003 is going to focus on various dynamical phenomena occurring with atomic clusters. The experimental investigation of clusters requires their ionization, which can be easily induced by electron bombardment. It is therefore of interest to examine the response of immers or clusters with respect to its electron impact ionization. A semi empirical investigation has been done in this regard by Maerk group in Austria [1]. In the present theoretical investigation our main interest is in the total inelastic cross section $Q_{inel.}$ It is not accessible directly in experiments, so we extract out total ionization cross sections Q_{Ion}, which is experimentally measurable quantity. In order to determine Q_{ion} from the calculated Q_{inel}, we consider $E_i \geq I$ and define the following quantity for a given target.

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}, \qquad 0 \leq R \lesssim 1 \tag{1}$$

For number of stable molecules [2] we have observed that

$$R(E_i) \cong R_p, \quad \text{for} \quad E_i \cong E_p \tag{2-a}$$

$$\cong 1, \quad \text{for} \quad E_i > E_p \tag{2-b}$$

where, E_p stands for the incident energy at which the calculated Q_{inel} attains its maximum and the value of R_p varies from 0.7 to 0.8 depending on the target and the ionization threshold. It is convenient to represent [3] the ratio R as a continuous function of energy ($E_i > I$) in the following manner.

$$R(E_i) = 1 - C_1\left[\frac{C_2}{U + a} + \frac{\ln(U)}{U}\right], \quad U = \frac{E_i}{I} \tag{3}$$

PS-21

Figure 1

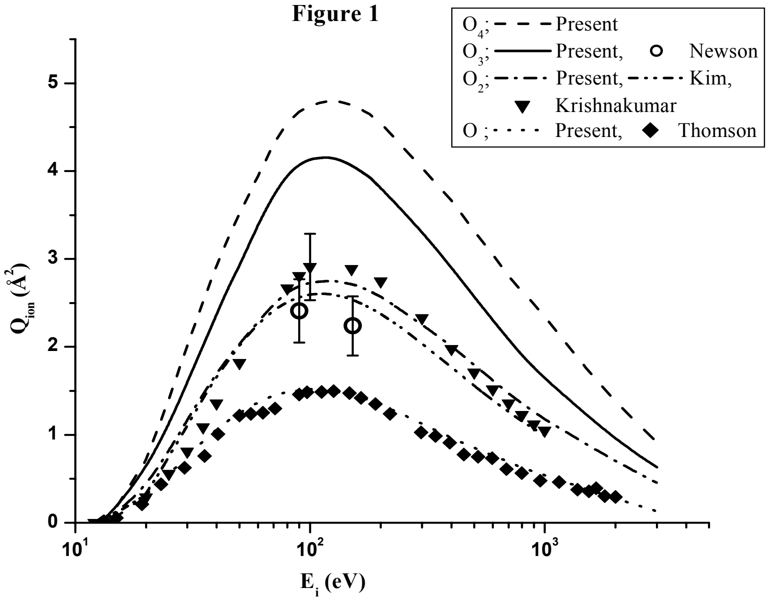

Figure 1 reveals details of the present total ionization cross-sections for all the Oxygen targets. The present calculations on the Q_{ion} for O_2 molecule find a good accord with the measurements of Krishnakumar & Srivastava [4], within their 10% error margin. Also shown here for comparison, are the present total ionization cross sections of O_3. These are larger than those of O_2, and we find from our results that at the peak position near 100 eV,

$$\frac{Q_{ion}(O_3)}{Q_{ion}(O_2)} = 1.52$$

The above value is quite close to the ratio 1.5 of the respective total number of electrons.The present investigation includes our study on the electron scattering and ionization of the *dimer* $(O_2)_2$, about which nothing much is known at present. The motivation for this study comes from the fact that dimers and clusters are exotic forms of matter, and that their investigation requires electron impact cross sections including those of ionization. All the present total ionization cross sections given in this figure are consistent with the respective target properties of the oxygen species, viz. ionization threshold, the bond lengths and the total number of target electrons.

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PS-22

LOW-ENERGY SMALL CLUSTER – SURFACE IMPACT: NANO-HILLOCK AND CRATER FORMATION STUDY

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Because of the novel properties of ionised clusters and their unique interactions with surfaces, compared to monomer ions, beams of cluster ions can be a very powerful tool for solid surface modification, which is in great demand for modern nanotechnology and nanoelectronics. Upon impact, energetic cluster ions can cause multi-collisional highly inelastic processes in a very shallow surface layer of solids. Very smooth thin films can be produced using such a technique of Energetic Cluster Deposition [1]. High intensity ion cluster beams (ion fluences 10^{14}-10^{16} ions/cm^2) produced from gaseous precursors and accelerated to high energies are also very efficient for smoothing of originally rough solid materials [2]. In spite of a rapidly growing interest in this field both in experiment and in theory there is no clear understanding of the processes occuring during the cluster-surface impact.

In this paper recent experimental results on surface bombardment by Ar_n^+ and $(N_2)_n^+$ cluster ions are presented. Si (111) samples (1x1cm) with a native oxide layer thickness of about 1-2 nm were chosen as a target material. The ion cluster beam with typical mass distribution in the range of n = 1-100 atoms for argon and n = 1-50 molecules for nitrogen was produced by a pulsed supersonic valve (Even-Lavie) with an ioniser mounted on its outlet. Produced cluster ions were then accelerated to energies from 2 up to 18 keV/cluster, focused, mass selected and steered towards the Si substrate orientated normally with respect to the beam axis. The cluster ion beam fluence after manipulation with ion optics, mass selection and aperturing the beam was in the range of $1 \cdot 10^8 - 5 \cdot 10^9$ ions/cm^2. Implantation was perfomed in vacuum of about $1 \cdot 10^{-6}$ Torr [3]. Finally, the implanted surfaces were studied using atomic force microscope in tapping mode.

Typical results of Ar_n^+ cluster collisions with a Si (111) surface are shown on the Figure.1a,b. The formation of pillar-like structures or hillocks of a few nm in height is observed for the smaller $Ar_{12\pm1}$ clusters impacting on Si (Fig 1a). Together with hillocks the presence of craters on the same implanted surfaces are found and with an increase of the cluster size up to $Ar_{55\pm1}$, while keeping the same energy per mass value the crater formation process starts to be dominating over the hillock formation (Fig 1b). There is some intermediate regime when the hillock is formed in the very center of a crater or the hillock is surrounded by a rim (Fig 1a). In general, the shape of the nanostructures is highly dependent on the cluster specie, size and implantation energy. The results of systematic measurements is presented and possible formation mechanisms for hillocks and craters is discussed.

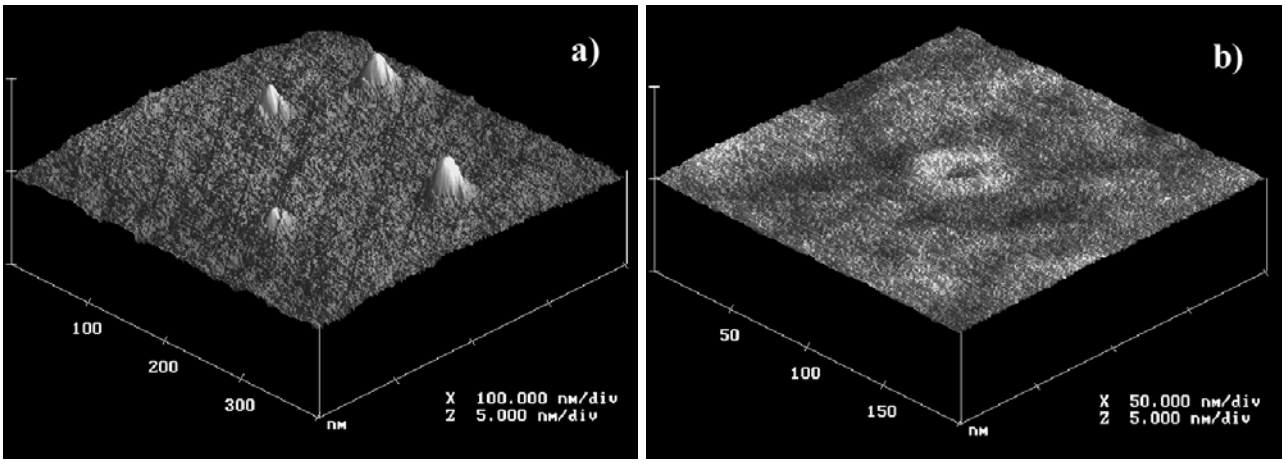

Figure 1: The results of the impact of Ar_n clusters on the Si (111) substrate oriented normally with the respect to the beam: a) hillock fomation after the $Ar_{12\pm1}$ impact with energy E = 3 keV/cluster; b) crater formation due to the $Ar_{55\pm1}$ impact with energy E = 15 keV/cluster.

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PS-23

DETECTION OF TWO-PHASE STATE IN FREE ARGON CLUSTERS

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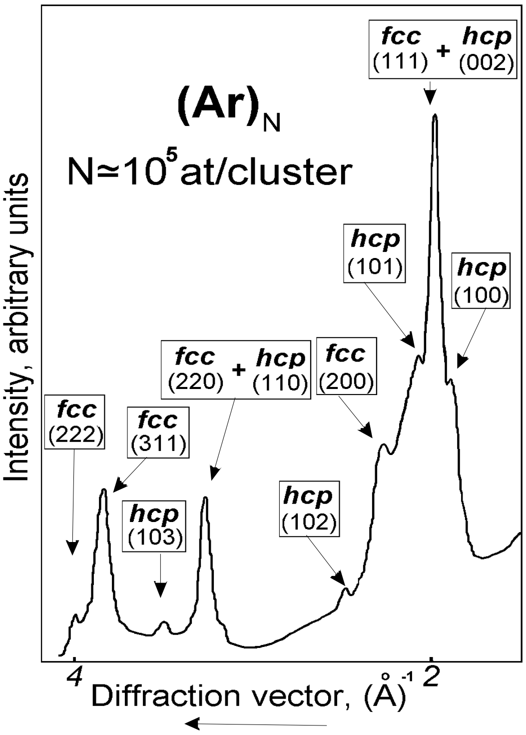
It is known that bulk inert gases (except for helium) can crystallize into the *fcc*-lattice. This experimental fact is not trivial at all since the calculation allowing for the pair atom interaction predicts high stability for the *hcp*-structure. Only the effects of the multiparticle interaction provide a small energy gain for the *fcc*-lattice. Since the *fcc-hcp* structural transition entails a certain decrease in the surface energy at the faces perpendicular to the (111) plane, the *hcp* phase has long seemed plausible in small atomic inert-gas aggregations, where the surface contribution is quite appreciable. The idea however has to be substantiated experimentally. It is most correct to investigate the dimensional structural effects on complexes (clusters) formed in an adiabatically expending gas jet. Such clusters always have equilibrium structures and they do not interact with the substrate.



Earlier structural investigation of crystalline inert gas clusters of (10^3 - 10^4) at/cluster have detected an *fcc*-structure with stacking faults [1] which may be considered as nuclei of the *hcp*-phase. In this study the structure of argon clusters is investigated in a wider range of the mean size N. The electron diffraction observation was performed using a supersonic cluster beam generator. The mean cluster size was varied form 10^4 to 10^5 at/cluster. The diffraction from the N≈10^4 at/cluster corresponded to the *fcc*-structure, the resolution of the (111) and (200) peaks was however poor. As simulation of the diffraction function shows [2], such situation can appear when the atomic packing contains the *hcp* arrangement along with the *fcc* one. As the cluster size increases to 10^5 at/cluster, the character of the diffraction pattern changes. Along with the *fcc*-structure, the (100), (101), (102), (103) peaks are observed, which are typical only for the *hcp*-structure (fig.).

We may anticipate the following mechanism of the formation of the *hcp*-phase. The stacking faults of the *fcc*-lattice are small nuclei of the *hcp*-phase. When their density is high, supercritical nuclei become probable. The growth of such nuclei is favoured by the rather high temperature (~50K) of large clusters.

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PS-24

PROPERTIES OF GOLD AND SILVER CLUSTERS DOPED WITH TRANSITION METAL ATOMS

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Properties of small metal clusters are governed by the interplay between electronic and structural effects. A wide range of physical properties often could be explained on the basis of shells of electrons, with valence electrons moving freely in an effective model potential, or shells of atoms where geometric aspects dominate. More information on this interplay can be deduced from the study of *bimetallic clusters* consisting of simple element atoms (e.g. coinage metals) and more complex atoms (e.g. transition metals). In such systems the number of itinerant electrons and the number of atoms can be varied independently. Also, different interatomic interactions between the heteroatoms will determine the electronic and geometric structure.

We investigated bimetallic clusters consisting of transition metal dopant atoms embedded in coinage clusters (Ag_NX and Au_NX^+ with N<45, X = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Zn), produced with a dual-target dual-laser vaporization source [1]. Abundances as a function of cluster size and composition were recorded using reflectron time-of-flight mass spectrometry following photofragmentation with high fluence UV laser light (> 10 mJ/cm², 193 nm). These data were used to deduce size and composition dependent cluster stability information.

Quantum chemical computations were performed to elucidate the factors that control the structure and stability of bimetallic systems composed of noble metal atoms and transition metal atoms. We have focused on neutral Zn-doped Au clusters and their cations. Stable structures for each cluster size (N=2-6) were investigated by using ab initio molecular orbital calculations.

In this contribution we will discuss composition-dependent stability features observed in the abundance spectra in terms of electron delocalization. In particular we will focus on: (i) the *dopant and size dependent* number of delocalized electrons [2], (ii) the relation between the amplitude of the *odd-even abundance staggering* and the energy difference between a $3d^x4s^2$ to a $3d^{x+1}4s$ electronic configuration of the dopant atom [2], (iii) *composition-dependent* magic numbers corresponding to spherical (3D) and planar (2D) closed electron shells [3], and (iv) quantum chemical calculations predicting *planar ground state structures* for Au_NZn^+ (N=2-6) [4].

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PS-25

CATALYTIC FORMATION OF WATER ON FREE PLATINUM CLUSTERS

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The adsorption of oxygen and hydrogen on small platinum clusters has been investigated in a cluster beam experiment [1]. A beam of clusters seeded in He gas is generated in a pulsed laser-vaporisation source. After expansion the beam passes a skimmer and then two collision cells, in which a low pressure of a reactive gas can be maintained. The clusters, with or without adsorbed molecules, are detected with laser ionisation (λ=157 nm) and time-of-flight mass spectrometry. By measuring the number of molecules adsorbed on the clusters as a function of pressure in the collision cells, the reaction probability in a cluster–molecule collision can be determined using a pseudo-first-order kinetic model [2].

Pt_7 is the smallest cluster for which we detect a stable Pt_nO_2 product and then the reaction probability for the first O_2 molecule increases with n up to $n \approx 14$, where it reaches a value of approx. 0.25. This value is in the same range as the reaction probability measured for Pt_4^-–Pt_7^- [3]. For clusters with $n>15$ also products with more than one O_2 molecule are detected. The reason for measuring a lower reaction probability on the smaller clusters is probably that these are more likely to fragment as a consequence of the heat released by the exothermic reaction [2]. For hydrogen adsorption we cannot distinguish any Pt_nH_2 peaks, since the width of the Pt_n-peaks are, due to the isotope distribution, broader than the mass difference of adding a hydrogen molecule even if the heavier deuterium isotope is used. However, from observing a shift to higher masses of the combined Pt_n, Pt_nD_2, Pt_nD_4, etc. peak we can conclude that D_2 adsorb on the platinum clusters, though an accurate determination of the reaction probability is difficult.

When one reaction cell contains O_2 and the other one D_2 the resulting mass spectrum deviates from a simple co-adsorption spectrum in which the respective contribution of the two gases would be added. Instead, we observe that the number oxygen atoms adsorbed on the clusters decreases with increasing D_2-pressure. The only reasonable explanation for this is that D_2O molecules form and desorb from the cluster surface. This reaction takes place throughout the investigated cluster size-range Pt_7-Pt_{30} and with a high efficiency. In a similar way as the reaction probability for the addition reaction is determined, the probability for the removal of an oxygen atom after a collision between a Pt_nO_m cluster and a D_2 molecule can be evaluated. The oxygen removal probability varies between 0.15 and 0.35 with no distinct trend with size.

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PS-26

MD SIMULATIONS OF HIGH-ENERGY NANOPARTICLE IMPACT AND PENETRATION PROCESS ON DIAMOND SURFACE

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By using molecular dynamics (MD) simulations, the cluster impact process on a diamond surface was studied in order to investigate highly energetic cluster-surface interactions. In addition to the surface erosion and polishing, a possiblity to use accelerated metal clusters in order to implant supported cluster dots on a graphite surface is indicated [1]. The authors have performed large-scale MD simulations of single Ar_n or $(CO_2)_n$ ($n \cong 960$) cluster impacts on a diamond (111) surface with the impact energy E_a from 10 up to 100 keV/cluster [2], and the formation of a hemispherical crater and two or three-layered induced shockwaves were observed at the early stage of the impact process at $E_a = 100$ keV. Rebounding hot fluidized carbon material was then seen to replenish the transient crater very quickly until 2 ps, with a central peak appearing as a long time phenomenon only in the case of a CO_2 cluster impact. In addition, the number of carbon atoms emitted from the target was much larger for a CO_2 cluster impact than for an argon cluster impact with a factor of 3.35 at $E_a = 100$ keV, and that corresponded well to our experimental results [3].

Figure 1 shows the comparison of CO_2 and heavy cluster impacts at $E_a = 100$ keV, where only the mass of the carbon atoms in the heavy impact cluster is substituted by that of tungsten (183.84 amu). The brightness of carbon atoms corresponds to the velocity here. The CO_2 cluster has reached the bottom at 0.7 ps [Fig. 1(a-i)], while the heavy cluster still goes into the solid surface as shown in Fig. 1(b-i). The heavy cluster finally stops penetration at about 1.5 ps [Fig. 1(b-ii)], when the fluidized carbon material has already replenished part of the hole above the cluster, and the embedment of a heavy cluster is thus achieved using the accelerated heavy cluster. The dependence of penetration depth on the cluster size, density, and acceleration energy will be considered.

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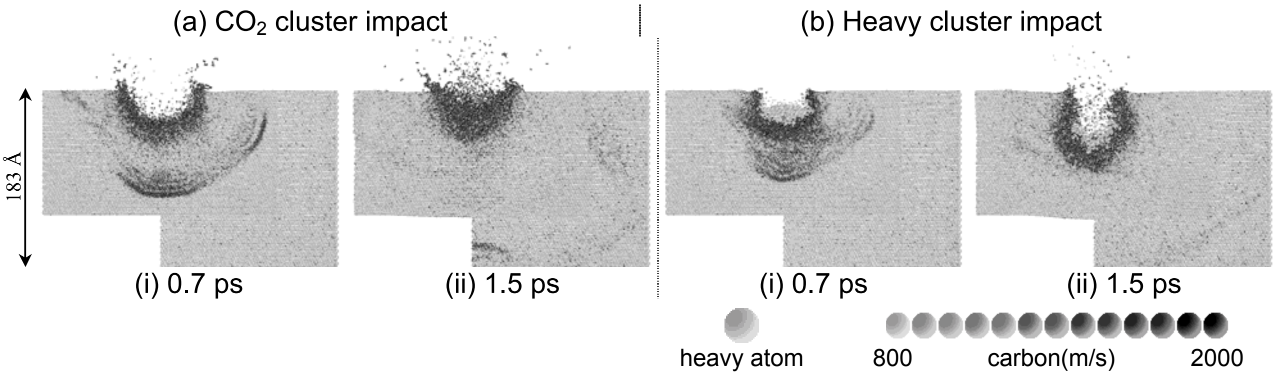

Figure 1: Comparison of CO_2 and heavy cluster impacts at an acceleration energy E_a of 100 keV/cluster (10 Å cross section).

PS-27

CHARGE TRANSFER AND FRAGMENTATION AT ION-FULLERENE COLLISIONS.

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Electron capture of one or several electrons from C_{60} molecule by projectile ions H^+, He^{2+} and Ar^{6+} in KeV energy range was studied. The capture can be followed by a number of processes connected with additional ionization and fragmentation of the C_{60} molecule. All these processes can be divided into four groups :

$$Ar^{z+} + C_{60} \to Ar^{(z-q)+*} + C_{60}{}^{q+}* \to \begin{cases} Ar^{(z-s)+} + C_{60}^{(s+r)+} + re^-, & (1) \\ Ar^{(z-s)+} + C_{60-2n}^{(s+r)+} + C_{2n}^{0} + re^-, & (2) \\ Ar^{(z-s)+} + C_{60-m}^{(s+r-k)+} + C_m^{k+} + re^-, & (3) \\ Ar^{(z-s)+} + \sum\limits_{m,k} C_m^{k+} + re^-, & (4) \end{cases}$$

where (1) is capture with ionization, (2)- the same supplemented by detachment of neutral clusters consisting of even number of carbon atoms, (3) –asymmetric breaking up into light and heavy positively charged fragments, (4) – multiple breaking up into several light charged fragments. ($Ar^{(z-g)+*}$, $C_{60}{}^{q+*}$ are intermediate excited charged states of particles).

Because of differences between ion-molecule collision time and life-times of various exited and autoionizing states the accompanying ionization can occur both during the collision in quasimolecule and after collision in separated particles.

The employed experimental technique enabled to measure the mass-composition of ions formed from a fullerene molecule in collision when the projectile have captured a definite number of electrons and thus to study the correlation between capture processes and relative probabilities of ionization and fragmentation processes (1)- (4).

As an example of obtained results Fig.1 shows the time-of-flight (TOF) mass-spectra of fullerene fragment ions registered in coincidence with projectile ions captured certain number of electrons S which was changed consequently from 1 to 6. As regards ionization so it is seen that the capture of one electron S=1 can be followed by additional ionization leading to formation of multicharged ions $C_{60}{}^{2+}$ and $C_{60}{}^{3+}$. The same situation takes place at one electron capture by protons as projectiles. This fact as well as formation of two and more free electrons in the case of multicharged projectiles can not be explained by formation of projectile ions in autoionizing states. The cross section of direct ionization at collision condition under study are small so the observed additional ionization is connected, probably, with autoionizing states of fullerene ions.

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Fragmentation processes for proton projectile have small cross sections and are connected mainly with detachment of neutral clusters (reaction 2) . However intensive

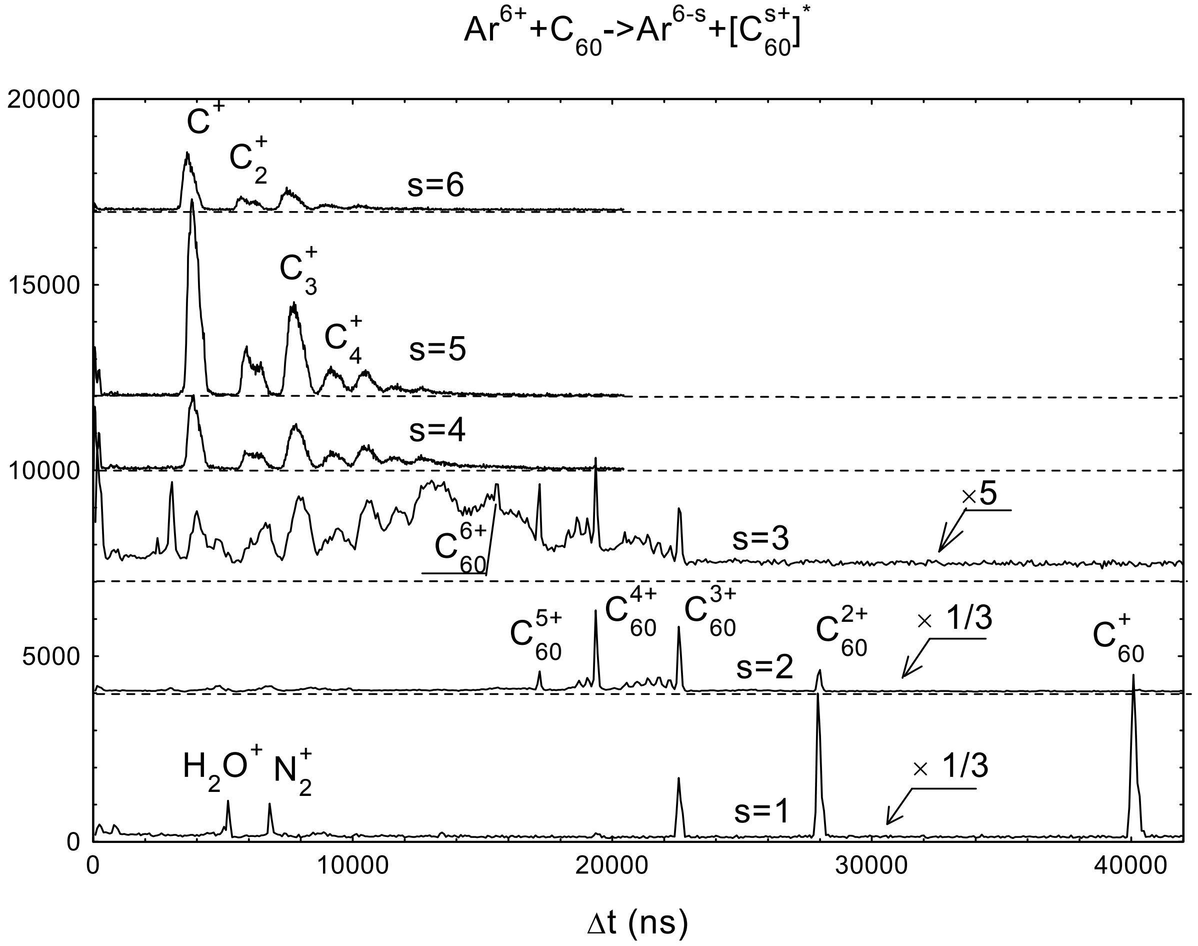

Fig. 1. TOF coincidence mass spectra of fragment ions for 60 KeV Ar^{6+} collisions with fullerene C_{60} at certain number S of captured electrons. Zero lines of spectra with different number stabilized captured electrons are indicated by dotted lines and shifted on Y axis.

fragmentation corresponding to all processes (1)-(4) take place at two-electron capture by He^{2+}projectile, where process (4) dominates. In the case of Ar^{6+} projectile the fragmentation processes following Fig.1 capture of more then two electrons (s>2) and at capture of 4-6 electrons leads to mainly to multiple fragmentation (process 4).

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CHARGE TRANSFER FROM FULLERENES TO ATOMIC IONS

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Charge transfer processes in slow collisions between C_{60} and noble gas ions: Ar^{q+} ($q \geq 4$) and He^{2+} have been investigated. We used two different models. The first model is as follows: the fullerene is being described as an infinitely conducting sphere (ICS) with the radius of 8.52 a.u. Atomic ions are assumed to be point masses. The charge transfer process is considered as a transition of electron through and over the coulomb potential barrier formed by the atomic ion and ICS (image potentials have been taken into account). The decay model [4] has been used to account for the time-dependence of the potential. The process of multiple charge exchange is considered as succession of single charge exchanges. Partial wave decomposition has been employed and we assumed that the partial phase shifts were mostly dominated by the elastic scattering processes. For the calculation of the transition coefficient, the method previously developed [3] has been used.

In the second model we start with the two close-coupling equations. Using the asymptotics of the fullerene ground state wavefunction, the exchange matrix elements have been calculated. They are then reduced to one second-order differential equation that has the form of the barrier transition equation with the complex potential. We solve the equation using a newly developed approach and obtain the charge transfer S-matrix elements.

Differential, total and partial (in the number of the transferred electrons) cross sections for the charge transfer have been calculated using the two models. We have compared the results and it turned out that in case of highly charged ions ($q \geq 4$) and low relative velocity ($v_{rel} \leq 0.5$ a.u.) both models provide practically the same results (the use of the first model is preferable here because it requires much less time for calculations), but in case of higher velocity ($v_{rel} \geq 0.5$ a.u.) or low charge of the atomic ions the first model fails to reveal the correct velocity behavior of the cross sections while the second model gives better predictions. In figure 1 we present the total cross sections for the following charge-exchange process: $C_{60}^{+} + He^{2+} \rightarrow C_{60}^{2+} + He^{+}$. The original experimental data will be presented at the conference. The results for collisions of fullerenes with Ar^{q+} are in good agreement with the experimental data [1], [2].

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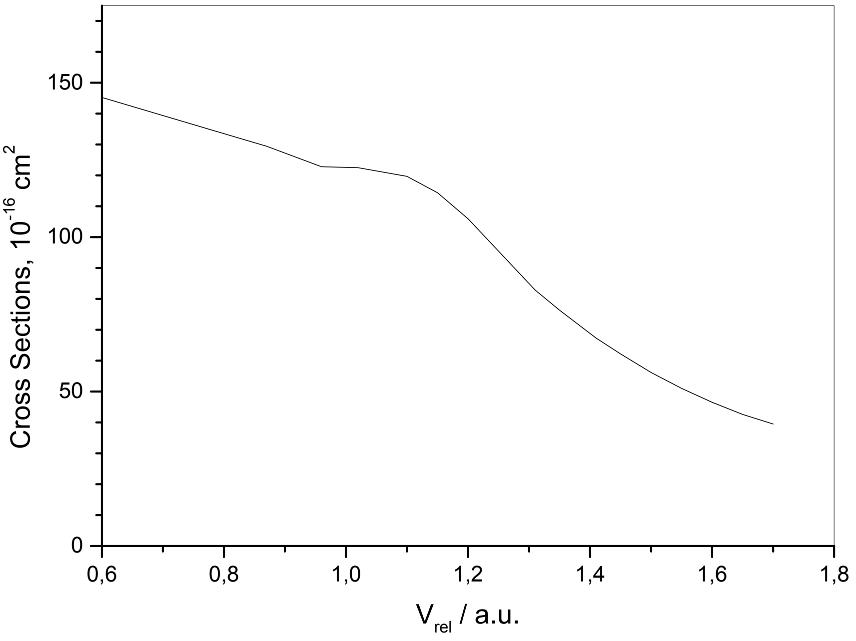

Figure 1: Total cross sections for the process $C_{60}^{+} + He^{2+} \rightarrow C_{60}^{2+} + He^{+}$ as functions of the relative velocity calculated using the second model.

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PS-29

THEORETICAL STUDY OF DISSOCIATION ENERGIES OF C_n^{q+} ($50 \leq n \leq 60$) FULLERENES FORMED IN ION–C_{60} COLLISIONS.

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In the last decade a huge number of experimental studies have been devoted to the study of C_{60} and its fragmentation process (see for instance, [1] and [2]). These efforts have led to significant theoretical advances in order to understand its structure and high stability against fragmentation. The unusual stability of C_{60} among carbon clusters is due to the high symmetry of the carbon cage: a truncated icosahedron. In contrast, our knowledge of fullerenes with low or no symmetry is still limited. Theoretical modeling of these clusters is more involved because one cannot rely on symmetry to simplify the search for a global energy minimum.

The dissociation energy of C_{60} into C_{58} and C_2 has been the subject of intense controversy and debate for almost a decade (see e.g. [3]). In contrast with the large number of experimental and theoretical works devoted to determine the binding energies of C_{60} and C_{60}^+, there have been much less attempts to determine these quantities in smaller fullerenes, either neutral or positively charged. From the theoretical side, the most complete calculation of dissociation energies for fullerenes containing less than 60 atoms have been performed by Zhang et al. [4], but only for neutral systems. These authors have determined dissociation energies for fullerenes as small as C_{20} by using a tight-binding method. Except for the C_{60} and C_{60}^+ (studied extensively by Scuseria et al. [5]), high level theoretical calculations of binding energies and geometries have not yet been carried out for smaller fullerenes and larger charges.

In this communication we present accurate DFT calculations (B3LYP/6-31G(d)) of the structure and energies of different C_n^{q+} fullerenes. We have performed geometry optimizations at DFT level for the neutral, singly–charged and doubly–charged fullerenes for n =50, 52, 54, 56, 58 and 60. In all cases several isomers have been considered in order to determine which is the most stable conformation. From these calculations dissociation energies and ionization potentials for the different species have been obtained. This information is essential to analyze the fragmentation patterns observed in collisions of fullerenes with various targets: atoms, molecules, and ions [1]. Our results compare fairly well with the available experimental data for the dissociation and ionization energies and permits to understand the tendencies observed in these quantities as a function of the size and the charge of the initial cluster.

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PS-30

ELECTRON CAPTURE IN C_N^+ CLUSTER - ATOM COLLISIONS AT INTERMEDIATE VELOCITY (N≤9)

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In this work, dissociative and non dissociative electron capture in C_n^+ clusters- atom collisions at intermediate velocity (v=2.6au) has been studied. This work is an extension, to n=9 and for different target atoms, of a previous study restricted to n=5 (cross sections), n=4 (dissociative branching ratios) and Helium atom as a target [1]. Here, thanks to a new experimental tool based on shape analyses of current pulses delivered by semiconductor detectors [2], all branching ratios of de-excitation could be measured, up to n=9 [2,3].

In figure 1 and 2 are reported measured branching ratios for all de-excitation channels of, respectively, C_5 and C_9 following electron capture in C_5^+, C_9^+ -> He collisions, plotted as a function of calculated dissociation energies (DFT-B3LYP calculations [4]). The dominance of dissociative fragmentation, amounting to 85%-90%, is surprising and must be attributed to a cluster effect since, in the ion atom collision C^+->He at the same velocity, electron capture occurs predominantly into the ground state as calculated within Continuum Distorted Wave theory [5].

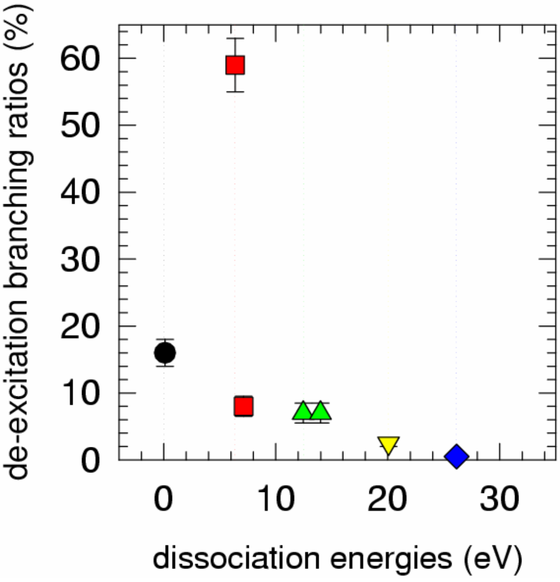

Figure 1: Measured de-excitation branching ratios of C_5 as a function of calculated dissociation energies. Circle: intact C_5; Squares: two-fragments channels (C_3/C_2 and C_4/C); Triangles up: three-fragments channels ($C_3/2C$ and $2C_2/C$); Triangle down: four-fragments channel ($C_2/3C$); diamond-shape: five-fragments channel (5C).

In order to understand this phenomenon, the following procedure has been followed. Using the predictions of the Weisskopf statistical theory [4], an energy distribution has been extracted for C_n clusters from measured branching ratios. This energy is the sum of the internal energy prior to the collision (initial temperature) and the energy deposited in the system by electron capture. The internal energy of clusters, of the order of 0.3 eV by degree of freedom, is determined confidently from cluster intensities obtained at the cluster source. The obtained value is consistent with the value extracted by other means, in particular analysis of branching ratios of de-excitation of C_n^+ and C_n^{++} as well. Having subtracted this internal energy part, it turns out that electron capture is still found to bring in all cases energy to the system, of the order of 5/6 eV (C_5 case). Possible explanations and associated theoretical work will be presented at the conference.

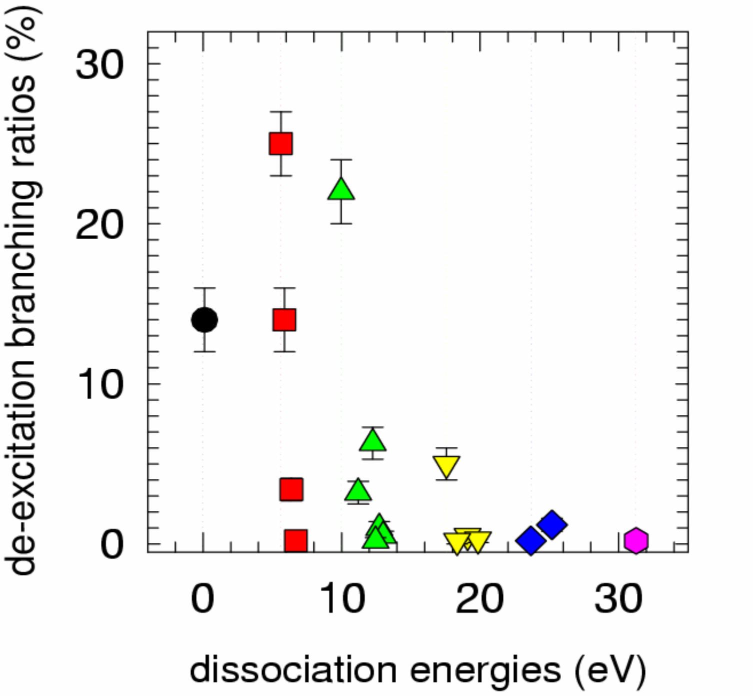

Figure 2: Measured de-excitation branching ratios of C_9 as a function of calculated dissociation energies [3].

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PS-31

EVAPORATION DYNAMICS OF MIXED LENNARD-JONES CLUSTERS : AN ENHANCED ACCESS TO THE MELTING TRANSITION

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The unimolecular evaporation process in homogeneous clusters has been studied by different authors using microcanonical simulations during the last few years [1]-[6]. In particular, it has been demonstrated that the evolution of the mean kinetic energy release as a function of the initial internal energy can be affected by the solid-liquid like phase transition in the product cluster [3],[6].

In this contribution, we present numerical results obtained from Molecular Dynamics (MD) simulations, which have been run to study the evaporation process of a model mixed Lennard-Jones cluster, namely Ar_nX_m, in which X is an artificial atom whose properties can be adjusted [7]. The influence of changes in its Lennard-Jones parameters (binding energies D and distance σ) and its mass has been explored in a systematic way in the case of various 7-atom clusters on: i) the outcome of Ar_3X_4 evaporation (chemical composition of the product cluster) and ii) the evaporation rate constant in the series of $Ar_{7-m}Kr_m$. It is shown that a proper choice of the X atom parameters allows to enhance the evaporation rate constant of Ar_nX in a way which enables to explore by MD the dynamics at much lower values of internal energy. Consequently the "melting" transition in Ar_7 and Ar_{13} product clusters can be directly investigated by the analysis of the mean kinetic energy release. In the latter case it is shown to be in excellent agreement with phase space theory predictions.

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PS-32

STATISTICAL EVAPORATION OF ROTATING CLUSTERS

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During these last years, phase space theory has shown its ability to describe accurately the evaporation process for nonrotating clusters [1],[2]. However, rotation can strongly affect the structure, dynamics and thermodynamics of molecular systems. In addition, angular momentum cannot be experimentally constrained to be zero.

In this contribution, unimolecular evaporation in rotating clusters is investigated using phase space theory (PST) and molecular dynamics simulations [3]. The rotational densities of states are calculated in the sphere+atom approximation [4], and analytical expressions are given for a radial interaction potential with the form $-C/r^p$. The vibrational densities of states are calculated using Monte Carlo simulations, and the average radial potential at finite temperature is obtained using a recent extension of the multiple range random-walk algorithm [5],[6]. These ideas are tested on simple argon clusters modelled with the Lennard-Jones (LJ) interaction potential, at several total energies and angular momentum of the parent cluster. Our results show that PST successfully reproduces the simulation data, not only the average kinetic energy release but its probability distribution, for dissociations from LJ_{14}, for which the product cluster can effectively be considered as spherical. Even for dissociation from the nonspherical LJ_8, simulation results remain very close to the predictions of the statistical theory.

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PS-33

INFRARED MULTIPLE PHOTON DISSOCIATION SPECTROSCOPY OF CLUSTERS AND CLUSTER ADSORBATE COMPLEXES

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Nanosized particles are important for industrial applications, such as heterogeneous catalysis or future electronic devices. However, their structures on an atomic scale are mostly unknown and little information has been inferred by indirect experimental methods. A more direct method to acquire structural information on these particles is based on the measurement of vibrational spectra of isolated gas phase clusters, in combination with complementary quantum chemical calculations.

Recently, vibrational spectra of metal oxide and carbide clusters in the gas phase have been obtained via IR resonance enhanced multiple photon ionization (IR-REMPI) spectroscopy [1,2]. IR multiple photon dissociation (IR-MPD) spectroscopy complements the ionization spectroscopy and extends the range of materials that can be studied in their cluster state as well as allows for studying of weaker bound cluster complexes [3].

In this study, IR spectra of metal oxide cluster cations and cluster adsorbate complexes are measured using IR-MPD spectroscopy. For example, structures of selected group Vb (V, Nb, Ta) metal oxide clusters can be identified by comparison with quantum chemical calculations [4]. The metal oxide clusters form complexes with hydrocarbons, which may be intermediates for hydrocarbon oxidation. In the case of small niobium and vanadium oxide clusters, IR spectra of ethylene - cluster adducts lead to the identification of the binding sites of the hydrocarbon.

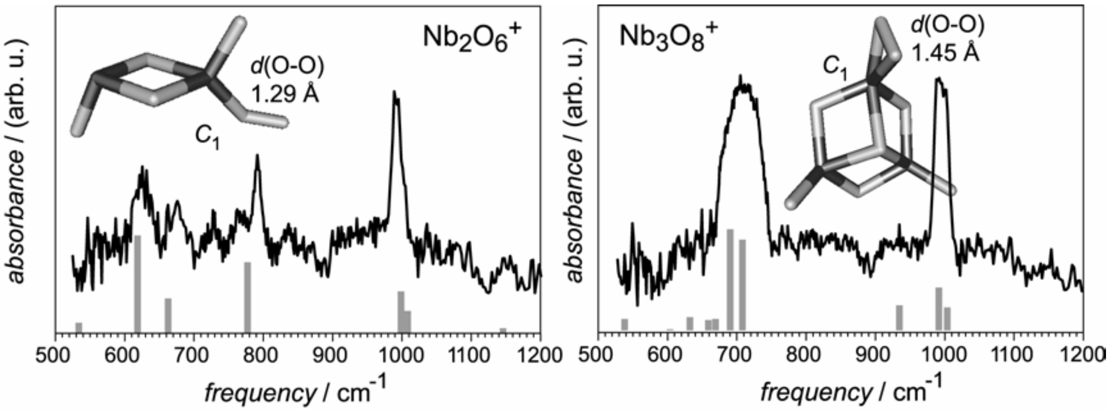

Figure 1: Experimental infrared spectra of small niobium oxide cluster cations obtained via IR multiple photon dissociation in comparison to the calculated spectra for the most stable isomers.

Furthermore, IR spectra of carbon monoxide adsorbed on neutral and cationic rhodium clusters are presented. These spectra give insights in the binding situation of the CO and open a method for probing the structure of metal cluster structures. Through comparison with known properties of CO adsorbed on single crystal surfaces and highly dispersed supported particles the studies of gas phase clusters are directly relevant for the understanding of metal cluster - support interactions.

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PS-34

IONIZATION AND FRAGMENTATION OF C_{70} BY SLOW HIGHLY CHARGED IONS

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Here, we report on the first detailed study of electron capture, ionization, and fragmentation measurements in collisions between slow highly charged ions and C_{70}. The experiment yields coincidence information on the number of electrons stabilized on the projectile, the projectile scattering angle, and the final kinetic energy distributions of intact and fragmented C_{70}. The experimental technique is identical to the one reported earlier for similar collisions with C_{60} [1, 2]. The mass distribution for a given number of electrons stabilized on the projectile have similar features, relating to evaporation ($C_{70}^{r+}\rightarrow C_{68}^{r+}+C_2$) and asymmetric fission ($C_{70}^{r+}\rightarrow C_{68}^{(r-1)+}+C_2^{+}$), as those recorded earlier for C_{60}. Fig. 1 shows a mass spectrum taken in coincidence with one, two and three electrons stabilized ($s = 1 - 3$) on 70 keV Xe^{23+} after colliding with C_{70}. However, for lower projectile charges the C_{60} fragment ions becomes a more prominent product in the decay of C_{70}-ions. The highest observed charge state of C_{70} is 9+, which again is similar to the observations using similar ionization methods for C_{60}.

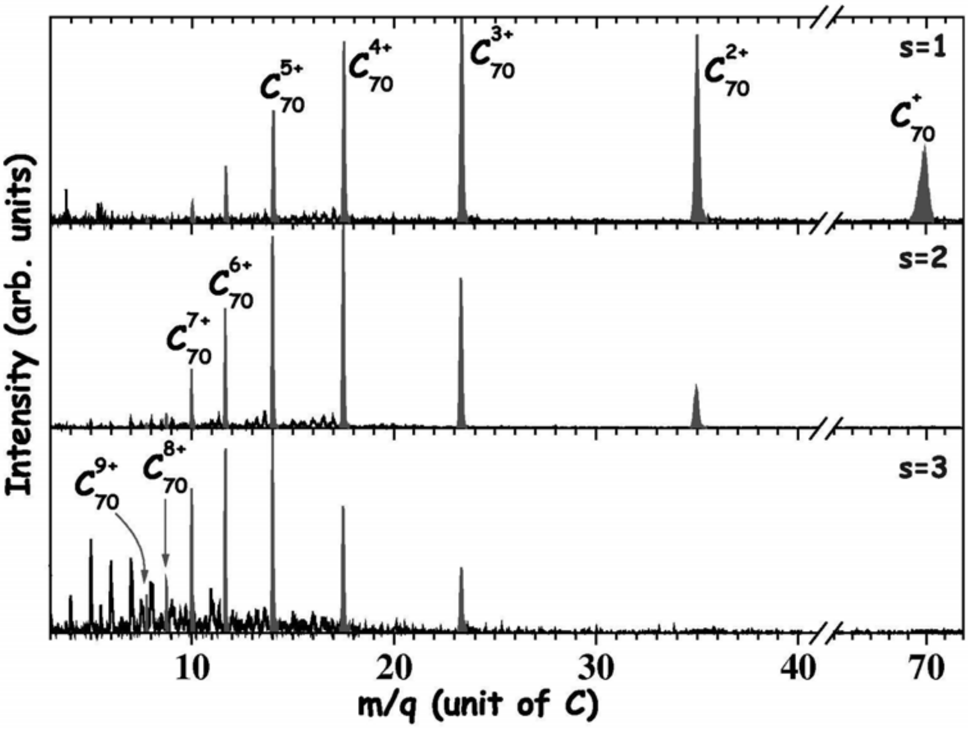

Fig. 1. Mass spectra of the collision products from 70 keV Xe^{23+} collisions with C_{70} taken in coincidence with one, two and three electrons stabilized on the projectile.

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We have further measured kinetic energy releases (KER) in asymmetric fission and evaporation using a novel technique in which the initial momentum distribution of the C_{70} molecules are strongly limited in collisions with highly charged ions [1, 2]. From the two-dimensional position distributions on a recoil detector at the end of a linear time-of-flight mass spectrometer, it is possible to extract the kinetic energy releases for emitting a single C_2-unit (charged or neutral). In Fig. 2 we show the measured KER values for the process where C_{70}^{r+} emits a single C_2^+-unit or a neutral C_2 as a function of the final C_{68}-fragment charge state. This is compared with earlier measurements using the MIKE-scan technique (Mass-analyzed Ion Kinetic Energies) [3, 4]. The measured KER values for $C_{70}^{r+} \rightarrow C_{68}^{(r-1)+} + C_2^+$ are significantly different from previous measurements [3]. Furthermore, there is a clear difference in the KER values obtained after fragmentation induced by Xe^{8+} and Xe^{16+}/Xe^{23+} collisions. This signals different energy transfers in the two cases - a feature which was not clearly observed so far for C_{60} fragmentation following different excitation schemes. Our obtained KER values for C_{70}^{r+} are very similar to the ones for C_{60} ions when it comes to asymmetric fission [5], which can be understood through similarity in sizes. This may further suggest that the fission barriers for C_{70} ions are close to those for C_{60}-ions, under the assumption that the C_2 activation energies and ionization potentials for C_{70} are similar to the corresponding values for C_{60}.

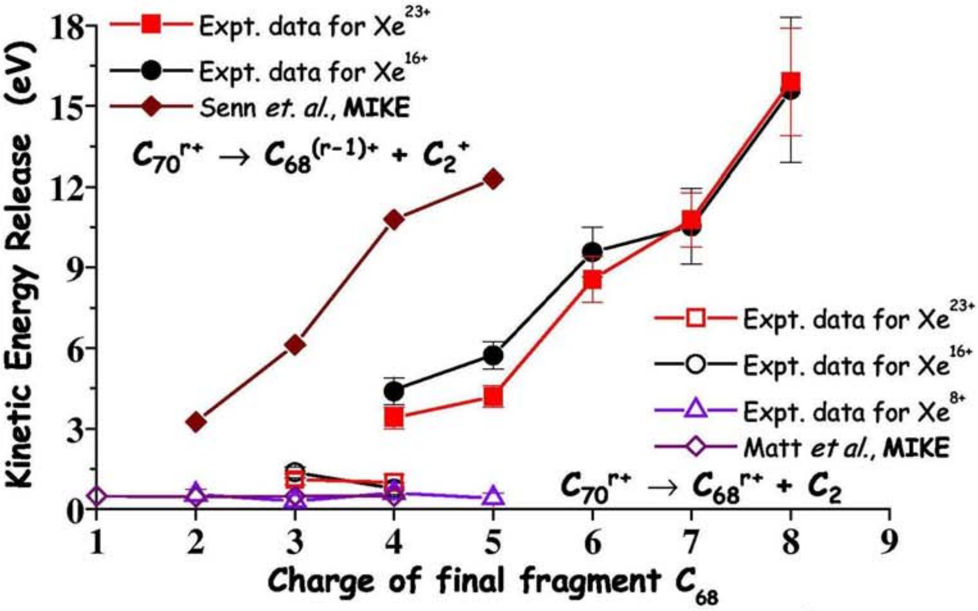

Fig. 2. Experimental kinetic energy releases for the process where C_{70}^{r+} emits a single C_2-unit (charged or neutral) using different projectiles, compared with existing measurements [3, 4]. Solid points: fission; Open points: evaporation.

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PS-35

DOUBLE PHOTOEMISSION OF FULLERENES AND METAL CLUSTERS

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Plenty of electronic states delocalized over the surface of the fullerene molecule or metal cluster make them particularly interesting candidates for the investigation of the electronic correlations. Scattering reactions dominated by electron correlations is the multiple ionization by the photon or electron impact. In double photoionization (DPI), a single photon with sufficient energy ionizes two electrons simultaneously. In order to take part in such a process, electrons of the target have to be strongly correlated. For the description of the multiple photoionization of free nanoparticles, we used two different approaches. In the first one we calculate the DPI cross section and the ratio of double to single photoionization probabilities in the lowest order of perturbation theory, including photon-electron and electron-electron interactions only once. The second approach used in this work is the statistical energy deposition model [1]. After the absorption of the photon by one of the target electrons, its kinetic energy is transferred and distributed among electronic excitations of the cluster, after which the system autoionizes to reach its final n-fold ionization state. The quantum states of the cluster are constructed within the Hartree-Fock approximation. In order to efficiently deal with the non-local Fock integrals, we use the method, relying on the variable-phase approach, described in [2]. The matrix element of the electron-electron interaction is calculated within the random phase approximation with exchange [3].

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PS-36

CORRELATION BETWEEN MULTIPLE IONIZATION AND FRAGMENTATION OF C_{60} INUDUCED BY MeV-ENERGY ION IMPACTS

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Recently, an increasing number of studies have been performed concerning collision processes between energetic ions and fullerene molecules. Fragmentation mass spectra of C_{60} have been extensively investigated using various projectile energies, charge states and projectile species. In most collisions, the degree of fragmentation is found to have a fairy good correlation with the amount of energy transfer into a C_{60} molecule. Although the amount of energy transfer is one of the most important parameters governing the fragmentation process, it is still difficult to know the details of the fragmentation mechanism only from the energy transfer. This is due to the reason that the transferred energy may be spent on various inelastic processes such as ionization, electronic excitation and vibrational excitation. In general, two mechanisms are considered as the trigger of the fragmentation. One is the coulomb explosion of highly ionized intact C_{60} ions and the other is the fragmentation from high internal energy states. The relative importance between these two mechanisms is expected to depend on the collision conditions. For instance, the internal excitation play an important role for fast projectile ions with low charge states as reported in our paper [1].
The purpose of this work is to know the relative importance of these two mechanisms in more detail. Simultaneous measurements of fragment ions and the number of emitted electrons (n_e) were performed with a time-of-flight (TOF) coincidence method. The present experimental technique, which is similar to [2], can provide information about initial charge state (r_i) of transient states ($C_{60}{}^{ri+}**$) as well as fragmentation patterns decayed from $C_{60}{}^{ri+}**$. It would also answer a question whether the fragmentation pattern is determined only by r_i or not. Furthermore, it should be noted that the r_i-distribution obtained experimentally corresponds to the relative probability of multiple ionization of C_{60}. Thus, such information is definitely useful to develop model calculations of the multiple ionization, which is important in atomic collision physics and in radiation physics involving complicated polyatomic materials.

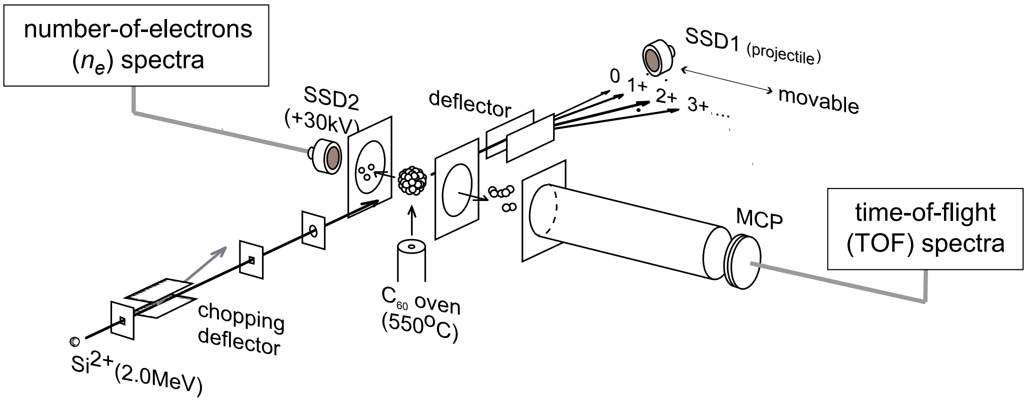

Figure 1: Experimental setup of the TOF-n_e coincidence experiment.

The experiment was performed at the 1.7 MV tandem accelerator facility of Kyoto University. A schematic diagram of the experimental apparatus is shown in Figure 1. The projectiles were Li^+, Si^{2+}, and $Au^{1\text{-}4+}$ ions in an energy range from 0.4 to 6.0 MeV. The TOF measurements were carried out using two different start-trigger modes; a beam chopping mode and a charge-changing mode. In the first mode, inclusive TOF- and n_e-spectra for all collision processes were obtained. The n_e-spectra were obtained by measurements of energy spectra from a solid state detector (SSD_2) biased to +30 kV. Namely, emission of simultaneous n_e-electrons leads to a total energy deposition of $30n_e$ keV into the SSD_2 detector.

Figure 2 shows a typical example of TOF-n_e coincidence map obtained in the chopping mode. Projection onto the X-, Y-axes gives total TOF- and n_e-spectra, respectively. An inset in the n_e-spectra represents the n_e-distribution determined by taking account of the electron backscattering effect at the detector surface [3]. One of notable features is that the n_e-distribution has a hump around $n_e = 10$, which is connected with collision events producing C_n^+ (n =1-3). One may say that the origin of the hump is the cage-penetrating collisions. The present n_e-distribution reflects certainly a new type of ionization profile which may be a typical characteristic of giant molecules like C_{60}, showing double structures originating from distant collisions and cage-penetrating collisions.

Another important result is that the fragmentation pattern from $C_{60}^{ri+}{**}$ of the same initial charge state (r_i) depends significantly on the charge-changing condition. In 2 MeV Si^{2+} collisions, for example, intensity ratios (R_f) between total fragment ions and all produced ions from $C_{60}^{3+}{**}$ (r_i =3) are 39% and 73% for $1e^-$-capture and $1e^-$-loss collisions, respectively. The difference of R_f at the same r_i indicates that the internal excitation energy is different significantly. Since the electron capture itself scarcely contributes to the increase of internal energy, it is obvious that the value of R_f for $C_{60}^{ri+}{**}$ in $1e^-$-loss collisions should be compared to that for $C_{60}^{(ri+1)\ +}{**}$ in $1e^-$-capture collisions. This is confirmed safely because the value of R_f, calculated to be 71% for $C_{60}^{4+}{**}$ in $1e^-$-capture, is nearly equal to R_f (73%) for $C_{60}^{3+}{**}$ in $1e^-$-loss collisions mentioned above. Thus, it is concluded that the internal excitation is the predominant mechanism leading to fragmentation of $C_{60}^{3,\ 4+}{**}$ in 2 MeV Si^{2+} collisions. On the other hand, for higher r_i (>4), relative importance of the coulomb explosion mechanism appears to increase in the same collision system.

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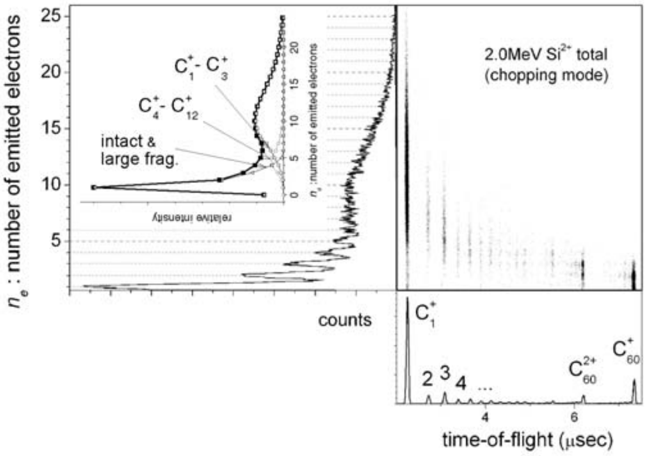

Figure 2:
TOF-n_e coincidence map obtained for 2.0 MeV Si^{2+} projectiles in the chopping mode.

FRAGMENTATION OF NEUTRAL C_n CLUSTERS ($n \leq 9$) : EXPERIMENTAL AND THEORETICAL INVESTIGATIONS.

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Recently a new experimental tool has been developed for fragmentation studies of high velocity clusters, based on shape analyses of current pulses delivered by semiconductor detectors [1]. Using this tool, branching ratios of de-excitation of neutral C_n clusters formed by electron capture in C_n^+ ->He, Ne, Ar collisions at V_p=2.6 a.u have been measured for n=3,5,7,9 (see also the companion work [2]). As an example, we show in figure 1 measured branching ratios for de-excitation of C_7 (C_7^+->He collision) as a function of calculated dissociation energies. This large set of data represents a unique opportunity to test precisely fragmentation theories. Two types of statistical theories, carrying a different fragmentation dynamics, are currently applied to the fragmentation study of these C_n systems:

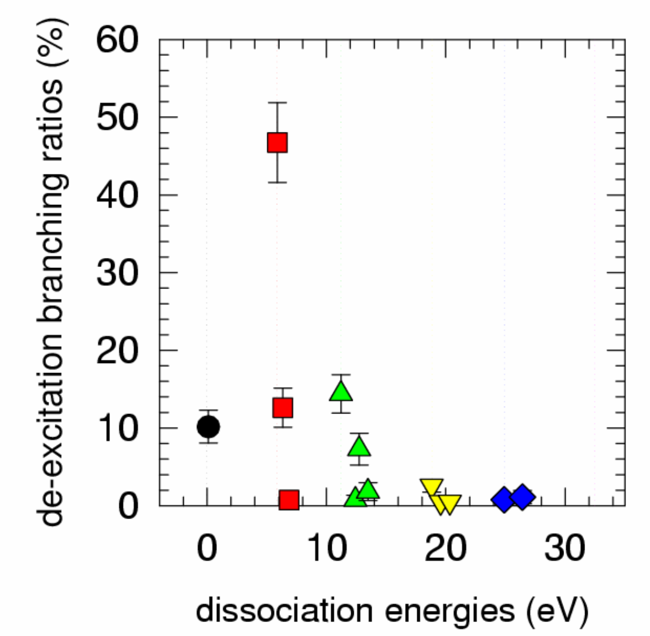

Figure 1: Measured de-excitation branching ratios of C_7 as a function of calculated dissociation energies. Circle: intact C_7; Squares: two-fragments channels (C_4/C_3, C_5/C_2, C_6/C); Triangles up: three-fragments channels ($2C_3/C$, $C_3/2C_2$, $C_4/C_2/C$, $C_5/2C$); Triangles down: four-fragments channels ($C_3/C_2/2C$, $3C_2/C$, $C_4/3C$); diamond-shapes: five-fragments channels ($2C_2/3C$, $C_3/4C$).

(1) For a given total internal energy, the evaporation rate constants have been evaluated in the framework of the microscopic and microcanonical statistical theory of Weisskopf as introduced by Hervieux et al [3]. The basic ingredients of this theory are the dissociation energies and the

density of states of the different fragments. The former have been evaluated by using DFT (B3LYP) and CCSD(T) ab initio calculations while the latter have been obtained in the framework of the harmonic approximation. Harmonic vibrational frequencies have been calculated at DFT level for all fragments. Rotational effects have been neglected. The rate constants obtained are then introduced in a sequential evaporation scheme and the probability of each channel is calculated in function of the energy deposited and the time of flight.

(2) We have also adapted the Microcanonical Metropolis Monte-Carlo (MMMC) model presented in [4] for the study of metal cluster multifragmentation to the case of small carbon clusters. This model allows the quantitative study of the fragmentation in systems where a large number of fragmentation channels are possible. All the points of the phase-space are treated simultaneously to calculate the probability of each channel at a given total energy of the system.

We present the theoretical results obtained with both models and a comparison with the experimental findings for the fragmentation of the following systems: C_4, C_4^+, C_5, C_5^+, C_7 and C_7^+. As an example we show in figure 2 the branching ratios for all the possible fragmentation channels of C_7 calculated within the MMMC framework.

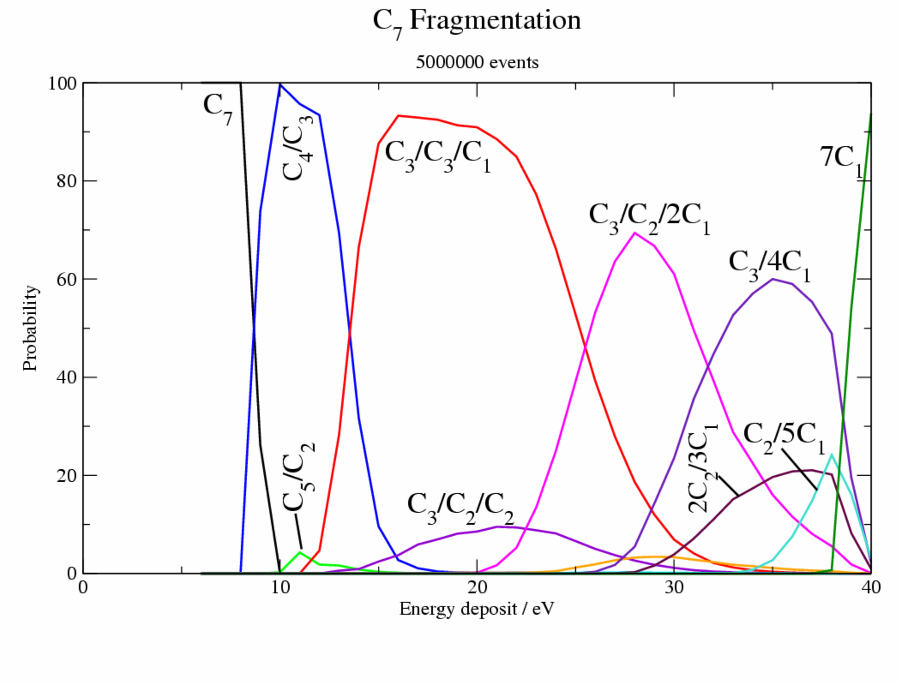

Figure 2: Probability of the different fragmentation channels in function of the energy deposit in the C_7 cluster

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PS-38

THE RESONANCE THEORY OF ALPHA – AND CLUSTER DECAY.

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Prefission emission of alphas and light charged particles provides with a source of information about the time scale in the fusion-fission reaction. In atomic clusters, experimentally observed fission usually proceeds through emission of dimers, mono- or trimers. On the other side, theoretical description of the processes is usually made in terms of the inverse cross-section. Such an approach assuming time reversibility of the process leaves out of the scope a possibility of its profound experimental check. This is in contrast with a number of indications that violations of the reversibility may arise due to back-transparency of the inner slope of the potential barrier in the ingoing channel [1], or different response of the nuclear surface on the interaction with the emitted and the same incoming particle, or due to temperature effects on the barrier distribution [2], as in the ingoing channel experimental fit of the optical model parameters is only possible for cold nuclei [3].

Moreover, traditional decay theory deals with tunnelling through a barrier of a particle which is in the quasistationary state. This does not involve important cases when a virtual proton or cluster is between the quasistationary states, as in alpha decay from compound systems formed in fusion reaction.

Our approach allows one to calculate the decay width at any energy of the emitted particle. Strong resonance effects are, specifically, predicted in alpha spectra from compound systems produced in heavy-ion collisions.

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PS-39

SILICON CLUSTER LATTICE SYSTEM (CLS) FORMED ON AN AMORPHOUS CARBON SURFACE BY SUPERSONIC CLUSTER BEAM IRRADIATION

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Vacuum synthesis of nanostructures by cluster beam irradiation has a large advantage to build up fine structure systems in nanometer scale, because one can control the building block in nanometer scale efficiently and characterize the growth mechanism. The irradiated clusters diffuse at significantly high speed comparable with atoms and juxtapose with neighbor clusters to form stable fine structures in nanometer scale. When the magnitude of the induced dipole moment of clusters proportional to the cluster size becomes uniform, equivalent periodic dipole potentials form cluster lattice systems (CLSs) with long range ordering. We have developed a new laser ablation type cluster source, “spatiotemporal confined cluster source (SCCS)”, which gives well-defined thermo-dynamic conditions in the cluster growth area locally confined both in space and time by using a laser-induced shock wave. A supersonic silicon cluster beam with a characteristically narrow size distribution, $\Delta N/N<5\%$, has been successfully generated [1].

The supersonic silicon cluster beam was irradiated at a velocity of 2.8km/s on a surface of an amorphous carbon (a-C) film with 3nm in thickness supported by a copper micro grid under room temperature. The images got by Z-contrast scanning transmission electron microscope (STEM, HD2000 Hitachi) show a good contrast of silicon clusters with the carbon background (Fig. 1). The silicon components of imaging particles are identified by the energy dispersive X-ray spectrometry (EDS). The a-C surface is fully covered by a unit cluster mono layer (CML) in the density of $1.0\times10^{13}\text{cm}^{-2}$ with silicon clusters of 2-3nm in diameter. In the lower density at 0.2CML, silicon clusters make pairs randomly oriented. In progress of coverage at 0.7CML, silicon clusters tend to partially form tetragonal or hexagonal closed packed structures by coalescence of cluster pairs. In further progress of coverage up to 1.0CML, silicon clusters form a c(2×2) with lattice constant of 4.0nm or closed pack structures. The ordered clusters form CLS without any commensurate interaction with the substrate surface, because the surface of a-C has no ordered structure. It was also revealed with ultra high resolution transmission electron microscope (UHRTEM) imaging that the silicon nanostructured fine particles have a crystallographic structure.

PS-39

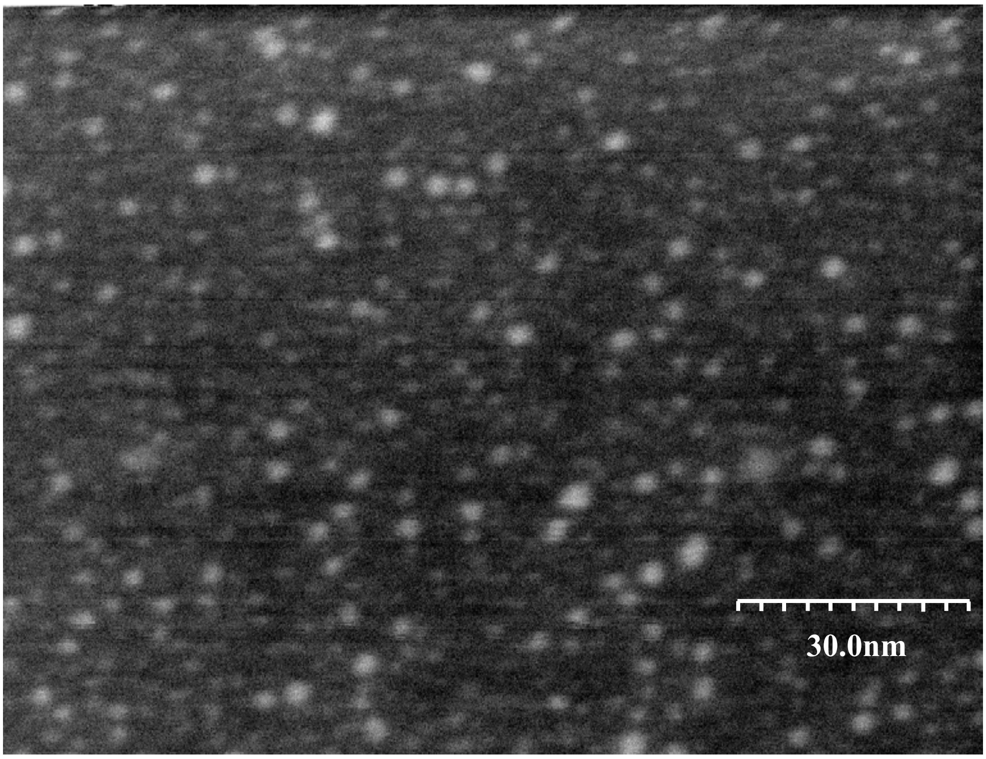

Figure 1: Z-contrast STEM images of Si_N clusters on an a-C thin film in the density of a unit cluster mono layer (CML). c(2x2) lattice structure with lattice constant about 4.0nm is observed.

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PS-40

FRAGMENTATION OF AGGREGATED FULLERENES C_{60} BY SYNCHROTRON RADIATION

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A lot of important results about fragmentation of fullerenes induced by ion bombardment have been obtained recently whereas information about the fragmentation under irradiation is rather scanty. Fragmentation of free fullerenes induced by strong laser field and modification of aggregated fullerenes under ultraviolet radiation have been only observed. This work aimed for revealing processes of modification and fragmentation of aggregated fullerenes C_{60} by Synchrotron Radiation (SR).

Thin films (3-4 ML) of fullerene C_{60} condensate were grown *in situ*. Then fullerenes were exposed at different doses Q of a nonmonochromatic SR provided by "zero diffraction order" mode. Photoelectron spectra of valence electrons and of C1s core-level, C KVV Auger electron spectra and energy loss spectra of C1s photoelectrons of the fullerenes were measured using monochromatic SR. These spectra represent themselves mainly the spectra of separate fullerenes [1] because fullerene molecules in such an aggregated state are weakly bound by van der Waals couplings. Fig.1 shows photoelectron spectra of the valence electrons of pristine fullerenes (1, $Q = 0$), of modified (2, $Q > 0$) fullerenes and of amorphous carbon (3), which was prepared *in situ* by ion bombardment of the film of aggregated fullerenes. The spectrum of pristine fullerenes (1) shows prominent molecular peaks (HOMO) and very low continuous background. Comparison of this spectrum with that of irradiated fullerenes shows that intensities of the molecular peaks diminish under SR irradiation and continuous background increases towards the spectrum of amorphous carbon. In addition "red" shift of the molecular peaks is observed. The revealed transformation the spectra of valence electrons evidences for the transformation of electron and atomic structure of fullerenes towards that of amorphous carbon. Analogous transformation of loss spectra, “red” shift of the spectra of C1s photoelectrons, “blue” shift of Auger electrons confirm this conclusion.

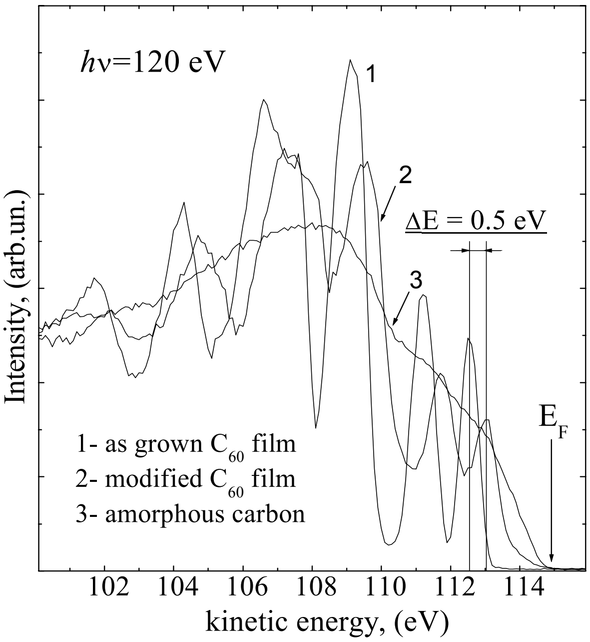

Fig.1: Photoelectron spectra of the valence electrons of pristine fullerenes (1, Q = 0), of modified (2, Q > 0) fullerenes and of amorphous carbon (3).

The mechanism of such a radiation-induced modification of fullerenes includes by analogy with electron-induced modification an excitation of valence electrons, creation of intermolecular chemical bounds, losing small fragments and decreasing high symmetry of large fragment [2]. Excitation of valence electrons is induced by photoelectrons and a swarm of secondary electrons. As a result, the density of delocalized electrons near the Fermi-level increases resulting into increase of the relaxation energy. The increase of the relaxation energy is known to be the reason of decrease of the binding energy ("blue" shift of the core-level and molecular peaks) and of the increase of the Auger electron energy ("blue" shift). Thus, modification of fullerite C_{60} by continuous SR has been revealed for the first time. Spectra of fragmented fullerenes were sdudied. Preliminary results of the initial stage of modification of fullerite by monochromatic x-rays (hv = 130 eV) have been obtained. The project was supported by BESSY-II, INTAS grant № 2136, and NWO grant № 047.009.012.

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PS-41

NEGATIVE ION IN A CAVITY, IN A CAGE, OR IN FRONT OF AN INSULATOR CLUSTER SURFACE

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A standard approach to construct a model for a compressed atom, or an atom confined to a cavity, is to impose the boundary condition on the electron wave function $\psi|_S = 0$ on the cavity surface S. This is equivalent to infinitely high confining potential wall (see, for instance, Ref. [1] and more bibliography in Ref. [2]). A similar formulation was employed recently to model an insulating cluster [2]. We combine this model with approximating atomic core in a negative ion by a zero range potential (ZRP) [3]. Solving the Schrodinger equation in this case amounts to finding the Green function with appropriate boundary conditions. Hence the known methods of Green function construction might be applied.

We solve a number of quantum problems within this framework, describing a negative ion in front of impenetrable spherical surface or inside impenetrable sphere. The former system was considered previously [2] as model of negative ion interaction with a insulator cluster, but only in case of zero energy. In the latter case, when a negative ion is confined to a spherical cavity of radius *R*, the electron binding energy is a function of the ion displacement *d* from the cavity center. This provides a 'potential curve' *U(d)* in which the ion nucleus moves. The curve attains minimum at *d = 0*. Hence the ion oscillates around its equilibrium position at the cavity center. The function *U(d)* is defined by transcendent equation, albeit its curvature at *d=0* is found in a simple analytical form:

$$U''(0) = \frac{2\kappa^3 R}{3[\alpha/(\alpha^2+\kappa^2)+R](1+\alpha R)}$$

Here $-\kappa^2/2$ is bound state energy in spherically symmetrical configuration, i.e. in the case *d=0*. The parameter κ is governed by equation

$$\kappa\, ch\, \kappa R = \alpha\, sh\, \kappa R\,,$$

$\alpha>0$ is ZRP parameter; $\alpha^2/2$ is affinity of the negative ion; we consider solution with $\kappa \to \alpha$ for $R \to \infty$. The vibrational spectrum in harmonic approximation vibrational spectrum is given by formula

$$E_n = \omega\,(n+3/2)\,,$$

where ω is vibrational frequency, $\omega^2 = U''(0)/M$, M is an ion mass, $n = 0, 1, 2 \ldots$.

Beyond the harmonic approximation, the vibro-rotational spectrum is found by numerical integration of the Schrodinger equation for the potential *U(d)*. In the other application we replace the infinitely high wall by a potential step of finite height, or by a spherical delta-function. The latter system models an endohedral ion, i.e. an ion inside the quasi-spherical fullerene cage.

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PS-42

DELAYED IONIZATION OF C_{60}

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The determination of dissociation energy of C_{60} for the C_2 loss channel has been the subject of numerous experimental reports. Theoretical calculations predict 10 to 12 eV whereas experimental studies have given 4 to 12 eV. Recently, it has become clear that most of this uncertainty is due to the lack of knowledge concerning the pre-exponential factor A in the Arrhenius expression for the decay rate, $k = A\exp\left(-E_d/k_BT\right)$. At first, it was believed that this factor should be of order $A \sim 10^{13}$ s^{-1}, while there is consensus now that it should be much larger, and a value $A \sim 10^{19}$ s^{-1} is often assumed. The breakthrough in this development was the analysis by Hansen and Echt [1] of delayed ionization of laser excited C_{60}. Ionization competes with neutral C_2 emission and provided that ionization is a weak channel the ion yield as a function of the delay time should follow a power law with a power equal to minus the ratio of the ionization and dissociation energies. Since the ionization energy is known, the dissociation energy could be derived without a knowledge of the value of A. The analysis gave a higher value for the dissociation energy for C_2 emission from C_{60} (11.9±1.9 eV) than obtained from previous experiments.

Recently Rohmund *et al* [2] have extended these measurements to longer delay times and found a strong cut off of the ion yield in the range from 10 to 100 μs . They argued that geometrical effects due to thermal motion of the excited molecules were negligible and that also quenching by radiative cooling should play a minor role. Instead they suggested that the ion yield is dominated by electron emission from molecules in the lowest triplet state with about 1.7 eV electronic excitation and that the cut off is due to exponential decay of this state with a lifetime of order 40 μs.

We have studied delayed ionization of C_{60} in a setup where geometrical effects are avoided by excitation of the molecular beam with a collinear laser beam. We have measured ions in coincidence with emitted electrons, which makes it possible to distinguish C_{58}^+ from C_{60}^+ and to measure the ratio of the yields of these ions. With this ratio, we can determine not only the dissociation energy of C_{60} but also the pre-exponential factor A. Our numerical analysis resulted in a dissociation energy of C_{60} of 10.7∀0.5 eV and a pre-exponential factor for neutral C_2 emission from C_{60}, $A=10^{21}$ s^{-1}. This is a considerably higher value than used earlier. We have also found that the exponential cut off of the C_{60}^+ yield is at longer delay times (~ 100 μs) and our analysis indicates that it can be explained by radiative cooling of the molecules [3].

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PS-43

DEFORMED JELLIUM MODEL FOR METAL CLUSTERS

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This work is devoted to the elucidation of the level of applicability of jellium model to the description of sodium cluster properties on the basis of the comparison of jellium model results with those derived within *ab initio* theoretical framework and experiment. On the basis of the deformed Hartree-Fock and the local-density approximation jellium model (see, e.g., [1, 2] and references therein) we have calculated the binding energies per atom, ionization potentials, deformation parameters and the optimized values of the Wigner-Seitz radius, r_s, for neutral and singly charged sodium clusters with $N \leq 20$ [3]. In the present work, we investigate in detail how the clusters ionization potential are influenced by the deformation parameter.

The calculated characteristics are compared with the results derived in [4] from the *ab initio* all-electron simulations of cluster electronic and ionic structure based on the density-functional theory as well as on the post Hartree-Fock perturbation theory of the forth order on many-electron correlation interaction.

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