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BOOK OF ABSTRACTS

Low-dimensional materials: theory, modeling, experiment

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Low-Dimensional Materials: theory, modeling, experiment

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THE EXTENDED HUBBARD MODEL PHASE DIAGRAM STUDY WITHIN LATTICE QMC

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The extended Hubbard model is of a large interest for the condensed matter community because of its possible application to description of various high-temperature superconductors. The interaction in the system is described by the on-site $U\hat{q}\,\hat{q}$ interaction term and $V\hat{q}_i\,\hat{q}_j$ nearest-neighbors interaction term. In the UV–plane, the system has three phases: Mott Insulator, Fermi liquid and Charge ordered phase. The tricritical point is located in the region of strong coupling where no controllable analytical approximations can be applied. We apply the Quantum Monte-Carlo method for first-principle study of this system. The method proven reliable in study of QCD, graphene and many other problems. In particular, we are interested in shapes and positions of phase-transition curves in the UV–plane.

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THE INFLUENCE OF STRUCTURAL DISORDER IN CARBON NANOMATERIALS ON THE LOW TEMPERATURE THERMAL AND ACOUSTIC PROPERTIES

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We illustrate the influence of the disorder in carbon nanomaterials (fullerite C_{60} and carbon nanotubes) on the thermal and acoustic properties at the low temperature. The physical properties of fullerite C_{60} are largely determined by the dynamics of the rotational motion of the C_{60} molecules. Below 90 K the reorientational motion of the C_{60} molecules is frozen and fullerite changes to the state of orientation glass. The calculation of glass contribution to the heat capacity and low temperature dependence of the speed of sound, was carried out. It was found that the low energy tunneling states that are located at the boundaries of domains may apparently lead the main contribution to the low-temperature effects in the heat capacity and the speed of sound.

In the investigations of the low-temperature transport properties of disordered metallic nanotubes have been shown that the short-range-order atomic reconstruction can apparently lead to the gap in the electronic density of states (DOS) on the Fermi level, the inverse of temperature dependence of electrical conductivity and the nonlinear thermopower. In this work the approach of the shortrange-order was used to describe the features in the low-temperature behavior of the specific heat and speed of sound in disordered nanotubes and was shown the strong influence of the structure changes in nanotubes on these properties. The expression for the electron-phonon interaction time in systems with local short-range order has been obtained:

$$\frac{1}{\tau_{e-ph}} = \frac{\zeta_0 \tau \varepsilon^3}{\hbar^2 p_F \tilde{c}}$$

where ζ_0 - electron-phonon interaction constant, τ - electron relaxation time (depends on T), $\varepsilon \sim kT$, p_F - electron momentum at the Fermi level, $\tilde{c}$ - sound speed. It follows from expression that a decrease in the speed of sound in disordered systems, which are carbon nanosystems, significantly increases the scattering of electrons by phonons.

STRUCTURAL STABILITY OF COPLANAR 1T-2H SUPERLATTICE MoS_2 UNDER 300 keV ELECTRON BEAM

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Coplanar heterojunctions composed of van der Waals (vdW) layered materials with different structural polymorphs have drawn immense interest recently due to low contact resistance and high carrier injection rate owing to low Schottky barrier height. Present research has largely focused on efficient exfoliation of these layered materials and their restacking to achieve better performances. We present here a microwave (MW) assisted easy, fast and efficient route to induce high concentration of metallic 1T phase in the original 2H matrix of exfoliated MoS_2 sheets, thus facilitating the formation of a 1T-2H hybridized phase. Absorption and Raman studies carried out before conducting any TEM measurements clearly suggest that the induction of 1T is a MW assisted transition. High resolution (HR) TEM measurements exhibit the formation of a highly crystalline coplanar 1T-2H heterogeneous superlattice phase with a higher concentration of 1T than 2H. Evidence of surface ripplocations within the same exfoliated layer of MoS_2 is also observed in the HRTEM investigations. In this work, the structural stability of 1T-2H superlattice phase during HRTEM measurements under an electron beam of energy 300 keV is reported [1]. Theoretically, it was shown that the thermodynamic stability of the hybrid 1T-2H phase is more, almost comparable to that of the semiconducting 2H phase [2]. Upon hybridization, the overall increase in the system energy compared to 2H phase is as small as 0.03 eV which defines the stability of the 1T-2H phase [2]. The metallic nature of the hybridized state was asserted from the fact that the total density of states of Mo *d* orbitals couple with that of the *Sp* orbitals and cross the Fermi level showing high conductivity [2]. Our experimental observations of the structural stability of hybridized 1T-2H phase could be either associated to the change in electronic configuration or to the formation of the surface ripplocations. Surface ripplocations can act as an additional source of scattering centers to the electron beam and also it is possible that a pulse train of propagating ripplocations can sweep out the defects via interaction from specific areas of MoS_2 sheets [3]. Coexistence of both the phases in the same MoS_2 nanosheet can have potential applications as homojunctions for spintronic devices, electronic transport and could provide viable solution to the contact issues in 2D electronics due to Ohmic behavior of the 1T phase and the homojunction.

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FARADAY ROTATION IN GRAPHENE

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We considered a graphene sheet encapsulated in a two-dimensional (2D) metallic grating and a substrate (Al_2O_3) and subjected to an external magnetic field, perpendicular to graphene. The grating consists of a thin and perfectly conducting metal film perforated with a 2D periodic array of square holes. We have demonstrated that, if the width of the perforation holes is close to the array period (i.e., the grating looks like a thin metallic net), the incident electromagnetic wave is strongly screened by this structure in the low-frequency range $\omega < 5$ meV. It results in a decrease of the Faraday rotation angle φ of the transmitted wave, in comparison with bare graphene.In contrast, if the wave frequency is close to that of the magnetoplasmon resonance in graphene, one can expect an increase of the Faraday rotation angle, which is a result of the magnetoplasmon-mediated transmission. The maximum of the Faraday rotation angle is shifted to higher frequency when the period of the grating decreases. An important advantage of the graphene-based structure with 2D grating is that it introduces lower ellipticity ρ (in comparison to bare graphene) of the transmitted wave and for some frequencies it can vanish, which means maintaining the linear polarization. The effect introduced by the grating is even more substantial for the magnetic circular dichroism[1], which is quantified by the difference in the extinction between left-hand and right-hand circular polarized waves. We notice that the dichroism can be tuned by adjusting magnetic field and also the graphene Fermi energy that determine the magnetoplasmon dispersion curve.

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STUDY ON THE INTERFACIAL INTERACTION BETWEEN CARBON NANOTUBES AND CATALYST: THE EFFECT IN TUBE DIAMETER

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Single-walled carbon nanotubes (SWCNTs) are seamless cylinders of graphene that have been at the forefront of nanotechnology research for the past two decades. They possess a range of exceptional properties including high strength (~37 GPa), thermal conductivity (~3500 W/m/K) and ballistic electronic transport. Importantly, they can have semiconducting, semi-metallic, or metallic conductivity depending on their chiral angle (χ), i.e. the angle between the tube axis and the edge of the graphene lattice. While mass-produced SWCNT powders are adequate for some applications, many emerging applications require stricter control over SWCNT properties and architectures, necessitating targeted growth, i.e. tailoring the physical properties of the SWCNTs (diameter, orientation/architecture, etc.) during synthesis to match the requirements of a particular application.

This project attempts to prove the key role of the catalyst – graphene interaction in the chirality selectivity of carbon nanotubes (CNT) and therefore, the intrinsic relation between catalyst size and nanotube diameter. We work on the assumption that the curvature energy is one of the most influential factors in the nanotube's formation reaction and a decisive step to determine the diameter of the nanotube during the growth. The calculation of interlayer binding energies using density functional theory (DFT) and pseudopotential functions has been valuable to find the transition diameter between fullerene and tube. Also, we propose a new relation that links theory to measurable thermodynamic properties such the surface tension, and surface energy. This is just the first step to bring light to the yet undiscovered reigning principle in the nanotube's diameter stability during nucleation.

INVESTIGATION OF PHASE BEHAVIOR AND STRUCTURAL PROPERTIES OF CHOLESTEROL-CONTAINING LIPID MEMBRANES

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The primary component of phospholipids as building blocks of cell membranes is carbon. Carbon's molecular structure allows it to form different kinds of bonds with distinct elements thus forming the backbone of all essential compounds of living matter. Due to their amphiphilic structure phospholipids form bilayers, into which various functional macromolecules, such as proteins, cholesterol, hydro-carbons, etc., are being incorporated.

Lipid membranes may be considered as two-dimensional systems. This feature introduces some simplification of the theoretical description of these objects and the determination of their mechanical characteristics.

In this work Differential scanning calorimetry analysis of fluid samples of synthetic phospholipid SOPC with different water content (10, 20, 33 weight percent) in presence of cholesterol was carried out to study the phase behavior of pure SOPC and cholesterol-containing membranes over a wide temperature range. The experimental thermograms during heating and cooling regimes at various water contents and for all studied systems are analyzed at different scan rates and the phase transition characteristics are determined.

Scanning electron microscopy on a series of images of the surface and the profile of thin SOPC lipid layers containing 0% – 50% of cholesterol are made to explore the change of the layer structure with the increase of cholesterol in the system. The evaluation of the phase transition properties, such as critical temperature, enthalpy etc. gives us the possibility to apply molecular dynamic simulation for assignment of the new physical and structural characteristics of the complex lipid membranes.

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SELF-CONSISTENT DESCRIPTION OF GRAPHENE QUANTUM AMPLIFIER

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High level of dissipation in normal metals makes challenging development of active and passive plasmonic devices. One possible solution to this problem is to use alternative materials. Graphene is a good candidate for plasmonics in near infrared (IR) region. In this paper we develop quantum theory of a graphene plasmon generator. We account for the first time quantum correlations and dissipation effects that allows describing such regimes of quantum plasmonic amplifier as surface plasmon emitting diode and surface plasmon amplifier by stimulated emission of radiation. Switching between these generation types is possible in situ with variance of graphene Fermi-level or gain transition frequency. We provide explicit expressions for dissipation and interaction constants through material parameters and find the generation spectrum and correlation function of second order which predicts laser statistics.

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MODEL CALCULATIONS OF THE POSITRON ANNIHILATION CHARACTERISTICS FOR MULTILAYER GRAPHENE FILM

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Using a Two-Component DFT with a solver from the MIKA-Doppler program package [1], we study a folded graphene structure. For the AA and the AB stacking arrangement of the carbons in the neighbouring layers [2] the electronic and the positronic densities relevant for the positron emission experiment are calculated, obtaining Positron Lifetimes of 151.5 ps in AA and 143.6 ps for the AB stacking. In addition, we consider defect such as a vacancy, H, He, and an Oxygen substitutes. To build the cluster of defects, a unit cell of 6 layers of graphene with a size of 6x6 a.u. is used. We also attempt to extend the code in order to include possible magnetic effects [3]. One use of this calculations can be in the analyses of the possibility of creating a graphene coating on a tungsten material, a step in developing tungsten-graphene plates for the use for the divertor in a fusion reactor like ITER [4].

This work is supported by the joint project ISSP(BAS)-LTF(JINR) ”Synthesis and theoretical studies of graphene nanostructures” (Theme 01-3-1115-2014/2018).

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KINETIC PROCESSES IN DOPED SEMICONDUCTOR NANOSTRUCTURES

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Electron-electron interactions in a single highly doped heterojunction are considered taking into account both intra- and intersubband transitions. Expressions are derived for the time of electron-electron interaction, matrix elements of the full screening potential and dynamic dielectric function in a 2D electron system with the fine structure of the energy spectrum, and for the electron density spatial distribution.

Our analysis of e-e interaction is based on the calculation of the conduction band energy structure $E_c(z)$. Similarly to [1], we approximate the potential well of the heterojunction by a triangular profile with the sharp bends at the size-quantized levels $E_m = E_c(d_m)$ and $E_p = E_c(d_p)$. To within the second order in the external potential $V_{tot}(q,\omega)$ in the perturbation theory expansion, the time required for the e-e interaction to change the state $\langle k|\, p\rangle$ into $\langle k+q|\, p-q\rangle$ is given by a well-known expression [2],

$$\frac{1}{\tau_{ij}^{ee}} = \int_{-\infty}^{\infty} d\omega \sum_{k,m}\sum_{q} \left|V_{tot}^{ijkl}(q,\omega)\right|^2$$

$$\sum_{k,p} \delta\left(E_j(k+q) + E_l(p-q) - E(k) - E_k(p)\right) f_k f_p \left(1-f_{k+q}\right)\left(1-f_{\mathrm{p-q}}\right)$$

where indices *i, j, k, l* run over the set consisting of symbols *m* (main component) and *n, d* (satellites of the n_p-component) which label the electron transition type.

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LASER INDUCED PERIODICAL SURFACE STRUCTURES ON MULTILAYER GRAPHENE

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Single and multi-layer graphene is known as a unique novel material with outstanding electronic, optical and mechanical features with high potential for fundamental studies and numerous applications. In addition, the ability to controllably form patterns is very important for flexible electronics and energy devices. This ability as well as high transparency, make graphene a desirable material for the formation of laser induced periodic surface structures (LIPSS) by femtosecond laser beam [1] .

We study the formation of LIPSS on multilayer graphene samples (from 3 to 15 layers) generated by action of femtosecond laser with 840 nm excitation wavelength, 150 fs pulse duration, 76 MHz repetition rate and 4.3-4.4 mJ/cm^2 fluence, presented in the work [1]. The orientation of LIPSS is related to the polarization direction of the laser radiation, and their spatial period depends on the laser wavelength and the number of pulses delivered. Experimental results concerning LIPSS period and some other peculiarities can be treated consistently by use of plasmon-polariton mechanism. However, some questions are still open. In order to understand and explain experimental results we propose theoretical model based on equations describing the nonlinear interaction of an ultrashort pulse with graphene sample and the substrate, electron density evolution, heat conduction, and thermo-elasticity.

We gratefully acknowledge the financial support of the BRFFR (project: F16SRBG-003).

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3D/2D TRIONS WITHIN FADDEEV AND HYPERSPHERICAL HARMONICS APPROACHES

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Excitonic effects in two- and three-dimensional (2D and 3D) nanostructures are determined by energies of excitons, trions, biexcitons and the electron-hole interaction have garnered considerable interest. In particular, the binding energies of charged exciton complexes such as negative and positive trions which are formed when a single exciton is correlated, respectively, with an additional electron in a conduction band or hole in a valence band are the subject of recent theoretical and experimental studies.

We present a theoretical study of trions in 2D monolayers of a transition metal dichalcogenide and 3D bulk materials in the framework of effective-mass model by employing the method of hyperspherical harmonics and the Faddeev method in configuration space, respectively. The binding energies of trions in monolayer nanostructures are calculated using the Keldysh potential, while the binding energies of trions in 3D semiconductors are obtained when electrons and holes interact via the Coulomb potential.

We investigate the mechanism of formation of the bound positively and negatively charged trions by considering the purely three-body term, that presents the mass polarization effect [1], and the screened Coulomb (Keldysh) potential. The relation between the binding energies of a positively and negatively charged trions was found. We show, how the mass ratio of the electron and hole affects stability of positively and negatively charged trions in 3D nanostructures.

The calculations show that the binding energy of negatively and positively charged trions is strongly enhanced in 2D structures due to the size-confinement effect, the screening effect of the Keldysh potential and small deference of the electron and hole effective masses. The latter two lead to a weaker electromagnetic repulsion between the identical particles and give the bound positively charged trion. The conditions for stability of a positive trion in bulk and 2D materials are considered. The comparison of our results for the binding energy of trions with those calculated via different theoretical methods and experimental data are presented.

This work is supported by US NSF by HRD-1345219, DMR-1523617 awards.

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ANGLE DEPENDENCE OF MAGNETORESISTANCE EFFECTS IN ARRAY OF BISMUTH NANOWIRES

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The issue of conductive surface states in bismuth is still under discussion. Our work is focused on detection of the surface states contribution using magnetotransport measurements. Previously we investigated an array of electrochemically grown bismuth nanowires in a longitudinal magnetic field [1] and observed several effects of magnetoresistance: broad maxima in fields 9-10T, sharp increase in low fields (0-0.5T), which is connected to antilocalization, and magnetooscillations with period close to hc/e through the cross-section of nanowire. These magnetooscillations resemble the Aharonov-Bohm effect on surface states, the result recently found in wires of a topological insulator [2]. The last two effects were detected for the first time on an array of bismuth nanowires.

In this work, we have measured magnetoresistance on the similar samples at different angles (α) between magnetic field and axis of nanowire. With an increase of α, the magnetoresistance increases drastically. The negative magnetoresistance region disappears at α = 20-25°. In low magnetic fields, the magnitude of the anomaly is practically independent on the angle. The analysis of angular dependence of Aharonov-Bohm oscillations was performed using Fourier transform. It was shown that the positions of the maxima of the Fourier spectra of oscillations as a function of the angle α are extrapolated well by the curve $Y = 0.53/\cos(\alpha)$. This confirms our assumption that the oscillations observed are Aharonov-Bohm-type.

The work was supported by the Russian Science Foundation (Project No. 16-12-10411).

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LOW-THRESHOLD FIELD ELECTRON EMISSION FROM CARBON STIMULATED BY LOCAL SURFACE DEFORMATION IN ELECTRIC FIELD

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It presents the results of a study of the HOPG surface behavior in a strong electric field. It is shown that the influence of electric field (1-100 V/μm) leads to the microdeformation of the surface takes place. In this case, there is a exfoliation of nano regions of the surface [1, 2]. The results are obtained using scanning electron microscopy, Raman spectroscopy and field emission microscopy. Studies were made in the stationary and pulse (nanosecond range) modes, in the direct and opposite sign of the field action. It is shown that the deformation does not depend on the polarity of the electric field.

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FIELD EMISSION FROM CARBON STRUCTURES ENHANCED BY INSERTING DIPOLE NEGATIVE-U CENTERS

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There is a very strong effect found in the study of field emission from carbon. This is a low-threshold emission, excited in fields 3-4 orders of magnitude lower than metals and semiconductors. The work is devoted to the construction of a theoretical model of this phenomenon.

The most interstitial- and vacancy-related centers in low-dimensional semiconductor structures appear to exhibit negative-U properties in the presence of the local vibration mode that gives rise to the spontaneous decay of the one-electron states with the formation of the reconstructed dipole centers. Specifically, a series of dipole centers that created inside fluted and suspended regions within the preparation of carbon structures seem to result in nanostructures and nanotubes responsible for the spin-dependent quantum transport phenomena. Moreover, the reconstruction of dipole centers under the application of the external electric field allows the model of the enhanced field emission from carbon-related structures. Indeed, the dipole centers appear to result in the surface band bending, with the creation of the deep triangle quantum well and corresponding Fermi level pinning varied by the value and the orientation of the external electric field. Besides, the dipole centers under applied voltage seriously control the characteristics of the delta-barrier that determine the parameters of the electron emission. Thus, the model suggested allows the explanation of the findings of small domains on the emitting surface in which the electric field is able to exceed the value of 10^8 V/cm taking account of the dimensions of dipole structures. The energy distribution of the emitted carriers reveal the specific maxima the positions of which are in a good agreement with the electron subbands, E_1, E_2 in the induced quantum well. Finally, this model provides also the quantum effects in the enhanced emission in external magnetic field as well as by varying the value of the longitudinal electric field.

FIELD ELECTRON EMISSION OF BILAYER GRAPHENE

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Low-threshold field emission in stationary and pulsed electric fields on a bilayer graphene is investigated. It is shown that the current-voltage and kinetic characteristics of field emission behave in full accordance with the effects of earlier observed on highly oriented pyrolytic graphite (HOPG), nanotubes, multilayered graphene-like structures [1].

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THEORETICAL ANALYSIS OF A LABEL-FREE GRAPHENE FET APTASENSOR FOR DETECTION OF LEAD IONS IN HUMAN BLOOD

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In this work an electrolyte-gated graphene field effect transistor (EG-FET) where graphene is functionalized by 8-17 DNAzyme is studied. This type of aptasensor is proposed by Wang et al. in [1] to detect different Pb^{2+} ions concentrations in the solution gate. Authors show that this sensor device has two important advantages: (i) high sensibility - detection limitation is below 37.5 ng/L which is three order lower than the safe blood lead level (100 μg/L) and (ii) excellent selectivity over other metal cations such as Na^{+}, K^{+}, Mg^{2+}, and Ca^{2+}.

In order to model the influence of specific binding Pb^{2+} ions by 8-17 DNAzyme molecules adsorbed on graphene surface on graphene conductivity vs liquid gate voltage characteristics. We use Boltzmann's transport approach and Grahame's theory of the electrical double layer similarly to [2]. As a result we extract from experimental curves charge carrier concentration in graphene for each Pb^{2+} concentrations to obtain the dependence of charge neutrality point shift on Pb^{2+} concentrations.

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REDUCED GRAPHENE OXIDE AEROGELS WITH POLYMERS AND CARBON NANOPARTICLES

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The main purpose of this study is a study of aerogels based on reduced graphene oxide with a high surface area and electrical conductivity, stable under cyclic electrochemical reactions, which are promising materials for supercapacitor electrodes, and are also considered promising carbon carriers for metallic nanodimensional catalysts.

The influence of various modifiers (aqueous polymer suspensions, polymer solutions, carbon nanoparticles, etc.) on the structure of aerogels from reduced graphene oxide was studied. The SEM method shows that the approach used makes it possible to obtain aerogels with a uniform distribution of fillers in the material structure. It has been found that the modification of the initial suspension of graphene oxide with polyvinyl alcohol leads to a fundamental change in the morphology of the aerogel - instead of the layered regular structure it acquires a fractal irregular character (Figure 1) and is accompanied by a significant increasing of the specific surface area.

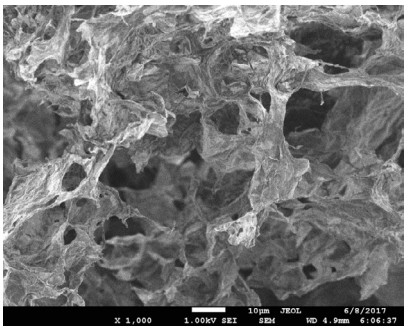

Fig. 1. *SEM aerogel shot: reduced graphene oxide + 20% polyvinyl alcohol*

A fundamentally new regimen for the reduction of graphite oxide, an explosive reduction initiated by hydrazine vapor at room temperature, has been developed. Comparison of graphene-like materials obtained during the initiation of explosive reduction of graphene oxide by thermal shock and hydrazine vapor, using IR spectroscopy, elemental analysis, and SEM showed that they have a close elemental composition, morphology, and a set of residual functional groups.

DFT STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF $MoS_{2(1-X)}Se_{2X}$ ALLOY

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Semiconducting transition metal dichalcogenides (TMDs) represent a class of layered materials. TMD monolayers such as MoS_2, $MoSe_2$, WS_2, WSe_2 are direct band gap semiconductors (with optical band gap of 1-2 eV). Owing to a nonzero band gap, rich physics and promising applications in electronic and optoelectronic devices transition metal dichalcogenides have attracted much attention.

In the present work first-principles calculations have been performed to study the structural features of the monolayer $MoS_{2(1-x)}Se_{2x}$ alloy and its electronic properties. We have studied the effects of relative positions of Se atoms in a real monolayer alloy. It was demonstrated that the distribution of Se atoms between top and bottom chalcogen planes is most energetically favourable. The concentration dependence of the band gap has been analysed with percolation theory. For more probable distribution of Se atoms $MoS_{2(1-x)}Se_{2x}$ monolayer alloy is a direct semiconductor with the fundamental band gap equal 2.35 eV (calculated with GVJ-2e method [1-3]). We also evaluated the optical band gap of alloy at 77 K (1.86 eV) and room temperature (1.80 eV), which is in good agreement with the experimentally measured band gap of 1.79 eV.

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QUALITATIVE ANALYSIS OF MAGNETIC WAVEGUIDES FOR TWO-DIMENSIONAL DIRAC FERMIONS

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We focus on the confinement of two-dimensional Dirac fermions within the waveguides created by realistic magnetic fields. Understanding of their band structure is of our main concern. We provide easily applicable criteria, mostly depending only on the asymptotic behavior of the magnetic field, that can guarantee existence or absence of the energy bands and provide valuable insight into the systems where analytical solution is impossible. The general results are employed in specific systems where the waveguide is created by the magnetic field of a set of electric wires or magnetized strips.

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CHEMICAL VAPOR DEPOSITION GROWTH AND CHARACTERIZATION OF GRAPHENE LAYERS

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Graphene layers were grown by different chemical vapor deposition (CVD) methods on copper foil. The obtained samples were characterized by Raman spectroscopy. Effects of the Cu surface roughness and orientation on the quality and the Raman response of the grown layers were studied. The obtained data are compared with the Raman signal of graphene after transfer on glass substrate revealing the complex interaction of graphene with the Cu catalyst.

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TERAHERTZ GENERATION IN NANOCOMPOSITES

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It is well known that nonlinear properties of nanocomposites depends on not only features of nanoparticles embedded into a matrix but also on parameters of the matrix inself. We study exciton states in nanocomposites consisted of semiconductor metal-oxide quantum dots (QD) incorporated into a dielectric non-centrosymmetric matrix accounting for large permanent dipole moment (PDM) of QDs and quadratic nonlinearity of matrix. We suppose, that the QD dielectric permittivity is substantially higher than the dielectric matrix one and the QD sizes are large enough. According to our calculations starting from the critical QD radius the electron-hole binding energy asymptotically approaches the binding energy of corresponding 2D exciton. Another reason of the large value of electron-hole binding energy and stability of exciton states, formed by spatially separated charges, is the dielectric enhancement effect originated from the field produced by the nanoparticles in matrix. In such nanostructures the PDM and transition dipole moment between exciton states in QDs may be two orders larger than corresponding parameters in volume semiconductors. Below we present the results of our theoretical analysis of the frequency down-conversion processes in nanocomposites with the PDM via resonant and nonresonant optical rectification mechanism.

We suppose that phase-matching conditions are fulfilled due to the Zakharov-Benney resonance between terahertz (THz) harmonic and the pump pulse. THz generation by a femtosecond laser pulse being in resonance with the QDs and out of resonance with dielectric matrix is investigated. The resonant mechanism of THz generation is shown to be more effective than non-resonant one. One- and two-photon resonances as well as local field effects are accounted for. THz generation efficiency is estimated in coherent and incoherent light-matter interaction regimes allowing possible phase modulation of the pump pulse and phase capture of THz harmonic. As is shown when the PDM influence is weak and one-photon transitions predominate the dependence of the THz field on the pump pulse is quadratic. In this case the THz generation efficiency does not exceed 10^{-3}. With increasing the PDM magnitude the underlying two-photon transitions lead to stronger dependence of low frequency harmonic on the pump pulse providing more efficient frequency conversion. For prevailing two-photon transitions the THz generation efficiency can reach 16-17% under phase capture conditions. Figure 1 demonstrates THz generation process in nanocomposite material with large PDM at input pump pulse area $\Theta_1=5\pi$.

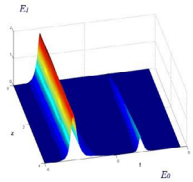

***Fig 1**. THz generation process in nanocomposite material with large PDM at $\Theta_1=5\pi$: E_1 (t, z) - propagating pump pulse, E_0 (t, z) - generated THz wave*

NANOMECHANICS OF GRAPHENE

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Graphene is a famous example of a crystalline membrane with a thickness of one atomic layer. The talk is focused on discussion of the unique elastic properties of this material, which are closely related to the question of the thermodynamic stability of 2D systems. Thermal fluctuations tend to bend the graphene membrane and destroy the long-range order in the system. There is, however, a competing effect of a strong anharmonic interaction between the flexural and longitudinal phonons, which tends to stabilize the membrane. Due to this competition, isolated membrane can exhibit a number of critical phenomena, including two phase transitions: the transition from the flat to crumpled phase — the so called crumpling transition (CT) — and the transition associated with loss stability of a flat phase under the action of external compression [buckling transition (BT)].

It turns out that CT is substantially analogous to the transition of a magnet to a ferromagnetic state. In this case, in complete analogy with the magnet, spontaneous symmetry breaking occurs: a spherically symmetric «crumpled phase» transforms into a flat phase with some arbitrary orientation of the plane. Surprisingly, the effects associated with CT significantly change the elastic properties of membranes, in particularly, graphene-based membranes, even far from the transition point, deep in the flat phase. For example, the bending rigidity of graphene flake grows with its size, and the coefficient of thermal expansion is negative and with a good accuracy constant up to extremely low temperatures. At present, the material that possesses such unusual properties is unknown. No less unusual are the manifestations of BT. In particular, it turns out that the ordinary linear Hooke's law for graphene is not satisfied. The stretching of an isolated graphene sheet grows with the applied stress in a power-law manner, with the exponent given by the critical index of BT.

This talk presents an overview of recent works, both theoretical and experimental, devoted to the description of the critical behavior of graphene-based membranes.

MECHANICAL PROPERTIES OF FUNCTIONALIZED POROUS CARBON NANOSTRUCTURES

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The glassy-carbon is a porous carbon structure (PCS), in which the density varies from 1.06 g/cm^3 to 1.55 g/cm^3. To use glassy-carbon as a material for autocathodes and sorbents, it is necessary to investigate the mechanical properties of the material. It was shown in paper [1] that porous structures with pore size of 10-15 nm and a density of 1.4 g/cm^3 have a Young's modulus of 30 GPa.

The purpose of this paper is a theoretical study of the change in the Young's modulus of porous carbon nanostructures with a density of 1.4 g/cm^3, depending on pore size and concentration of oxygen atoms. The studies were conducted by means of a molecular-mechanical method with use of energy potential AIREBO.

For a study of mechanical properties of the constructed three atomistic models of porous carbon nanostructures: pore size of 2.7 - 5.5 Å, pore size of 6.2 - 7.3 Å, pore size of 8.5 - 14.9 Å. The oxygen atoms in the cavity of the porous carbon nanostructures were located chaotically. Studies were conducted with using elementary elements, taking into account periodic boundary conditions.

On the basis of results presented in this paper and paper [1], it was established that the Young's modulus of porous carbon nanostructures decreases with increase porosity of the structures. Young's modulus of a porous carbon nanostructure with pore size: from 0.4 nm to 0.8 nm is 1.45 TPa, from 0.2 nm to 1.12 nm - 732 GPa, from 0.7 nm to 1.3 nm - 661 GPa. The values of the Young's modulus increase with increasing concentration of oxygen atoms with their chaotic arrangement in the pores of the PCS cell.

At a study, the change of values of the Young's modulus of the EXY component depending on concentration of oxygen atoms located layer-by-layer in the PCS, two methods with different arrangement of oxygen atoms in the cell are considered. It is established that depending on increase in concentration of oxygen atoms with their parallel arrangement concerning the plane of stretching (XY), the values of Young's modulus (EXY) are increased, and for perpendicular arrangement of oxygen atoms relative to the plane.

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MAGNETORESISTIVE SUPERFERROMAGNETIC SENSORS

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Superferromagnets (SFMs), e.g., magnetic nano-crystal self-assemblies and/or arrays, represent promising candidates for Lab on a Chip systems including many laboratory tasks. Such soft magnetic systems provide an opportunity to develop new materials with characteristics far beyond traditional solids. The randomly jumping interacting moments (RJIM) model, see [1] and refs. therein, gives useful framewok for studies of SFMs. In particular, it provides a basis for developing analytical tools employed in order to specify, quantify and analyse respective magnetic structures. Such tools explore correlations of magnetic noise amplitudes and allow for quantitative definition, description and study the SFM origin, as well as self-organized criticality in the response properties. In this contribution we briefly overview some results for a sensor mode of SFM reactivity associated with spatially local external fields, i.e., a detection of magnetic particles. Favorable designs of superferromagnetic systems for sensor implications are revealed.

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LATTICE STUDY OF PHASE DIAGRAM AND CHIRAL MAGNETIC EFFECT IN DIRAC SEMIMETALS

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Recently discovered Dirac Semimetals Na_3Bi and Cd_3As_2 provide perfect opportunities for investigation of phenomena which were usually attibuted to high energy physics. The reason for that is the existence of two massless Dirac fermions in the quasi-particle dispersion relation for these materials. We formulate the discretized version of the effective field theory for low energy excitations in Dirac Semimetals. Within lattice effective field theory approach we investigate the phase diagram of Dirac semimetals in the plane effective coupling constant - Fermi velocity anisotropy and the conductivity of these materials in external magnetic field. One of the manifestations of the chiral anomaly, Chiral Magnetic Effect, can be be observed in these materials as a large magnetoconductivity. Our results confirm the existence of Chiral Magnetic Effect in Dirac Semimetals.

GRAIN BOUNDARY INDUCED PHONON SCATTERING IN POLYCRYSTALLINE GRAPHENE

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We have investigated theoretically the phonon scattering due to grain boundaries of different shapes in polycrystalline graphene based on the deformation potential approach. Grain boundaries are represented as repeated rows of 5-7 disclinations dipoles. This approach allows us to obtain the exact analytical results for the mean free path of phonons in the Born approximation [1], [2]. For closed configurations such as the Stone-Walls defects the momentum dependence of the mean free path is found to be k^{-3}, while for straight grain boundaries it varies as k^{-1}. The thermal conductivity as a function of temperature and the grain boundary size is studied numerically within the Callaway's approach [3] where normal phonon processes are taken into account. We found that the role of grain boundaries is of importance in a wide temperature range including room temperatures.

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STRUCTURE AND STABILITY OF SILICON OXIDE NANOCLUSTERS

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Silicon nanoparticles are promising for many applications including nanoelectronics, optoelectronics, solar cells, biomedical imaging sensors, etc. The exploration of Si-O clusters is also of interest for astrophysics and geophysics as it can bridge the gap between the presence of SiO molecules in the circumstellar space and the dominance of silicate minerals in the Earth crust.

We present a systematic study of the structural, electronic and thermodynamic properties of Si_nO_m clusters in a wide range of compositions ($1 \le n \le 10$ and $0 \le m \le 20$). The lowest-energy structures for all n and m were found by the evolutionary algorithm (the USPEX code) combined with density-functional calculations. The most stable clusters were determined using two criteria: (1) the minimum second derivative of the total cluster energy by the number of silicon and oxygen atoms; (2) the minimum energy of the cluster decomposition into two fragments. In addition to the expected $(SiO_2)_n$ clusters, a number of structures with unexpected stoichiometry were found to have a high stability.

It was shown that under normal conditions in oxygen atmosphere the nanoclusters are in the oxygen-enriched form (in comparison with the stoichiometric compositions $(SiO_2)_n$). For example, among the Si_7O_m clusters, the most stable cluster is Si_7O_{19}. The additional oxygen atoms exhibit magnetic properties and form reactive oxygen species at the surface (in particular, peroxide, ozonide ions and oxo-radicals). This can explain the high toxicity and carcinogenicity of silica dust [1].

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NEW PHASES AND CONTROLLING IN 2D EXCITON SYSTEMS

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Electron-hole bilayers based on semiconductor nanostructures, graphene and topological insulators, superfluidity and strongly correlated states will be reviewed (see also [1-11]). Role of the hybridization will be analyzed. Drag effect, Cooper electron-hole pair fluctuations and fluctuational internal Josephson effect in the system will be considered. Anisotropic superfluidity, instabilities and strong correlated phases in dipole systems will be analyzed. Anisotrpies of helicity modulus, superfluid mass density, speed of sound and quasicondensate luminiscence are predicted for a two-dimensional system of interacting dipole excitons in a periodic potential at T = 0. Presence of supersolid properties in the system considered is shown. Physical realizations of the model are discussed. For a system of two-dimensional dipolar excitons in an electrostatic lattice estimates for the magnitude of the predicted effects are given and a method to control superfluid component and measure helicity modulus in dipolar systems is presented. Roton instability of dipole exciton system in semiconductor film is discussed. Strong correlated phases of dipole excitons (or dipole atoms) will be discussed. Experimental manifestation of the predicted effects will be analyzed. Instabilities in the system of dipole excitons (excitons with spatially separated electron and holes) will be analyzed. Possible crystal and supersolid phases in dipole exciton systems will be discussed. The transition of the exciton system from the superfluid state to a non-superfluid state controlled by gate and its manifestation by light scattering will be analyzed.

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MANY-ELECTRON EFFECTS IN SMALL SILICON NANOCLUSTERS BY GW METHOD

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In the first-principles calculations, an evident source of systematic errors is the exchange-correlation (xc) contribution, that is subject to approximation. Moreover, good xc approximation for the bulk often is not applicable to nanoobjects. The atomic structure of small nanoclusters generally differs great from that of the bulk and relatively big particles. The nanocluster structure varies widely with cluster sizeand composition. Surface atoms constitute a significant part of a small nanoparticles and also have a strong impact on its properties. All these features affect the Coulomb screening and require a suitable description of the many-electron effects in nanoobjects. On the example of small silicon clusters, the energy ordering of isomers, as well as the features of plasma excitations, are considered in the framework of the GW method.

The first-principles prediction of stable nanocluster structure is often hampered by the existence of many isomer configurations with energies close to the ground state. Thus xc contribution can change a subtle energy order of competitive structures. To analyze this problem, we consider the energetics of silicon nanoclusters passivated by hydrogen $Si_{10}H_{2n}$ ($0 \le n \le 11$), where passivation changes the structure from compact to loosely packed and branched. Our calculations confirm a considerable sensitivity of isomer energy ordering to many-electron effects.

Plasma oscillations in silicon nanocrystals Si_{16} - Si_{60} and Si_4H_{10} - $Si_{35}H_{36}$ were also considered by the GW method. An analysis of the results obtained and effectiveness of the method for the indicated problem is given. As in the bulk crystals, GW spectral function noticeably overestimates distance between quasiparticle peaks and corresponding satellites. However, peaks in the self-energy function fit well experimental curve for the plasmon frequencies depending on nanocluster size. Volume and surface plasmons demonstrate significant dependence on the size, structure and passivation of hydrogen.

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THE YOUNG'S MODULUS OF PILLARED GRAPHENE

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The pillared graphene is a material based on graphene sheet connected with vertically aligned carbon nanotubes (CNT). In the scientific literature there is already an established opinion, mainly due to the result of computer simulation that the column graphene is able to prove itself as an effective filter or as membrane for the separation of gas mixtures, or as a hydrogen storage [1]. In this paper, we have carried out theoretical research of dependence the value of the Young's modulus of the cluster-pillared graphene based on zigzag-CNT upon size of graphene sheet and CNTs' length.

The research was carried out for composites, CNTs' diameter of which was the same and was equal 5 Å. Length of zigzag-end of graphene sheet in all over the researching composites was equal 16.4 Å. Length of armchair-end of graphene sheet was changing from 33.5 Å to 136.3 Å. Length of CNTs stayed constant within each composite, but in series of studies CNTs' length were changing from 3.3 Å to 31.6 Å. We have defined the optimal condition by the molecular mechanic method [2].

At the researching the dependence of the value of the Young's modulus upon the CNTs' lengths, we discovered that the Young's modulus were increasing at the increasing of the CNTs' lengths. This result coincided with result for pillared graphene based on armchair-CNT by the type of the dependence [3].

We propose that showed structures will be perspective material for nano electronics for high mechanical strength.

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HIGH HARMONICS GENERATION WITH 2D METALLIC CARRIERS OF TOPOLOGICAL INSULATOR

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Along with graphene topological insulators (TI) recently emerged as a central theme in condensed matter physics and has attracted enormous interest due to their unique electromagnetic properties. Three-dimensional TIs are bulk insulators with robust 2D metallic surface states. These states are massless with linear Dirac like energy dispersion. The unique properties of the surface states are responsible for their exotic nonlinear electromagnetic properties. One of the most desirable nonlinear optical processes is the high-harmonic generation stimulated by an intense coherent electromagnetic radiation. Hence, it is of interest to investigate multiphoton excitation and subsequent high harmonic generation process in TIs.

In the present work, we develop a nonlinear microscopic theory of the interaction of 2D metallic carriers confined on the surface of the 3D topological insulator with coherent electromagnetic radiation toward generation of high harmonics. In the scope of dynamic Hartree-Fock approximation the set of integrodifferential equations for the interband polarization and carrier occupation distribution is solved numerically. It has been shown that by THz radiation of moderate intensities, one can control interband multiphoton transitions in 2D metallic surface states of TI on time scales 100 ps. Furthermore, we have shown that along with multiphoton transitions there is an intense radiation of high harmonics at the interband (particle-hole annihilation) and intraband transitions induced by a pump wave. The obtained results certify that the process of high-harmonic generation for THz photons can be already observed for intensities 0.2 kW/cm^2.

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BULK BOUNDARY CORRESPONDENCE AND DYNAMICAL PHASE TRANSITIONS IN ONE DIMENSIONAL SPT SYSTEMS

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We study the Loschmidt echo for quenches in open one-dimensional lattice models with symmetry protected topological phases [1]. For quenches where dynamical quantum phase transitions do occur we find that cusps in the bulk return rate at critical times are associated with sudden changes in the boundary contribution. For the Su-Schrieffer-Heeger model, we show that these sudden changes are related to the periodical appearance of two eigenvalues close to zero in the dynamical Loschmidt matrix. We demonstrate, furthermore, that the structure of the Loschmidt spectrum is linked to the periodic creation of long-range entanglement between the edges of the system.

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MODELING AND SIMULATIONS OF GRAPHENE PSEUDOSPHERES

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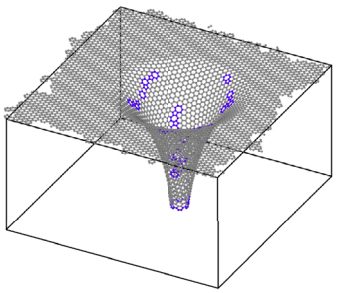
In a previous work it was shown that the realization of the graphene topology on a Beltrami pseudosphere can lead to the analogue realization of the Hawking-Unruh effect [1]. This effect predicts that quantum fields in curved space-time with an horizon exhibit a thermal character due to the quantum vacuum and to the relativistic process of measurement. The aim of this work is thus to produce a 3-coordinated carbon structure on a Beltrami pseudosphere to find the minimal energy configuration of the atoms on this surface, showing that it is energetically stable and, thus, that can be obtained experimentally. Heptagonal and pentagonal defects (represented in blue in the figure below) emerge on the surface due to the negative curvature [2]. We devise a new algorithm to scale-up the pseudospehere dimensions reaching a radius R~100 nm of the event horizon. Next, we study the curvature effects on the electronic properties of the system, which should bring about a thermal spectrum in the form of finite temperature electronic Local Density of States [1].



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SPIN CURRENT OF CORRELATED 2D ELECTRONS SYSTEM IN THE PRESENCE OF RASHBA SPIN-ORBIT INTERACTION

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In order to understand effects of Coulomb correlations on the spin current and spin Hall current in a semiconductor film with strong Rashba spin-orbit interaction (Rashba medium), a model of two particles, which move in a two-dimensional (2D) Rashba medium and correlate through Coulomb potential, is studied. We show that the problem can be solved exactly for the both cases of Coulomb repulsion and attraction. In the case of Coulomb attraction between an electron-hole pair, the energy spectrum is found, which is similar to the spectral series of hydrogen atom, where each energy level is split into three sublevels due to spin-orbit interaction. The problem of Coulomb repulsion of two electrons in the Rashba medium is solved exactly too. The obtained evident form of the wave function allows us to calculate an equilibrium spin current.

FLUORINATED GRAPHENE FILMS IRRADIATED BY SWIFT HEAVY IONS: CHANGES IN ELECTRIC AND STRUCTURAL PROPERTIES

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Fluorinated graphene (FG) is known to be one of the most stable, dielectric graphene derivative. It turned out that such chemical and thermal stability causes some problems for developing of FG-nanostructuring pathways. We used swift heavy ions to create new graphene-based, nanostructured material from partially fluorinated graphene films.

The studied films were prepared from a fluorographene suspension by applying onto the surface of silicon substrates. It was experimentally shown that the following processes took place in the irradiated FG-films:

(i) thermal expansion of individual fluorographene particles with subsequent formation of hollow "bubbles",

(ii) particle nanostructuring (on increasing the fluence, we observed a decomposition of initial particles into granules sized ~ 20 - 50 nm), and

(iii) as suggested, formation of shallow (1.5 - 3 nm) graphene quantum dots in the fluorographene matrix. As a result of film nanostructuring, in the measured C-V and G-V characteristics of structures involving examined films there emerged peaks whose amplitude grew with decreasing the measurement frequency.

We suppose that the shock heating resulted in a substantial local change of structural and electrical properties of the films. The obtained granules may offer promise in biological and medical applications due to the stable properties of the "graphene quantum dots in fluorographene matrix" system.

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ORIGINS OF NONLOCAL RESISTANCE IN MULTITERMINAL GRAPHENE: SPIN HALL AND VALLEY HALL VS. OTHER COMPETING EFFECTS

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The recent experimental observation of nonlocal voltage, several microns away from the nominal current path, near the Dirac point (DP) in multiterminal graphene devices with adatom-induced spin-orbit coupling or in multiterminal graphene on hexagonal boron nitride (G/hBN) heterostructures has been interpreted as the result of the direct and inverse spin Hall effect (SHE) or the direct and inverse valley Hall effect (VHE), respectively [1]. However, subsequent experiments reproducing the nonlocal signal in graphene with adatoms have also demonstrated insensitivity to the applied in-plane magnetic field, thereby suggesting its disconnect with SHE physics or any other spin-related mechanism. The theoretical interpretation of nonlocal signal in G/hBN heterostructures in terms of topological valley currents carried by the Fermi sea states just beneath the gap opened in graphene due to inversion symmetry breaking does not explain the long-standing puzzle of why the highly insulating state of G/hBN is rarely observed. In this talk, I will show how to resolve these puzzles by using first-principles Hamiltonians of graphene with adatoms or G/hBN heterostructures combined with numerically exact calculations of the nonlocal resistance based on the multiterminal LB formula [2,3]. In the case of multiterminal G/hBN heterostructure, we demonstrate [3] the key role played by the Fermi surface edge states and the corresponding edge currents (which were missed in previous theoretical analyses based on simplistic Hamiltonian) that can explain both the nonlocal resistance and metallic-like resistivity observed in experiments while being in full accord with the very recent Josephson interferometry-based imaging of the spatial profile of edge supercurrents.

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ELECTRONIC PROPERTIES OF PARTIALLY FLUORINATED GRAPHENE

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The structure and composition of graphite fluorides are determined by the synthetic conditions, namely, crystallinity and particle size of graphite, reaction temperature, and fluorinating agent and two stoichiometric compounds with CF and C_2F composition are known. A layer of the graphite fluoride CF consists of trans-linked cyclohexane chairs in which sp^3-hybridised carbons combine with fluorine atoms by covalent bonds. Incorporation of two kinds of carbon atoms, linked with fluorine atoms and bare carbon, into graphite fluoride C_2F could give the various structures within a C_2F composition. Here, from the comparison of the experimental NEXAFS spectrum of graphite fluoride C_2F produced at room temperature and theoretical spectra plotted for three different models we show that the more preferable fluorine pattern is the formation of zigzag-like CF chains [1]. The models were calculated within density functional theory at the B3LYP/6-31G level. CK-edge NEXAFS spectrum was simulated using the so-called (Z+1)-approach, where a fictitious Z+1 compound with an additional proton in its atomic nucleus is introduced instead of the real Z compound containing a core level hole. Recent measurements revealed magnetic properties for the fluorinated graphite fluorides and results will be discussed [2, 3].

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NANOPATTERNING OF GRAPHENE OXIDE BY SWIFT HEAVY IONS

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We report the fabrication of nanometer-sized reduced graphene oxide (rGO) spots by swift heavy-ion (SHI) bombardment. Such structures can be considered graphene quantum dots (QDs) embedded in a non-conductingmatrix. Both the number density and the diameter of the rGO spots can be tailored by a suitable choice of irradiation parameters (i.e., ion type, fluence, and energy). The degree of graphene oxide defunctionalization by SHIs with different energies scaled well with the deposited electronic energy density. The resistance of the samples decreased nonlinearly with increasing ion dose, and, at fluences above 10^{13} cm^{-2}, was orders of magnitude lower than the initial value. An increase in the electronic stopping power of the ion resulted in:

(i) suppression of the structural ordering at low fluences,

(ii) increased amorphization efficiency and formation of sp-hybridized carbon chains of both polyynes and polycumulenes at high fluences.

The electronic structure and vibrational properties of these carbon-chain molecular junctions were investigated using density functional theory calculations. A hypothesis suggesting that the sp-C chains are bridges joining opposite sides of nanoholes created inside the track core and thus assuming the formation of a coupled QDantidot system is presented. These phenomena were found to be absent in comparative experiments with 200 keV Xe ion irradiation, i.e., in the nuclear stopping regime.

EXPANSION BEHAVIOR OF HOPG UNDER SWIFT-HEAVY-ION IRRADIATION

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We report the effects induced in highly oriented pyrolytic graphite (HOPG) by irradiation with swift heavy ions (SHIs). According to previous studies, the tracks formed in SHI-irradiated HOPG are supposed to be discontinuous, and for ions with an electronic stopping power (S_e) ranging from 7 to 18 keV/nm, the probability of defect creation on the surface is predicted to be < 1 [1]. Our STM measurements of 167 MeV Xe ion-irradiated HOPG (S_e ~ 17.3 keV/nm) revealed the presence of two types of nanohillocks on the surface. Atomically-resolved images showed that the first type refers to regions with damaged C lattice (point-like defects), whereas the second type represents distorted protrusionswith undamaged lattice. The protrusions are supposed to form due to damaged regions located a few layers below the surface, or interstitials between the two uppermost layers. The local near-surface expansion of damaged regions was confirmed by XRD and XAES measurements. The XRD patterns of Xe ion-irradiated specimens show that with increasing ion dose the interlayer distance increases up to 3.55Å. In the XAES spectra, the irradiation-induced changes are manifested by a gradual intensity reduction of a component at a kinetic energy of ca. 265 eV that represents interlayer p−p electron interaction. A complete disappearance of this component upon high-dose ion bombardment suggests that interlayer distance increases to such an extent that HOPG structure is transformed to loosely interacting graphene sheets. TEM investigations of cross-sectional view specimens provided a direct proof that (i) tracks in HOPG are really discontinuous, and (ii) the damaged graphene sheets partially overlap each other, thus causing the interlayer expansion to occur in immediate proximity to the damaged region. We propose, this effect is responsible for an atypical dependence of the Raman spectroscopy derived disorder parameter (ID/IG) on excitation laser energy.

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THE INFLUENCE OF STRUCTURAL DISORDER IN CARBON MULTI-WALLED CARBON NANOTUBES ON THE DENSITY OF STATES

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The change in the density of electronic states (DOS) near the Fermi level under doping, ionic and thermal treatments has been studied. On the basis of experimental data of the DOS near the Fermi level, a band structure model for MWCNTs containing various types of defects was constructed. In the framework of the method of temperature Green functions, an expression is obtained for the contribution to the DOS near the Fermi level for large-diameter MWCNTs with impurities and structural inhomogeneities (short-range order).

It is shown that doping of MWCNTs with nitrogen leads to an increase in the density of occupied states near the Fermi level, which indicates an increase in the number of free n-type charge carriers in the N-MWCNTs surface layer. It was found that annealing of N-MWCNTs in a vacuum leads to a more significant overlap of the bands, which is due to annealing of structural defects and an increase in the amount of electrically active nitrogen. It was determined that irradiation of N-MWCNTs by argon ions with an energy of 5 keV and a dose of ~ 10^{16} ion/cm^2 leads to the formation of a band gap (~1.2 eV) due to distortions of the MWCNTs crystalline structure and carbon oxidation with the formation of carbon-oxygen groups on the surface of carbon nanotubes.

Within the framework of the theory of short-range order and the method of temperature Green's functions, the observed features of the DOS are explained by a change in the of short-range order associated with rearrangement of the ordering-stratification due to doping, ion irradiation and thermal treatment. In the case of doping of MWCNTs with nitrogen, stratification is observed, that is, the impurity atoms will be located in the second coordination sphere (substitution). Irradiation of N-MWCNTs by argon ions leads to the appearance of additional functional groups, that is, ordering takes place (the impurity atoms are located in the first coordination sphere).

SPINTRONICS IN A RIPPLED GRAPHENE SYSTEM

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We analyze the transmission and reflection of an electron flow through a rippled system in an effective mass approximation when only the interaction between nearest neighbour atoms is taken into account. In our consideration a ripple consists of a curved graphene surface in the form of an arc of a circle. This (direct) arc is continuously connected to the inverse arc. The combined system (one element) is connected from the left-hand and right-hand sides to two flat graphene sheets. Considering the curved surface as part of the armchair nanotube, we have shown that the curvature-induced spin-orbit coupling [1] yields backscattering with spin inversion. This spin inversion is caused by the spin-orbit term that breaks spin symmetry in the effective Hamiltonian of the armchair carbon nanotube [2].

In the energy gap created by the curvature induced spin-orbit coupling there is a preference for one spin orientation, depending on the direction of the electron flow at normal incidence. The width of the energy gap depends in the inverse proportion of the radius of the ripple. One element acts as a semipermeable membrane in some energy range which is transparent for electrons with spin up travelling in one direction and for electrons with spin down travelling in the opposite direction [3].

We have found a cooperative effect of transmissions and reflections produced by a large number of the elements. The larger the number of consistently connected elements, the stronger the dominance of a specific spin component. Based on these results, we predict a strong spin filtering effect for a sufficiently large number of arcs in the rippled graphene system.

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MONODISPERSE FLUORESCENT CARBON NANODOTS WITH TUNABLE AGGREGATION PROPERTIES

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Fluorescent carbon nanodots (CNDs) have attracted increasing attention in the last decade due to their unique combination of bright photoluminescence (PL), easy functionalization, low toxcity and chemical inertness[1]. However, production of monodisperse carbon nanodots (MNCDs) having identical composition, structure, and size and possess in this way identical chemical and physical properties still remains to be a challenging task.

Herein we report a facile and effective route to obtain monodisperse carbon nanodots 3.5±0.9 nm in size[2]. The structural studies demonstrate that the synthesized MCNDs have a nearly spherical shape and are constituted by ~8–10 graphene layers that contain various oxygen-containing functional groups. Owing to their identical size and chemical composition, the MCNDs via coagulation form primary aggregates ~10–30 nm in size, which are, in turn, combined into secondary porous spherical aggregates with diameter of ~100–200 nm. The processes of coagulation of MCNDs and peptization of their hierarchical aggregates are fully reversible and can be controlled by varying the MCND concentration or the pH values. Moreover, the MCNDs show a bright visible luminescence that can be further enhanced by the factor of five by simple modification procedure with the use of hydrogen peroxide and ammonia. The thus obtained fluorescent MCNDs with their properties of formation of porous spherical aggregates are promising candidates for drug delivery as a self-disassembling container and bioimaging.

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GROWTH AND CHARACTERIZATION OF SINGLE- AND MULTILAYER GRAPHENE AND CARBON NANOTUBES

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Single- and multilayer graphene films were grown by chemical vapour deposition (CVD) on Cu foil. Plasma enhancement was included in the CVD process for growth of vertically aligned multiwalled carbon nanotubes using Ni nanoparticles as catalyst. The obtained samples were characterized by electrical measurements, atomic-force and Raman spectroscopy. Nature of defects in the samples and optimal growth conditions for high quality of graphene and carbon nanotubes are discussed.

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SPIN-VALLEY HALF-METAL IN 2D SYSTEMS WITH NESTING

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Half-metal is a system with full spin polarization of charge carriers at the Fermi surface. Such polarization usually occurs due to strong electron-electron correlations. Recently [1], we have demonstrated that doping of the material with the Fermi surface nesting also stabilizes the half-metallic states even in a weak-coupling regime. Among 2D systems with nesting, we would like to mention specifically AA bilayer graphene and biased twisted bilayer graphene, both of which are actively studied. In the systems under consideration, the spin or charge density wave is formed by four bands nested in the absence of doping. Each of these bands is characterized by charge (electron/hole) and spin (up/down) labels. We prove that only two of these four bands accumulate charge carriers introduced by doping, forming a half-metallic two-valley Fermi surface. It is possible to observe two types of such half-metallicity. The first type corresponds to full spin polarization of the electrons and holes at the Fermi surface. The second type, with antiparallel spins in electron-like and hole-like valleys, is referred to as a ``spin-valley half-metal'' and corresponds to complete polarization with respect to the spin-valley operator. We analyzed spin and spin-valley currents and possible superconductivity in the system under study. We show that spin and spin-valley currents can flow in both half-metallic phases at the applied magnetic field.

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TRANSPORT PROPERTIES OF BILAYER GRAPHENE IN ELECTRIC AND MAGNETIC FIELDS WITH BROKEN SYMMETRY STATES AND GENERAL GAP

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The results of a theoretical study of an influence of different kinds of the ground state energy gaps depending on spin s = ± *h/2* and valley ξ at the Dirac K (ξ = 1) and K' (ξ = −1) points in the quasiparticle spectrum on longitidunal and Hall optical conductivities of graphene AA- and AB-bilayers with help of quantum electrodynamic approach in (2+1)-dimensional space-time are presented.

The exact analytical expressions for optical conductivities in electric (leading to the gap of order 5-20 meV) and magnetic fields (3-10 Tesla) are derived with use of the 4-band microscopic U(1) -gauge-invariant. Dirac-type Hamiltonian

$$H=\xi\begin{pmatrix} \Delta_{\xi s} & \gamma_3 v_F\pi/\gamma_0 & \gamma_4 v_F\pi^+/\gamma_0 & v_F\pi^+ \\ \gamma_3 v_F\pi^+/\gamma_0 & -\Delta_{\xi s} & v_F\pi & \gamma_4 v_F\pi/\gamma_0 \\ \gamma_4 v_F\pi/\gamma_0 & v_F\pi^+ & -\Delta_{\xi s} & \gamma_1 \\ v_F\pi & \gamma_4 v_F\pi^+/\gamma_0 & \gamma_1 & \Delta_{\xi s} \end{pmatrix}$$

for $\Delta_{\xi s}=U+\xi\Delta_T+sU_T+\xi s\Delta$ (different for AA and AB-stacking) is linear with respect to covariant derivatives which include magnetic field potential perpendicular to bilayer sheets is suggested. The resulting conductivities are found with use of the Kubo formula together with limiting cases for the direct current conductivities and the relations among the Hall conductivities and Faraday and Kerr angles for the systems, including "AB(AA)-bilayer-substrate" The results predicted some regimes of ground states with broken symmetry realization under external fields control being useful for nano and microoptoelectronic devices on a base of graphene.

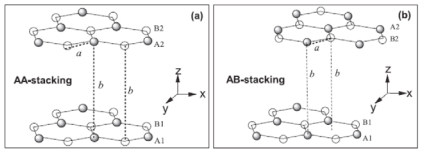

Fig 1*. (a) AA- and (b) AB-bilayer graphene*

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MICROWAVE ASSISTED SYNTHESIS OF MoS_2 NANOSTRUCTURES: OPTICAL AND ELECTRICAL STUDIES

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Transition metal dichalcogenides (TMDs) in their two dimensional (2D) and nanostructured forms are of fundamentally and technologically important. TMDs can exist in various forms like mono- or few layers or in nanostructures like- nanospheres or rod like- structures whose band gap energy and carrier concentration varies depending on the crystalline phase and the structure. A simple method involving liquid phase exfoliation of MoS_2 powder in organic solvents, followed by microwave treatment for the synthesis of MoS_2 nanostructures is reported here. The probe sonication and the microwave treatment play an important role in rolling and curling of the MoS_2 nanosheets[1] to give rise to MoS_2 spheres and rod/tube like-structures with diameter approximately 150–200 nm. The MoS_2 nanorods formed in this fashion are hollow inside with a wall thickness of 15–20 nm and the length of the nanorods is found in the order of several micrometers. Synthesis of such tailored MoS_2 nanorods by a simple and facile route of liquid phase exfoliation is not yet reported. Our observations suggest the 2H phase of bulk MoS_2 remains preserved in the nanostructures with high crystalline quality[2]. The electrical properties of these nanostructures will also be elaborately discussed.

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BIASED TWISTED BILAYER GRAPHENE: MAGNETISM AND GAP ENGINEERING

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Constant electric field applied perpendicular to a graphene bilayer is a useful tool to control various properties of the system. For example, the transverse field opens a gap in the electronic spectrum of the AB bilayer. Since twisted bilayer graphene (tBLG) [1] is in many ways similar to two decoupled graphene sheets, one might naively expect that a transverse bias introduces only trivial modifications to the electronic spectrum of the tBLG. Contrary to such an assumption, we demonstrate that biased tBLG exhibits more complex behavior. It is known that, when the twist angle is not very small, the electronic spectrum of the twisted bilayer consists of four Dirac cones inherited from each graphene layer. When the field is applied, two hole-like and two electron-like Fermi surface sheets emerge. Electron and hole components of this complicated Fermi surface demonstrate (almost) perfect nesting. When the electron-electron repulsion is present, the nested Fermi surface becomes unstable with respect to exciton band-gap opening. The exciton order parameter is accompanied by spin-density-wave order. The gap can be varied by the bias voltage. At constant voltage, the value of the gap is a monotonously decreasing function of the twist angle. The discussed system demonstrates the coexistence of (i) externally controlled gap and (ii) multicomponent magnetic order. This is interesting for both fundamental research and applications, and consistent with recent measurements [2].

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POSSIBLE MANIFESTATIONS OF GRANULAR SUPERCONDUCTIVITY IN GRAPHITE FLAKES VIA PERSISTENT CURRENTS

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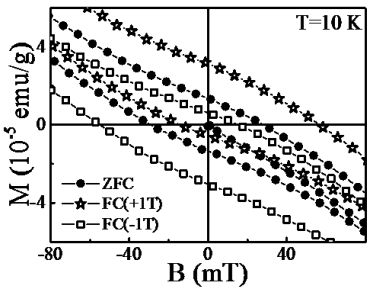
Recently, it has been claimed that slightly twisted graphite/graphene sheets containing flat energy bands could unlock the potential of high-temperature superconductivity in graphite layered system [1-3]. Following recent concepts, we obtained thin graphite flakes from bulk highly ordered pyrolytic graphite (HOPG) by an extended grinding process and then annealed in order to increase the probability of formation of such regions where superconductivity might be possible. Magnetization field dependence was obtained after the sample was cooled from 300 K down to 10 K in zero applied field (ZFC): the resulting hysteresis loop is found symmetric about the origin as indicated in the figure with bold circle symbols. The situation is changed on field cooling (FC) the sample to T = 10 K in a magnetic field of + 1T [FC(+1T) in the figure] and -1T [FC(-1T)] as denoted in the figure by star and empty square symbols, respectively. As a consequence, the FC curves have got shifted vertically (trapped moments) with respect to the ZFC curve. This shift persists up to 350 K, which in our opinion may be a manifestation of granular high temperature superconductivity via persistent currents.



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EMERGENT PHYSICS AND CHEMISTRY OF GRAPHENE

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The paper presents an overview of graphene electronic structure in light of a general concept of emergent phenomena that result from the quantum phase transition caused by continuous symmetry breaking. In the current case, the spin symmetry breaking is provided by a drastic enhancement of p_z odd electron correlation when the shortest distance between them, defined by C=C bond length, exceeds critical value R_{crit}. The UHF formalism clearly evidences the broken symmetry occurrence and perfectly suits to self-consistent description of the issue. Empirically supported and convincingly certified, the UHF emergents, such as (i) open-shell character of electron spin-orbitals; (ii) spin polarization of electron spectrum; (iii) spin contamination; (iv) depriving the spin multiplicity of electronic states; (v) local spin pool at zero total spin density, and so forth greatly extend the view on ground states of graphene and other sp^2 nanocarbons and not only give a clear vision of spin peculiarities of graphene chemistry but predictably point to occurrence of emergents related to graphene physics, such as ferromagnetism, superconductivity and topological nontriviality. The paper presents numerous experimental evidences supporting a deep interrelationship between emergent chemistry and emergent physics of graphene.

EFFECT OF THE GRAIN BOUNDARIES ON THE ELECTRONIC AND MECHANICAL STRUCTURE OF GRAPHENE

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Nowadays, the polycrystalline graphene is in the center of interest due to technological needs. However, its structure contains a lot of inevitable structure elements like vacancies, Stone-Wales defects, dislocations etc. They are mostly contained in the grain boundaries (Fig.1). So, it is important to know their influence on the properties of the material.

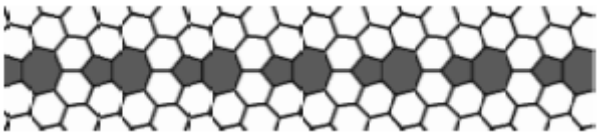

***Fig. 1**. Grain boundary containing Stone-Wales defects*

We will concentrate on different types grain boundaries which contain the Stone-Wales defects (heptagon-penatgon pairs). We will investigate different characteristics of their electronic structure: the conductivity, the charge mobility, density of states. Next we will look through the thermal properties.

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ORIGINS OF TERAHERTZ PHOTORESPONSE IN GRAPHENE TRANSISTORS: THEORY AND EXPERIMENT

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Graphene field-effect transistors (FETs) coupled to antennas can serve as efficient terahertz (THz) and sub-THz radiation detectors. The promise of graphene is due to possible plasmonic enhancement of photovoltage and a variety of rectification mechanisms (non-linearities) associated with linear electron-hole dispersion. The origin of THz rectification in graphene was argued to arise either from resistive self-mixing [1], photo-thermoelectric effect [2], or rectification by p-n junctions inevitably formed at the contacts. We present a combined experimental and theoretical study aimed to 'disentangle' various contributions to THz rectification in graphene FET-based detectors [3].

Our FETs were fabricated from exfoliated graphene encapsulated in hexagonal boron nitride. THz radiation was fed to log-spiral antenna connected to source and top gate terminals, the dc photovoltage was measured between source and drain. We have studied the dependences of photovoltage on carrier density and temperature. An increase in photovoltage near charge neutrality point with lowering temperature as well as temperature-independent shoulder of photoresponse at hole doping are consistent with rectification by Seebeck effect at p-n junctions near the contacts, and inconsistent with resistive self-mixing scenario. Extra peak in photovoltage near neutrality point appearing below T~100 K can be explained by rectification at p-n junction formed between top-gated and ungated regions. We also present a microscopic theory that quantitatively describes the observed photoresponse.

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FIELD THEORETIC STUDY OF ELECTRON-ELECTRON INTERACTION EFFECTS IN PLANAR DIRAC LIQUIDS

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The talk will review recent results related to interaction effects in condensed matter physics systems such as planar Dirac liquids, e.g., graphene and graphenelike systems, the surface states of some topological insulators and possibly half-filled fractional quantum Hall systems. These liquids are characterized by gapless bands, strong electron-electron interactions and emergent Lorentz invariance deep in the infra-red. We address a number of important issues raised by experiments on these systems covering subjects of wide current interest in low-energy (condensed matter) as well as high-energy physics. We shall consider in particular the subtle influence of interactions on transport properties [1, 2] and their supposedly crucial influence on a potential dynamical mass generation [3, 4]. The resolution of these problems will guide us from the thorough examination of the perturbative structure of gauge field theories to the development and application of non-perturbative approaches known from quantum electro/chromo-dynamics to address strong coupling issues.

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TOPOLOGICAL DEFECTS IN GRAPHENE AND OTHER 2D MATERIALS

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Grain boundaries and dislocations are intrinsic topological defects of polycrystalline materials, which inevitably affect their physical properties. In my talk, I will discuss the structure of topological defects in two-dimensional (2D) materials such as graphene and monolayer transition metal dichalcogenides [1]. I will first introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors and grain boundaries covering the complete range of possible misorientation angles [2] and discuss their thermodynamics in the light of our recent observation of buckling transition in polycrystalline graphene [3]. The rest of my talk will cover electronic transport properties of polycrystalline 2D materials with a special focus on the ballistic charge-carrier transmission across periodic grain boundaries. In this regime, the transport is governed primarily by momentum conservation giving rise to phenomena such as the perfect reflection of low-energy charge carriers [4] and valley polarization of charge carriers transmitted across line-defect structures that can be experimentally engineered [5]. Unlike graphene, monolayer transition metal dichalcogenides (MoS_2 and alike) combine a two-valley electronic band structure with strong spin-orbit effects. The latter can be employed for creating spin-polarized currents and adds yet another conservation law in the electronic transport across regular defects such as the frequently observed inversion domain boundaries [6,7].

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MANIFESTATION OF NOVEL MAGNETOPLASMON BRANCHES IN RESPONSE OF 2D ELECTRON SYSTEM ON ELECTROMAGNETIC IRRADIATION

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Plasmons in low-dimensional electron systems are of interest because of the gapless dispersion law, which depends on the geometry of the structure, and of the possibility of the continuous frequency variation using the gate voltage. Without magnetic field plasmons in 2D system with the dc conductivity $\sigma < 2\pi c$ in SGS units are strongly damping due to electron collisions with impurities and phonons [1]. The plasmons damping is decreasing with magnetic filed. In a recent paper [2] extraordinarily low damping branches in magnetoplasmon-polariton spectra of a 2D electron system were predicted. It was shown that effects of electromagnetic retardation is crucial and drastically change plasmon dispersion in the vicinity of light dispersion even in the case $\sigma < 2\pi c$. Since the magnetoplasmon dispersion presumably determines the poles of the denominator of optical coefficients, for instance absorption one, here we calculate the reflection, transmission and absorption coefficients for electromagnetic waves incident on the 2D electron gas, which is described by the dynamical Drude model with dissipation, in perpendicular to the plane magnetic field at an arbitrary angle of incidence.

Following [3,4] we calculate the scattering matrix and find the reflection, transmition and absorption coefficient. It turns out that the denominator as well as the numerator of the optical coefficients do not have poles on magnetoplasmon-polariton dispersion, however, the absorption coefficients nevertheless has features such as resonances in the dependence of absorption on angle of incidence.

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SPECIAL FEATURES OF FIELD EMISSION ELECTRON ENERGY SPECTRUM FROM CARBON NANOSTRUCTURES (HOPG, CNT, GRAPHENE-LIKE STRUCTURES)

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The features of the total energy distribution of electrons emitted from multi-layered graphene-like structures, multi-wall CNT and Highly Oriented Pyrolytic Graphite were studied experimentally. It was used the retarding potential technique. It was established that all the investigated objects demonstrate a noticeable shift of the maximum of their energy spectrum with respect to the Fermi level [1, 2]. The appearance of the second maximum, which is shifted by 2 – 2.5 eV from the main peak, was discovered. Half-width of the distribution broadens with the increase of the electric field for all investigated materials.

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