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Section

ATOMIC CLUSTERS

ON CREATION AND CONTROLLING OF ATOMIC CLUSTERS ON NANOSCALES SPACE-TIME IN SPIN GLASSES BY MEANS OF EXTERNAL ELECTROMAGNETIC FIELDS

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The formation and control of periodically modulated refractive index in media is one of the most important problems of solid state physics and material science. First of all it is related to the possibility of developing compact UV or X -ray Free-Electron Lasers based on emission of transition radiation (TR). The superlattice of dielectric constant also can be very interesting and perspective from the viewpoint of creation a new type multiqubit quantum register, where each qubit is formed from the four TR photons.

Recall that TR photons are generated at passing of electron beam via neighboring layers of media with different permittivities. As well known the radiation power in this case is proportional to $[\varepsilon R1\ (w) - \varepsilon R2\ (w)]2$, where ω is a frequency of radiation and $\varepsilon R1,2(w) = Re[\varepsilon 1,2(w)]$ designates the real parts of permittivities of corresponding layers. As follows from our recent research in a weak external standing electromagnetic fields, dielectrics of type amorphus SiO2 which are well described by the spin glass model demonstrate critical properties. In the result of these phenomena on the scales of space-time periods of external fields in the 3D media, regions with the extremely various dielectric constants are formed.

In this work we have considered the influence of external periodic electromagnetic fields on 3D medium, when the wave is propagated on one x direction. In particular as the exact numerical simulation of the problem has shown, even at weak external fields the polarizations of the system are frustrated on all coordinates. These frustrations of polarization for some cases are so large that lead to catastrophes of the Clausius- Mossotti's equation for the dielectric constant. The latter circumstance leads to the formation of quantum wires in the medium. Moreover, the research shows that these filaments can be formed as on coordinate of propagation of external wave as well as to perpendicular to the wave directions. We have investigated the size effects and the stability problems of formed structures depending on external fields parameters, when the length of quantum wires is about 25 atomic units. The dispersion properties of one-dimensional superlattice are analyzed in detail and is suggested specific areas for its application.

ABOUT APPLICABILITY OF THERMODYNAMIC PARAMETERS TO SMALL DROPS AND CLUSTERS

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There is a problem of applicability of thermodynamic parameters to small drop and cluster as these parameters are the macroscopic thermodynamic notions, but nanodrop is a microscopic system. An effective method of nanoparticles production is the condensation from supersaturated vapor. Nucleation, formation of critical nuclei, is the first stage of such condensation. The surface tension of small drops and clusters is the most important parameter in the nucleation theory, as it determines the work of the critical nuclei formation.

In our paper the results of molecular dynamics calculations of nanodrops are presented. The density profiles, the Irving-Kirkwood pressure tensors, the chemical potentials of the systems, the equimolar radii of the drops and the radii of tension, the mechanical and thermodynamic surface tensions have been calculated.

It is shown that both the mechanical and thermodynamic surface tensions decrease with the decrease of the equimolar radius of the drop, and reach zero at the same R0 depending on temperature. With the further equimolar radius decrease the surface tension becomes negative. It means that such droplet is metastable and that the notion of surface tension which is used in macroscopic theory can not be applied to such small drops. The dependence of the ratio of the surface tension of the drop to the surface tension of the flat surface liquid-vapor on the ratio of the equimolar radius of the drop to R0 is a universal function [1-2].

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THE STUDY OF PURE AND HYDROGENATED SILICON NANOTUBES AND NON-CONVENTIONAL TIGHT-BINDING METHOD

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It is known that silicon is the basis for microelectronics. However, more recently, carbon nanoparticles in the form of both nanotubes and graphene predicted to become the foundation of almost all, without exception, of future technologies. There was also the view that carbon replace silicon in the main areas of use - transistors and integrated charge. However, after the theoretical prediction of the existence of silicon nanotubes [1], such as carbon, they soon were found experimentally [2]. Then, in [3] showed that for the operation of hydrogen devices most effectively will have no carbon and silicon nanotubes. This discovery was particularly important when it became known that carbon nanotubes for one reason or another fall short of the majority of engineers working to develop hydrogen batteries. Thus, silicon nanotubes are the subject of intense research both theoretical and experimental methods.

Silicon, unlike carbon, does not tend to the formation sp1 and sp2 hybrid configurations in the form of one-or two-dimensional structures. In [4] showed that the nanotubes, which consist only of silicon atoms are unstable and is irreversibly transformed into a shapeless clusters. Stabilize the tubular structure can be achieved by encapsulation in a tube of transition metal atoms [5]. In addition, silicon nanotubes can be of varying diameter and length and structure. The stability of the nanotubes depends on all these parameters. However, until now a full investigation of various structures of silicon nanotubes are not carried out. In addition, silicon nanotubes as carbon, may be chiral, ie, crooked, zigzag and chiral. It should also be noted that the existing methods of calculations of large clusters also have their disadvantages and different results.

Thus, in this work is carried out quantum-chemical study of the structural and energy characteristics of pure and hydrogenated silicon nanotubes of different size combination of molecular dynamics and non-conventional tight-binding method

(TBM), the proposed Khakimov [6-7]. This method allows us to describe the geometry, binding energies, ionization potentials, electron affinities as well as silicon nanotubes containing up to 30 atoms, with almost strict accuracy of ab initio methods. In this case, the calculations are performed using the TBM to several orders of magnitude faster than calculations using ab initio methods.

To study the selected nanotubes of different diameters and lengths, such as a tube with the number of atoms in the longitudinal section 8 and 12 atoms. Number of units in the tube was 2, 3 and 4 rings interconnected to form regular hexagonal shapes on a sheet of the pipe. Thus, the constructed molecules have a tubular structure and the silicon atoms in them trehkoordinirovany. Furthermore, the built structures were placed in TBM-MD and performed molecular dynamic optimization of the spatial configuration of clusters. In the process of optimizing the geometry, the atoms moved from the initial positions and smooth tubular structures distorted and transformed into a curved configuration, where the angles between the bonds close to the corners of a tetrahedral shape. Most of the silicon atoms close to each other, thus increasing, and decreasing the coordination number of uncommitted portion of the valence electron orbital's of the dangling. Saturation of silicon atoms with hydrogen atoms produced in several ways, the complete saturation, partial saturation, where each silicon atom attached to one hydrogen atom and only the extreme saturation of the silicon atoms, closing up on both sides.

Summarizing the results, we conclude that the flat structure of most silicon nanotubes is unstable and they collapse to the transformation of nanotubes in the nanowire. The collapse of most atoms are the two edges of the tubes. How stable nanotubular configuration and formed nanowires, unlike carbon nanotubes, have an uneven surface. This is because the valence electron orbitals of the silicon atoms other types of atypical hybridization, except sp3, hence silicon will tend to form diamond-like connection the most. Nanotubes with diameters remain small shallow structure, whereas large-diameter tubes are flattened and the opposite atoms form a connection between. It should also be noted that short nanotubes with fewer units, less stable and become the no shallow shapeless structure. As the number of links in the chain, ie with an extension tube length probability conservation tubular increases.

Hydrogenation of carbon nanotube affects its stability as a function of its saturation with hydrogen, fully saturated nanotubes turn into shapeless hydrogenated clusters, whereas only marginal hydrogenation of silicon tube leads to the

conservation of its structure. Chorale annotate does not change during hydrogenation.

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MAGNETISM AND SELF-ORGANIZATION OF Co NANOSTRUCTURES EMBEDDED INTO Cu (100)

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Recent years have brought significant advances in experimental and theoretical studies of small magnetic clusters. The small magnetic clusters are current focus of intensive research due to both their importance in fundamental low-dimensional physics and the potential applications in nanoscale materials and devices.

The main goal of our work is to investigate the evolution of Co nanostructures embedded into a Cu(100) surface at the atomic scale. The present calculations using the kinetic Monte Carlo method with energy barriers of all relevant events calculated by means of the molecular-dynamics method with ab initio based interatomic potentials are performed. The atomic processes responsible for the linear and angular chain formations are identified. We demonstrate the key role of substrate vacancies in the motion of embedded Co atoms and investigate the self-organization of Co atoms in different conditions.

The interplay between structure and magnetic properties of small cobalt clusters (linear and angular chains) embedded in a Cu(001) surface is studied performing ab initio calculations in a fully relaxed geometry. We reveal that, despite the small macroscopic mismatch between Co and Cu, the strain relaxations at the interface have a profound effect on the structure of the clusters and the substrate. We show that the atomic relaxations strongly reduce the magnetic anisotropy energy (MAE) and the orbital magnetic moments of embedded clusters. The largest MAE is found for a single Co atom in the Cu(001) surface. A strong enhancement of the spin magnetic moments in embedded clusters as compared to a single atom of Co incorporated in the Cu(001) surface is found. This work was supported by Russian Foundation of Basic Researches, grant RFBR 11-02-12256. Computational resources were provided by the Research Computing Center of the Moscow State University (MSU NIVC).

FORMATION OF AU NANOCONTACTS AT THE ROOM TEMPERATURE: A KINETIC MONTE CARLO INVESTIGATION

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Gold nanowires have been the object of intense theoretical and experimental investigations in the last years [1, 2]. One of the mostly used ways to prepare stable nanowares is electron-beam irradiation on a gold thin film in an ultrahigh vacuum transmission electron microscope (UHVTEM) [3]. Neighboring holes are perforated in a gold thin film using a focused electron beam; further irradiation induces the diameter of the holes to grow until a nanometric bridge is formed. The generated gold neck showed a tendency to elongate, become thinner, and finally break. This process usually took 5-30 min at the room temperature.

We present the detailed theoretical investigation of the gold nanocontacts formation in an UHVTEM at the room temperature. For simulation of long-time evolution we used the following MD-kMC scheme. All relevant atomic events were calculated by means of the molecular dynamics (MD) method with ab initio based interatomic potentials. The evolution of the Au atoms system was simulated using the kinetic Monte Carlo (kMC) method. We consider different orientations of a gold thin film. Finally, we compare our theoretical results with experimental data.

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PHOTO-ELECTRON SPECTRA AND ANGULAR DISTRIBUTIONS FROM CLUSTERS

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We investigate from a theoretical perspective the dynamics of atomic clusters following a short and intense laser pulse. Ionic dynamics is unimportant for the fast electronic processes directly accompanying and following the laser pulse and will be ignored. First, we analyze the optical response which is the doorway for the coupling of the laser to the cluster. Then we look at the more detailed observables of electron emission: net ionization, photo-electron spectra (PES), and photo-electron angular distributions (PAD). We will briefly explain its computation and present results for PES and PAD from a variety of cluster systems.

LARGE-SCALE FIRST PRINCIPLES CONFIGURATION INTERACTION CALCULATIONS OF OPTICAL ABSORPTION OF SMALL MAGNESIUM CLUSTERS

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We have performed systematic large-scale all-electron correlated calculations on small magnesium clusters Mgn, to study their linear optical absorption spectra. Several possible isomers of each cluster were considered, and their geometries were optimized at the coupled-cluster singles doubles (CCSD) level of theory. Using the optimized ground-state geometries, excited states of different clusters were computed using the multi-reference singles-doubles configuration-interaction (MRSDCI) approach, which includes electron correlation effects at a sophisticated level. These CI wave functions were used to compute the transition dipole matrix elements connecting the ground and various excited states of different clusters, eventually leading to their linear absorption spectra. The convergence of our results with respect to the basis sets, and the size of the CI expansion were carefully examined. The contribution of configurations to many body wavefunction of various excited states suggests that the excitations involved are collective, plasmonic type.

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THE MULTISCALE PHYSICS OF NANOSTRUCTURES SELF-ASSEMBLING

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Structure, dynamics and properties of size selected clusters (S3C) have been intensively studied during the last decades both theoretically and experimentally. The very unique properties of clusters, having similarities with the finite systems like single nuclei, atoms or molecules on the one hand side and with the solid state systems on the other, as well as the evolution of the properties between the two limits, have been discussed in thousands of papers during the last three decades.

Nowadays the enormous knowledge gained in the S3C studies becomes more and more demanded in various applications. One of such topics is the nanoarchitecture design, i.e. the controllable, reproducible and economical fabrication of nanosystems with desirable morphology and properties. The rational design of the architecture of nanosystems, nanodevices, nanostructured materials with tailored properties opens a broad spectrum of applications in the modern nanotechnology and medicine.

The very promising approach to the smart fabrication of nanosystems is the so-called bottom-up approach [1] exploring the property of ensembles of atoms, molecules, S3Cs and nanoobjects to self-assembly into 2D or 3D structures with specific, well-defined and nanostructured morphologies.

In spite of the obvious importance the physics of these processes is not entirely understood [2-4] due to the complexity of systems and the multiscale nature of the phenomena involved. This explains the increasing interest towards the better understanding of structure formation and dynamics of systems on the nanoscale, http://fias.uni-frankfurt.de/mbn, http://fias.uni-frankfurt.de/dyson/.

In my talk there will be given a brief introduction to this field of research.

The talk aims to present the state-of-the-art analysis of the structural and dynamical properties of the size selected clusters that become essential for the formation of nanosystems with the particular nanoarchitecture. As a case study there will be discussed the process of formation and post-growth relaxation of nanostructures deposited on a surface [2-4]. There will be presented a detailed systematic theoretical analysis of the formation and the post-growth relaxation

processes of silver nanofractals on a graphite surface. There will be demonstrated that the kinetic processes involved determine the morphology of the created islands on a surface after post-growth relaxation. The dependence of stability of the created fractal structures upon several factors, such as the particles mobility and temperature [3-4], will be analyzed. Different scenarios of the fractal relaxation and the time evolution of the island's morphology will be discussed. Results of the theoretical model will be compared with the experimental data reported in [2]. Particular attention in this analysis will be devoted to the ways how to overcome the multiscale complexity of the outlined problem and to extend the computational limits by utilizing the rational coarse graining and model approaches. Further progress in this direction should allow one to controllably influence the self-organization processes of particles on a surface or in 3D, and on this way to find rational paths to create architectures of nanosystems with predictable and desirable properties.

Finally, I would like to devote some attention to the development of the software package MBN (Meso-Bio-Nano) Explorer, see http://www.mbnexplorer.com/, being a very useful tool in the exploration of multiscale physics of nanostructures self-assembling and design.

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COHERENT SPIN DYNAMICS OF NANOMOLECULES AND MAGNETIC NANOCLUSTERS

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The regimes of coherent spin motion of magnetic nanomolecules and magnetic nanoclusters are investigated. Spin dynamics of both separate nanoclusters as well as the assemblies of many nanomolecules and nanoclusters are studied. The role of external fields, resonators, magnetic anisotropy, dipole interactions, and other nanocluster properties are elucidated. The emphasis is on finding such conditions when nanomolecules and nanoclusters exhibit fast magnetization reversal. The possibility of realizing fast reversal is essential for a number of application of magnetic nanoclusters, e.g., for fast information processing.