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GRAPHENE / HEXAGONAL BORON NITRIDE COMPOSITE NANOPARTICLES FOR 2D PRINTED HETEROSTRUCTURES

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A peculiarity of the present study is the use of plasma for the creation of the flakes of graphene and hexagonal boron nitride (h-BN) without using substrates and catalysts. Application of the direct-current arc torch plasma jets provides the advantages of the property controllability and mass production of both types of flakes. The conditions for the formation of composite nanoparticles from graphene and h-BN flakes in suspension were worked out. Morphology and structure of the composite nanoparticles are found to change with an increase of graphene content in composition from (1) the multi h-BN clusters with a random structure on graphene to (2) the graphene flakes covered with the vertically arranged h-BN flakes, then (3) the graphene flakes encapsulated with a monolayer of h-BN flakes, and, at last, (4) the h-BN clusters decorated with graphene scrolls. Practically in all cases, the composite nanoparticle size was 150 -300 nm, this size corresponds to the ability to use them for inkjet 2D printing. The electrical properties of the films created from these composite nanoparticles are also strongly changed depending on their structure. The composite G:h-BN with content (10–6):1 demonstrates non-linear current-voltage characteristics with strong hysteresis (up to 4 orders of magnitude), whereas I-V curves for films with lower or higher graphene content are linear. The temperature dependencies of current in such composite layers show the transport with the activation energy of 27-34 meV most likely connected with bandgap formation due to graphene – h-BN van der Waals interaction. The strongly increased photocurrent was also observed for the composite films.

QUENCH DYNAMICS OF SUPERCONDUCTING NANOSTRUCTURES

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Recent development of the time-resolved spectroscopies (to picosecond precision) allows to probe dynamical processes imposed by the intrinsic effects or driven by the external potentials, giving an insight into the characteristic energy-scales realized in various systems of our interests. We study them here in a nanoscopic heterostructure, comprising the single and/or double quantum dot(s) embedded between the superconducting and metallic electrodes. We analyze the response of such setup to: (i) abrupt voltage applied across the junction, (ii) sudden change of the quantum dot energy levels, and (iii) their periodic driving. We explore evolution of the Andreev bound states (originating from the superconducting proximity effect) and discuss their signatures observable in the time-dependent charge currents. We discuss efficiency of relaxation processes and investigate the Rabi-like quantum oscillations, their beating patters and multi-photon features showing up in the tunneling conductance.

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THE CONCENTRATION DEPENDENCE OF HYDROGEN ON THE ROTATION ANGLE IN TWISTED GRAPHENE

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The concentration of adsorbate atoms dependence on the rotation angle between the layers of twisted bilayer graphene (tBLG) during hydrogenation was determined using simulation methods. Short-range order parameters for various types of defect complexes were calculated. The hydrogen concentrations at which the short-range and long-range order regions are formed for different adsorption centers have been determined. The calculation results are shown in Fig. 1. The obtained dependence of the hydrogen atoms concentration on the rotation angle tBLG is in qualitative agreement with the experimental data [1].

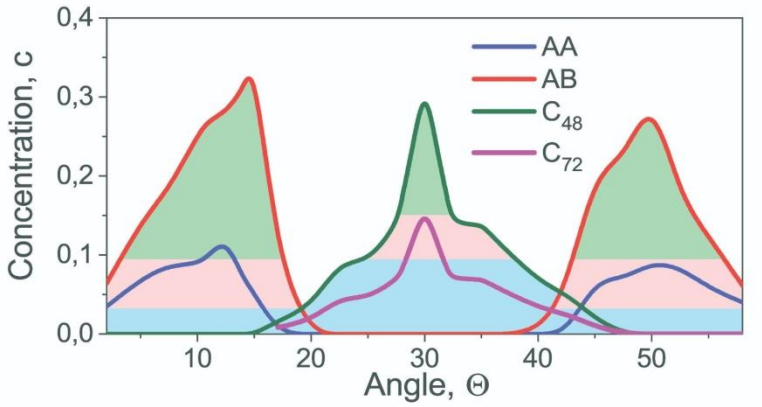

Figure 1. Calculated concentration of adsorbate atoms dependence on the rotation angle between the layers of tBLG. The fill color corresponds to a certain type of disorder: impurities are blue, short-range order is rose, long-range order is green.

The study was supported by a grant from the Russian Science Foundation (project No. 20-72-00138)

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CALCULATION OF BOUND AND RESONANT STATES OF SIZE-QUANTIZED ELECTRON AND HOLE USING A QUANTUM NETWORK MODEL

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Semiconductor heterostructures with quantum wells have been actively studied in recent decades. In this report, we consider the electron and hole in such a structure using a quantum network model [1]. It provides a clear interpretation of the problem and allows one to calculate both bound and resonant states in terms of poles of the extended scattering matrix [2, p. 155]. We use this model to study the energies of the charge carriers in InGaAs and AlGaAs-based heterostructures with quantum wells. The obtained results for the bound electron-hole states (excitons) are consistent with previous numerical calculations [3]. A dependence of the energies of the resonant states on a quantum well width is analyzed. We also show that our model can be used to study the quantum entanglement of an electron and a hole in semiconductor quantum wells.

The work is supproted by RFBR, grants No. 19-02-00576 and No. 20-32-70131.

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ENERGY SPECTRUM OF EXCITONS IN SEMICONDUCTOR QUANTUM WELLS

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Energies of the electron-hole bound states (excitons) and quasibound ones in GaAsbased quantum wells (QWs) of various widths are calculated [1]. This is achieved by studying the three-dimensional SchrËodinger equation for the exciton in a QW and, in particular, by determining the lower energy boundary of the continuous spectrum of the corresponding differential operator. The eigenvalue problem for the SchrËodinger equation is solved numerically by the finite-difference method [2]. The calculated quantum states of electron-hole pairs are classified based on the types of their dominant in-plane and quantum-confinement one-dimensional functions of the wave function factorized form. A dependence of energy levels on a QW width as a parameter is thoroughly studied for widths up to 100 nm. The accurate radiative decay rates for calculated *s*-like exciton states are also obtained using the exciton-light coupling theory of E.L. Ivchenko [3]. The nonradiative linewidths of the quasibound states are estimated [4]. Calculated energy spectra are confronted with the experimental reflectance spectra measured for high-quality InGaAs/GaAs heterostructures with QWs. The ground and, at least, a few excited states of the heavy-hole exciton in QW are identified in the experimental spectra.

The work is supproted by RFBR, grants No. 19-02-00576 and No. 20-32-70131.

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DENSITY OF ELECTRONIC STATES OF DISORDERED TWISTED GRAPHENE

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The analytical expression for the density of electronic states (DOS) of twisted bilayer graphene (tBLG) was obtained using theoretical calculations by the methods of quantum field theory (method of temperature Green's functions, quantum mechanical equations of motion). It includes the dependence on the concentration and configuration of defective complexes, the distance and angle of rotation between the layers, the temperature, and the magnitude of the external field (V). The calculated DOS for tBLG with defective complexes located in the 1st coordination sphere is shown in Figure 1. It is shown that, depending on the magnitude of V, metallization or dielectricization of TBLG can be observed. Our results are in good qualitative agreement with experimental data [1].

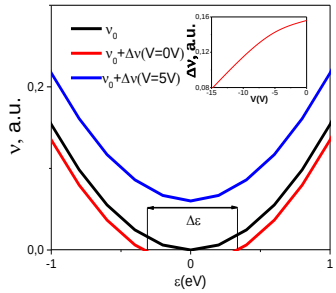

Figure 1. Calculated DOS of tBLG: ideal (black curve), with disorder at V=0V (blue curve), V=5V (red curve). Inset: the dependence of the contribution to the DOS on scattering by impurities and short-range order regions on V.

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TRIPLET SUPERCONDUCTIVITY INDUCED BY MOVING CONDENSATE

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It has been commonly accepted that electromagnetic fields suppress superconductivity by inducing the ordered motion of Cooper pairs. We demonstrate a mechanism which instead provides generation of superconducting correlations by moving the superconducting condensate. This effect arises in superconductor/ferromagnet heterostructures in the presence of Rashba spin-orbital coupling. We predict the odd-frequency spin-triplet superconducting correlations called the Berezinskii order to be switched on in ferromagnets at large distances from the superconductor/ferromagnet interface by application of a static magnetic field or irradiation inducing condensate motion in the direction perpendicular to structural anisotropy axis, what opens great perspectives for low-dissipative spintronics[1,2]. The effect is shown to result in the unusual behaviour of Josephson effect and photo-induced Josephson current.

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DIAMOND-LIKE 2D FILMS BASED ON A FEW LAYERED GRAPHENES: ATOMIC AND ELECTRONIC STRUCTURES, PREPARATION METHODS AND APPLICATIONS PERSPECTIVES

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Recently, graphene heterostructures have generated renovated interest for new findings on the induced chemical transformation of a few-layer thick epitaxial graphene into a new carbon all sp^3 2D films [1-3] earlier named diamanes [4] as fully hydrogenated (or fluorinated) bilayer graphene or a few layered graphene.

In this work we provide a review of theoretical [4-7] and direct experimental works about these materials. We consider also new modeled structures such as Moire diamanes, based on bigraphenes whith twistedangles near 30o [8,9]. Using state-of-the-art computational techniques electronic, mechanical as well as energy stability were estimated and comparison with periodic approximant and AB-stacked diamanes was performed. New structure of quasicrystalline diamane demonstrates wide band gap of 3.4 – 4.5 eV and unique mechanical properties which makes it stiffer and more brittle than AB-stacked diamane. We proposed also the first two-dimensional carbon quasicrystal composed entirely of sp^3 hybridized atoms – diamane quasicrystal, based on incommensurate twisted 30° bigraphene [10]. They could be fabricated through complete fluorination or hydrogenation of the bilayer graphene, similarly to synthesis of AB-stacked diamane by high pressure treatment.

It was shown that their metal-doped analogues, which cover the spectrum of their conductive properties from semiconducting to metallic (with the possibility of conversion to a superconductor) [11]. These dielectric films are interesting due to their unique mechanical and optoelectronic, heat-transport and conductive (upon doping) properties [12-14]. It was proposed that such diamanes could be realized on the base of bilayer hexagonal boron nitride, silicene and other fabricated by functionalization of the bigraphenes by different adsorbents including chlorine, bromine [15].

We discuss the prospect of using such diamond-like structures of nanometer thickness in mechanical, optoelectronic and electronic nanodevices.

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PROXIMITY INDUCED PHENOMENA IN NANOSTRUCTURES COMPRISING GRAPHENE-OXIDE INTERFACES

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The ability of graphene to be easily interfaced with different classes of magnetic materials (ferromagnets, magnetic insulators etc.) makes it extremely attractive for spintronics [1]. Numerous efforts have been devoted to inducing magnetism in graphene by different approaches including by means of magnetic insulator proximity effect [2]. Here we present recent developments on proximity induced magnetism in graphene including novel class of associated with it transport phenomena [3,4,5].

Using a combination of first-principles and tight-binding approaches, the influence of various magnetic insulators on electronic structure of graphene was systematically investigated. Five different insulators were considered: two ferromagnetic europium chalcogenides (EuO, EuS), two ferrimagnetic insulators (yttrium iron garnet (YIG), cobalt ferrite (CFO)) as well as bismuth ferrite (BFO). Large exchange-splitting values in graphene varying from tens to hundreds of meV depending on substrate are found [3,5]. These results were used then to for introduction of several proximity induced transport phenomena called proximity electro- (PER), magneto- (PMR), and multiferroic (PMER) resistance effects [4,5].

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HYDROGEN AND HELIUM INCORPORATED INTO VACANCY CLUSTERS IN GRAPHENE ON COPPER, IRON, TUNGSTEN SUBSTRATE STUDIED BY POSITRON ANNIHILATION

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Here we study defects created by irradiation with protons and α particles in graphene on different substrates. With the help of the Density Functional Theory and its Two-Component extension [1] the positron lifetime and the momentum distribution of the electrons in different combinations of volume defects was calculated. These results of the positron annihilation spectroscopy allow one to analyze the effect of structural defects like vacancies and vacancy clusters in the chosen material. For Cu substrate the calculations for a positron lifetime in perfect lattice give 131.3 ps, for carbon atom mono vacancy: τ =133.2 ps, for carbon divacancy: 138.1 ps. Also of great interest is the value of the positron lifetime with a copper atom vacation presented. For two carbon vacancies and one vacancy of copper we have τ =198.1 ps. For iron and tungsten substrates we have similar increase of the lifetime. These results show the correlation of the positron lifetime and momentum distribution of electrons with the electron density at the defects [2].

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SOME MODELS OF LASER BEAM SELF-CHANNELING IN RED BLOOD CELL SUSPENSIONS

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The problems of laser pulse deep penetration into biological tissues and suspensions are challenges because these media are turbid and laser radiation is subject to multiple scattering [1, 2]. It acts on a microparticles with a gradient force directed along the gradient of the field intensity and moving them into the high intensity area and concentrating along the optical axis. A change in the density of nanoparticles leads to a nonlinear modification of the effective refractive index of the medium, and, as a consequence, an effective waveguide is formed. Dynamic equilibrium is achieved through competition between optical pressure gradients and particle diffusion due to Brownian motion. Besides, the viscosity of liquid affects the particle movement and its mobility in the gradient force field. Another optical force responsible for laser radiation self-guiding in suspension is the scattering force (especially forward). Its impact on laser beam propagation substantially depends on particle size and shape. In this work we study the motion of an ensemble of microparticles in the field of a focused Gaussian laser beam under the action of a gradient force of light pressure and a scattering force is studied, taking into account the Brownian motion of bioparticles in a suspension.

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INAS/GAAS QUANTUM DOT/WELL COMPLEX AS TWO-LEVEL SYSTEM

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The single-electron tunneling properties of one dimensional (1D), 2D and 3D structures as well as double quantum wells (DQWs), double quantum dots (DQDs), and quantum rings (DQR) have been studied in with relation to the electron localization and tunneling between the objects [1,2]. In presented work, we focused on the resonance tunneling in 3D/1D and 2D/1D nanoscale InAs/GaAs dot/well complex having mixed dimensionality. Also, these complexes have the mixed spectral structure: discrete spectrum for QD (in 3D and 2D) and continuous spectrum for QW when this QW is considering in three- or two-dimensional space. Our modeling is performed by using the bandgap model based on effective potential [3]. The main effect of the optical PL experiments [4] was simulated in [5]. We describe the dynamics of localized/delocalized states of electron confinement spectrum related to geometry variations in the terms of two-level quantum systems. The wave function of an electron may be localized in one of the QDs or be delocalized when it is spread over the whole system. The mechanism of two-level quantum system creations will be presented by numerical modeling for the spectral distributions of localized/delocalized states in DQD and in QD/QW complex. A comparison of both results shows an obvious correlation. The tunneling states appear in QD/QW complex with the same energies as in DQD system. Thus, the tunneling in the QD/QW complex has the same discrete character as in the DQD. The perspective for using the dot/well arrays for modeling quantum qubits is discussed.

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ON INSTABILITY OF CHARGE QUBIT BASED ON DOUBLE QUANTUM DOT

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We present numerical model for qubits made of InAs/GaAs double quantum dot (DQD). The electron/hole localization and spectral distributions of localized/delocalized states are studied. The InAs/GaAs heterostructures are described, using the effective potential model proposed given in Ref. [1]. It was shown in [2], that the electron tunneling and spectral distributions of localized/delocalized states in this binary system are extremely sensitive to the shape symmetry violation. The coupling parameter Θ, defines the delocalized $(\Theta \approx \pi/2)$ and localized $(\Theta \sim 0)$ states of electrons. The parameter appears to depend on the energy difference Δ in the spectrum of the left and right QDs; τηε difference can be caused by a shape symmetry violation. The sensitivity of the parameter Θ to small variations of Δ is estimated to be:

$$\delta(\Theta/2) = \frac{1}{\Delta^2}\delta(\Delta). \quad (1)$$

Based on this approach and related findings, we propose a new interpretation for the quantum computing general problem of instability of qubits. Since the qubit is a two-level system, exactly like DQD, its extreme sensitivity is described by Eq. (1) as $\Delta \to 0$; this would include any fluctuation violations, leading to loss of "coherency" of the qubit or "tunneling state" in the qubit. One can propose an ideal bi-stable device (with the probability of 1/2 for each state) when $\Delta \to 0$. However, the model means, the more sensitive the qubit is, the more unstable the system. Results of the modeling will be given and discussed.

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INTERPRETATION OF THE LOW-THRESHOLD FIELD ELECTRON EMISSION FROM GRAPHENE-LIKE STRUCTURES

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It has been experimentally shown that an electric field can create ultrathin graphene-like layers in layered carbon structures. This seems to result from of an increase in the distance between the graphite layers in the electric field. In this case the quantum-dimensional regions arise been bounded by chains of point and extended defects with negative correlation energy. This defects are either in a positive or negative charged state even at room temperature [1].

In the case of a homogeneous distribution of centers with negative correlation energy, the vertical and horizontal networks are formed, similar to the Josephson networks, which restrict the transport of residual single carriers. The formation of such networks is accompanied by the suppression of the electron-electron interaction, which makes it possible to register macroscopic quantum phenomena up to room temperature. It is assumed that networks consisting of centers with negative correlation energy are promising for the formation of stable qubits.

When the electron-electron interaction is suppressed, the current to the barrier and through it is transferred ballistically. Moreover, the localization of single carriers inside networks with the negative correlation energy can provide currents of up to hundreds of milliamps. Thus, with a large number of parallel networks under conditions of ballistic carrier transport, even with a low carrier concentration, the possibility of obtaining large currents observed experimentally is substantiated [2].

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ELECTRONICS IN 2D MATERIALS WITHOUT BRIDGING COMPONENTS

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We propose a new paradigm of electronic devices based on electrodes of two-dimensional materials separated by a gap, i.e. without any functional element bridging them. In particular, we analyse the electrical response of narrow graphene nanogaps in search for transport signatures stemming from spin-polarized edge states [1]. We find that the electrical transport across graphene nanogaps having perfectly defined zigzag edges does not carry any spin-related signature. We also analyse the magnetic and electrical properties of nanogaps whose electrodes have wedges that possibly occur in the currently fabricated nanogaps. These wedges can host spin polarized wedge low-energy states due to the bipartite nature of the graphene lattice and give rise to interesting transport phenomena. We use a tight-binding model [2] to show that, depending on the structure of the edges at the nanogap, which changes the coupling between the surface and bulk states, several electronic functionalities can be achieved: ohmic behaviour, rectification, negative differential resistance, spinfiltering and magnetoresistance.

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EXCITONS IN TWO-DIMENSIONAL SEMICONDUCTORS

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Two-dimensional (2D) crystals attract great attention nowadays owing to their spectacular electronic and optical properties. The family of 2D transition-metal dichalcogenides, MX2, where M is the transition metal (typically Mo or W) and X is the chalcogen (S, Se or Te) host tightly bound excitons, Coulomb-correlated electron-hole pairs, with the binding energies on the order of several 100's meV and radiative lifetimes in the picosecond range. The excitons govern optical response of 2D MX2 crystals [1].

In my talk the key features of the excitons are presented and novel effects related to the 2D character of the transition-metal dichalcogenides and multivalley band structure are discussed. We address the specifics of the exciton Rydberg series accounting for the dielectric screening of the Coulomb potential and Dirac-like character of the charge carriers energy spectrum, and analyse the differences with the 2D hydrogenic model. We further address excitonic fine structure caused by the longrange exchange interaction between the electron and the hole and analyze the impact of the dielectric environment of the 2D crystal on exciton valley decoherence [2]. Finally, we study quantum transport effects on excitons in 2D semiconductors including the weak localization effect [3] and valley Hall effect [4].

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KWANT: A NUMERICAL TOOLBOX FOR QUANTUM NANOELECTRONICS

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The Kwant code for numerical quantum transport was released in 2013. Kwant is an open-source Python package aiming to be an user-friendly, universal, and high-performance toolbox for the simulation of arbitrary physical systems that can be described by a tight-binding model. The software was received well by the physics community: it has been used in research that has led to hundreds of peer-reviewed publications throughout the world.

The Kwant toolbox has been in continuous development since its inception. On one hand, it has become easier and more expressive to use for problems to which already the original version could be applied. On the other hand it is now possible to tackle a wider range of problems. Examples of improvements include: addition of the concept of models, comprising their creation (automatic discretization of continuum Hamiltonans), use, and analysis of their symmetries; operators and facilities to visualize their expectation values; new solvers like the kernel polynomial method. A special mention is reserved for tkwant, a separate but related package that extends Kwant to time-dependent quantum transport.

In my talk I will briefly introduce Kwant, present the most important improvements of recent years, and give a glimpse of ongoing and possible future developments.

RGO/UHMWPE COMPOSITE AEROGELS WITH TUNABLE ADVANCED PROPERTIES

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In this study, we propose a previously unknown template-directed polymerization strategy for producing graphene/polymer composite aerogels with elevated mechanical properties, the preservation of the nanoscale pore structure, the extraordinary crystallite structure and tunable electrical properties. We develop the novel approach of ethylene polymerization on the surface of reduced graphene oxide (rGO) sheets pre-structured as an aerogel template with the formation of ultra-high molecular weight polyethylene (UHMWPE). It is shown that the in-situ polymerization of ethylene on the surface of rGO sheets uniformly throughout the volume of aerogel. The polymer content variation allows to tune the electro conductive properties of the aerogel in in a wide range. The structural features of UHMWPE grown on rGO sheets were studied using XRD analysis. Such an approach will make it possible to create composite materials with ultra-high molecular weight polymers with highly developed nanostructural morphology and advanced properties controlled by the thickness of the polymer layer on the surface of rGO template particles. These composites can be used can be used in reconstructive surgery to replace unloaded bone parts, electroactive materials for supercapacitors and li-ion batteries, as well as heat insulating elements operating at very low temperatures in the space and aviation industries or in the far north conditions.

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TWISTED LAYERS, NARROW BANDS, AND NEW PHASES IN TWO DIMENSIONAL MATERIALS

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The discovery of superconductivity and other electronic phases in twisted bilayer graphene has led to an intensive study of similar properties in other arrangements of two dimensional materials. These systems are based on structures on scales much larger than typical inter-atomic distances (moiré structures), and they provide a fascinating connection between microscopic and mesoscopic physics. The origin of the unusual properties of twisted bilayer graphene, still not fully understood, is reviewed, with emphasis on new effects and interactions not encountered before in condensed matter physics. The similarities and differences with other materials with complex electronic phases will be emphasized.

FINE STRUCTURE OF THREE-PARTICLE STATES IN DOPED MONOLAYERS OF TRANSITION METAL DICHALCOGENIDES

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Monolayers of transition metal dichalcogenides (TMDCs) is a novel class of semiconductor materials with remarkable properties due to the interplay of valley and spin degrees of freedom. Optical spectra of those direct band-gap materials are influenced by a variety of complex multi-particle tightly bound excitonic states. We calculate the optical spectra of TMDC monolayers in presence of doping by diagonalization of a three-particle Hamiltonian within the Tamm-Dancoff approximation, where the doping effects are modeled by discretization of the Brillouin zone [1,2]. Our study reveals a fine structure of the lowest three-particle states and doping dependent spectral features in quantitative agreement with the available experimental data. At finite doping we observe brightening of the indirect dark exciton, whose oscillator strength becomes comparable to the trion and direct exciton states at moderately low doping levels, offering a novel interpretation of the observed complex spectra of TMDC monolayers. In our study of influence of the dielectric screening on the optical spectra of MoS2 monolayer we observe a coupling of dark and trion states which manifests itself as an anticrossing of spectral peaks and occurs within a range of parameters accessible experimentally.

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RESONANT "SUPERCOLLISIONS" AND HEAT TRANSFER IN GRAPHENE

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Graphene is a very good conductor and promising material with unusual properties. Modern technology allows to produce uniquely pure graphene samples that contain only a few impurities. Recent results on ultra-precise experimental thermal measurements [1] demonstrate that it is possible to probe local heating due to the remaining impurities. In the present work, we theoretically describe this phenomenon. Specifically, we study the effect of strong rare impurities on heat transfer in a coupled electron-phonon system in disordered graphene. A detailed analysis of the electron-phonon heat exchange assisted by such an impurity through the “resonant supercollisions”, i.e. combined collisions in which impurities and phonons are simultaneously involved, is presented. We further explore the local modification of heat transfer in a weakly disordered graphene due to a resonant scatterer and determine spatial profiles of the phonon and electron temperature around the scatterer under electrical driving. Our results are consistent with experimental findings of Ref. [1]. This work was supported by the Russian Foundation for Basic Research (grant No. 20-52-12019) –Deutsche Forschungsgemeinschaft (grant No. SCHM 1031/12-1) and the BAZIS Foundation for the Development of Theoretical Physics and Mathematics.

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FLUORINATED CARBON FULLERENES: STRUCTURES, OPTICAL PROPERTIES AND APPLICATION FOR DRUGS DELIVERY

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Fluorinated nano-materials containing OH-groups are used widely for drug delivery due to their high drug-loading capacity and intense near-infrared performance [1], but the structure of functionalyzed fullerenes is still controversy. In the presented study, DFT was used to find the optimal structures of functionalyzed fullerenes C_{20} and C_{60} with different concentrations of fluorine. As there are many ways to place fluorine atoms on the fullerene surface, genetic algorithm was used to find low-energy isomers. Two ways of optimizing resulted in different results were considered. The first way provides simultaneous optimizing of all fluorine atoms positions, whereas the second way implies adding of fluorine atoms one by one. Fullerenes with an even number of fluorine atoms were found to be more stable than the ones with the odd number. $C_{20}F_2$ and $C_{60}F_{48}$ configurations were proved to be the most thermodynamically stable. It was verified that there is no energy barrier in the reaction of single fluorine addition to partly fluorinated fullerenes. The instability of highly functionalized fullerenes [2] was explained. As all the carbon atoms in the pristine fullerene molecule are sp^2-hybridised, they make an almost flat surface. After partial fluorination, atoms that are bonded with a fluorine possess sp^3-hybridisation, which makes them tetrahedron shaped, almost like a methane molecule. Highly functionalized fullerenes deform the structures of fullerenes, making them unstable. This is why fully functionalized fullerenes are unfeasible. The presented study was performed with the financial support of the Russian Science Foundation (Grant No. 20-73-00245).

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ELECTRONIC STRUCTURE AND PROPERTIES OF BLACK PHOSPHORUS

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I will review some theoretical issues related to a recently discovered two-dimensional material, few-layer black phosphorus (for the case of single layer, also known as phosphorene). This is a direct-gap semiconductor with a gap in Γ point changing from roughly 2 eV in single layer to 0.3 eV in the bulk, with anisotropic and essentially non-parabolic energy spectrum. I will present tight-binding parametrization of electron energy spectrum and its application to large-scale simulations of optical and plasmonic properties. Strong anisotropy of electron spectrum can lead to appearance of hyperbolic plasmons, under strain or under laser pumping. At strong interlayer electric field (or potassium doping) electronic phase transition happens to semimetallic phase with anisotropic Dirac cones. I will discuss consequences of this transition for plasmon spectra and quantum Hall effect. I will also consider single- and two-phonon scattering processes and intrinsic limits on charge carrier mobility in single-layer black phosphorus which turn out to be much more restrictive than for graphene, as well as the "flexuronic" density-of-states tail due to the two-phonon processes. Electronic structure and properties of the defects on black phosphorus surface (such as vacancies, alkali-metal and transition-metal adatoms) will be also considered. The most interesting results are probably related to a switchable bistability of the electronic state of Co adatom at the surface of black phosphorus which opens a way to its use for the single-atom memory and realization of atomic Boltzmann machine. Also, a strong anisotropy of electron screening result in a formation of unusual chain-like structures of metal adatoms at the surface of black phosphorus.

CONDUCTIVITY ANISOTROPY ABOVE CRITICAL TEMPERATURE IN LOW DIMENSIONAL NON-HOMOGENEOUS SUPERCONDUCTORS

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In the majority of layered and strongly anisotropic superconductors the effects of superconductivity first appear along the least conducting axes [1-4] at T>Tc and then along other directions. The standard theory of superconducting fluctuation fails to elucidate this anisotropic onset of superconductivity. We explained it by assuming a heterogeneous superconductivity onset at T>Tc in the form of isolated islands inside the original phase [3-5]. As temperature decreases, the volume fraction of superconducting phase grows by increasing the number and size of superconducting islands. Finally at T=Tc the phase coherence of these islands establishes in the whole sample, making the system completely superconducting. For this kind of anisotropic heterogeneous systems with ellipsoid inclusions of arbitrary dimension we derived analytical formulas for resistivity by applying the Maxwell-Garnett and self-consistent approximations [3-6]. The results agree with experimental data on the temperature dependence of resistivity anisotropy above Tc in several layered conductors: FeSe, $YBa_2Cu_4O_8$, β-(BEDT-TTF)$_2$ I_3, and allow to estimate the size of superconducting islands, e.g. d ~ 1μm in β-(BEDT-TTF)$_2I_3$.

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EXCITON STATE FEATURES IN NANOCOMPOSITES WITH SEMICONDUCTOR QUANTUM DOTS AND METHODS OF THEIR CHARACTERIZATION

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The adjustable optical properties of semiconductor quantum dots (QD) open the doors for many applications. In particular, engineering their luminescence lifetime, making it longer is important from point of view of bioimaging, optoelectronics and so on. The remarkable feature of QDs is the presence of a permanent dipole moment (PDM). High spontaneous macroscopic polarization is revealed in InGaN/GaN QDs. The PDM and polarizability of both the neutral exciton and positive trion are found in a single InAs/GaAs self-assembled QD. The PDM magnitude of the CdSe QD is shown to exceed hundreds Debye. In [1] the authors have revealed in the experiment the very large PDM of excitons of InAs QDs in GaAs, corresponding to electron-hole separations up to 2.5 nm. ZnO QD has the advantage of having the PDM 11.4 times and 5,21 times larger than those of CdSe and CdS. Moreover, the exciton states in nanocomposites with semiconductor QDs can be controlled via corresponding choice of both matrix and QD susceptibilities. In this case exciton states are formed by spatially separated charges that provides transition dipole moment enhancement of one to two order of magnitude. Macroscopic and microscopic features of nanocomposite are actively studied, but the origin of observed effects is still under discussion. In our work we discuss the peculiarities of photon echo (PE) methods of nanocomposite characterization accounting for angular distribution function of the PDM orientations, and spatial dispersion of transition dipole moments. We have shown for the first time that PDM is responsible for signals generated at multiple frequencies which drastically depend on its angular distribution and dipole moment distribution function.

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SPIN-RELAXATION AND YU-SHIBA-RUSINOV STATES IN SUPERCONDUCTING GRAPHENE

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2D materials in the proximity of super-/semi-conductor are expected to host a wide spectrum of different phenomena. In my talk I will focus on spin-relaxation in graphene proximitized by an s-wave superconductor. In normal graphene the electron spin lifetime is surprisingly short, ranging from 0.1 to 10 ns, depending on the sample quality. Because of small intrinsic spin-orbit coupling the underlying mechanism for the fast spin relaxation had been an outstanding puzzle. Adatom impurities can affect spin-relaxation via locally enhanced spin-orbit coupling (SOC) [1], or local magnetic moments [2]. I will argue that quasiparticle spin-relaxation in superconducting graphene can disentangle those two contributions due to different doping and temperature dependence [3]. Moreover, I will analyze the stability of the induced local magnetic moments, and the emergence of Yu-Shiba-Rusinov (YSR) bound states in such proximity induced superconducting systems.

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Radiation-induced defects and hopping transport in two-dimensional MoS_2

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The novel two-dimensional material MoS2, as well as other transition metal dichalcogenides, were found to have edge states, similar to those of graphene [1]. We have investigated the electronic properties of monolayer molybdenum disulphide in the presence of randomly distributed nanopores of various diameter and shape (see Fig.1). We use the tight-binding Hamiltonian [2,3] that takes into account dz2,dxy,dx2-y2 Mo orbitals, as well as the spin-orbit interaction. Using the Green-Kubo real-space formalism, we have calculated the density of states of the 2D MoS2 sample with 0.5 million atoms with randomly distributed nanopores and single vacancies. We found electron states within the band gap that can be attributed to the edge states of the nanopores. Using the density of states, we estimate the possible resistance of the sample with defects in the variable-range hopping transport mode, which is actual for the MoS2 at low temperatures [4].

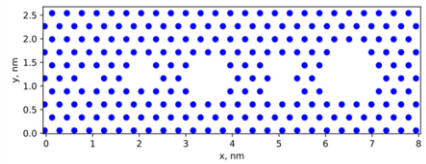

Fig.1: The types of nanopores considered: vacancies(left), and 0.32 nm to 0.96 nm nanopores(left to right). Only Mo atoms are shown.

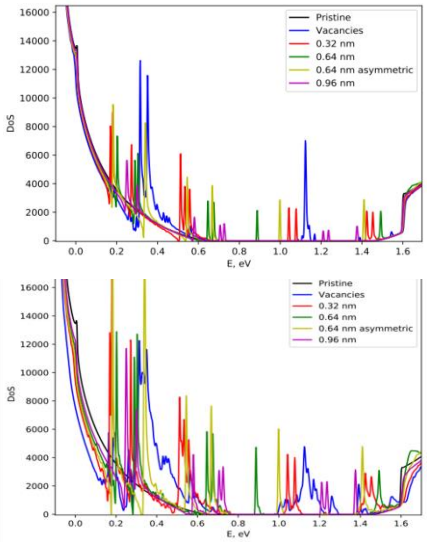

Fig.2: The density of states (avg. units) vs energy (eV), for 1% (top) and 4% (bottom) atoms removed.

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THE MECHANICAL PROPERTIES OF THE COMPOSITE THE PILLARED GRAPHENE: THE INFLUENCE OF THE GEOMETRIC CONFIGURATION

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Mechanical properties are one of the most important properties that a material should possess when used in nanodevices as an elemental base. A more detailed study of the mechanical properties of pillared graphene is necessary to expand the fields of application of this composite despite an active study of its mechanical properties.

The aim of this work is a theoretical study of Young's modulus when pillared graphene depending on the geometric parameters of the composite: length, diameter and chirality of the carbon nanotube (CNT), size of the graphene sheet. The deformation of the composite was carried out by 3%.

It was established during the investigation of the Young's modulus of the extended pillared graphene containing armchair nanotubes that [1]:

- Young's modulus of the composite increases when it is stretched along the normal to the graphene sheet and with an increase in the length of the CNT;
- Young's modulus of the composite decreases when it is stretched along the directions of the graphene sheet and with an increase in the length of the CNT of the composite.

It was revealed that the tensile strength in the direction of the graphene sheet (Young's modulus of 630 GPa) exceeds the tensile strength in the direction normal to the graphene sheet (Young's modulus of 150 GPa).

It was established during the study of the Young's modulus of finite-dimensional columnar graphene containing zigzag nanotubes that:

- Young's modulus in all composites increases with increasing CNT lengths;
- Young's modulus increases with increasing size of the graphene sheet in the composite.

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SUPERFERROMAGNETIC RESPONSE IN UNIFORM AND SENSOR MODES

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Many laboratory tasks cab be included in Lab on a Chip systems based on superferromagnets (SFMs), e.g., magnetic nano-crystal self-assemblies and/or arrays. Such soft magnetic systems provide an opportunity to develop new materials with characteristics far beyond traditional solids. SFM parameters for various applications can be analyzed by employing the randomly jumping interacting moments (RJIM) model, see [1] and refs. therein,. 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 demonstrate an importance of finite size effect in implications of these methods. We briefly consider SFM figures of merits for a sensor mode of a reactivity associated with spatially local external fields, i.e., a detection of magnetic particles, change of a temperature etc. Favorable designs of superferromagnetic systems for sensor implications are revealed.

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DEFECTS AND NEW PHASES IN TWO-DIMENSIONAL MATERIALS

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Following isolation of graphene, many other 2D systems, e.g., single sheets of transition metal dichalcogenides (TMDs) have been manufactured. All these materials contain defects and impurities, which may govern their electronic and optical properties. Moreover, defects can intentionally be introduced using beams of energetic particles – ions and electrons [1,2]. Formation of defects may also give rise to phase transformations in these materials. All of these calls upon the studies on defects and mechanisms of their formation. In my talk, I will present the results of our recent theoretical studies [3-5] of point and line defects (such as mirror twin boundaries) in 2D TMDs obtained in close collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D TMDs.

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THE INFLUENCE OF EXTERNAL RADIATION ON THE JOSEPHSON JUNCTION + NANOMAGNET SYSTEM

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We investigate Kapitsa-like pendulum effects in the magnetic moment dynamics of a nanomagnet coupled to a Josephson junction under external periodic drive. Generated by the Josephson junction and external drive magnetic field play the role of the oscillating force of the suspension point in analogy with the Kapitsa pendulum. The high frequency oscillations change the position of stability of magnetic moment. The magnetic field of the quasiparticle current of the Josephson junction determines the frequency dependence of the magnetic moment's stable position. We obtain simple analytical formulas for the stable position of magnetic system both under external periodic drive and without it. The influence of external periodic drive on the voltage value of complete reorientation have been demonstrated.

NEW METHOD FOR VARIABLE-COMPOSITION CLUSTER STRUCTURE PREDICTION. APPLICATION TO SILICON OXIDE NANOCLUSTERS

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We present a new evolutionary method for simultaneous prediction of atomic structure and stability of nanoclusters in a wide area of sizes and compositions. The resulting speedup is 5-50 times compared to current methods, which perform global optimization for each cluster composition independently [1].

We apply our method to fully first-principles global optimization of 315 Si_nO_m clusters with $1 \le n \le 15$ and $0 \le m \le 20$. We explore the stability of Si_nO_m clusters calculating minimal second-order differences of energy over Si and O atoms ($\Delta_{min}(n,m)$). The graph of $\Delta_{min}(n,m)$ and several stable clusters are shown at fig. 1.

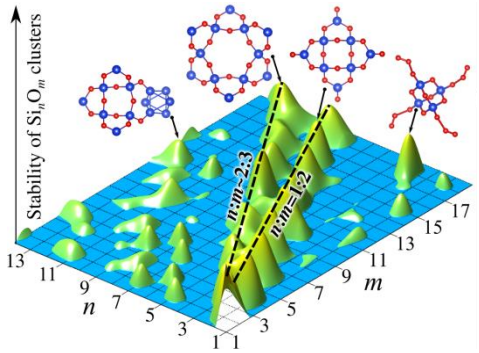

Fig. 1. The graph of $\Delta_{min}(n, m)$ as a function of n and m, showing the stability of Si_nO_m clusters. Regions of instability are marked in blue.

The obtained map of Si-O cluster stability shows the existence of the "ridges" and "islands", corresponding to the most stable clusters. In addition to the expected $(SiO_2)_n$, we found Si_nO_m clusters with $n:m \sim 2:3$, as well as a number of other stable ("magic") clusters (e.g., Si_4O_{18}), which can be important for various applications.

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NEW EFFECTS OF EXCITON SYSTEMS IN NOVEL 2D MATERIALS

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New effects in systems of excitons in novel two-dimensional (2D) materials and structures [1-4] reviewed (see also [5] and refs therein). We propose a method to increase the lifetime of 2D direct excitons by optical cavity engineering and show the possibility to observe their macroscopically coherent state at temperatures much higher than that of indirect exciton condensation [1]. For 2D material or quantum well embedded in photonic layered heterostructures with subwavelength period, we predict the exciton radiative decay to be strongly suppressed.
We propose the method to study dark 2D excitons (e.g. in 2D TMDC) by neighboring bright excitons in the neighboring layer [2]. We demonstrate that the interlayer interaction leads to a mixing between excitations from different layers which leads to the appearance of a second spectral branch in the spectrum of bright condensate. The excitation spectrum of the condensate of dark dipolar excitons then becomes optically accessible by luminescence of the bright condensate. We propose to control of electron-hole superfluidity in double layers of 2D material by an external periodic potential [3]. The second order phase transition between superfluid and electron-hole plasma, controlled by the external periodic potential, is studied ..

We predict the spin Hall effect for polaritons in 2D TMDC embedded in a microcavity [4]. *A* and *B* polaritons is formed due to the coupling of *A* and *B* excitons created in a TMDC monolayer and microcavity photons. Two counter propagating laser beams incident on a TMDC monolayer can split normal and superfluid polariton flows due to the generation the spin-dependent gauge magnetic and electric fields. We show that the polariton flows in the same valley are splitting: the superfluid components of the *A* and *B* polariton flows propagate in opposite directions along the counter propagating beams, while their normal components flows almost perpendicularly to the superfluid flows.

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THEORY OF MAGNETOTRANSPORT IN WEYL TYPE -II JUNCTIONS

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The transport properties of junctions of normal and superconducting Weyl semimetal (breaking Lorentz symmetry), in the presence of magnetization induced by magnetic strips are studied. The sub gap tunnelling conductance is found to be novel and robust in the presence of different orientation and strength of magnetization of the magnetic strips. In the thin barrier limit, the analytical results for the normal-magnetic-superconducting junction are obtained and these results are found to have no analogues to their conventional counterparts and junctions with Dirac electrons in two-dimensions. Possible experimental setups to test our theoretical predictions are discussed.

IDENTIFICATION OF BOND-DEPENDENT EXCHANGE PARAMETERS IN FRUSTRATED RARE-EARTH MAGNETS

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Due to interplay of spin-orbit coupling and crystal electric field, anisotropic exchange interactions are allowed in magnetic rare-earth insulators[1], and its combination with frustration of the triangular lattice leads to exotic long-range ordered ground states with pronounced quantum effects, as well as quantum spin liquid state with long-range entanglement and fractionalized excitations. That is why the identification of exchange parameters of recently synthesized materials is important task, which we illustrate with two examples.

First, we use field-dependent heat capacity measurements in rare-earth triangularlattice antiferromagnet CeCd3As3 at dilution fridge temperatures to trace the fieldevolution of the spin-excitation gaps throughout the antiferromagnetic and paramagnetic regions. The distinct gap evolution places strong constraints on the microscopic pseudo-spin model, which, in return, yields a close quantitative description of the gap behavior[2].

Another rare-earth triangular-lattice magnet YbMgGaO4[3] showed many promising spin liquid features but also possessed a high degree of disorder owing to sitemixing between the non-magnetic cations. To further elucidate the possible role of disorder and to explore the phase diagram in applied field, we use neutron scattering and sensitive magnetometry measurements of YbMgGaO4, as well as the closely related compound,YbZnGaO4.

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FORMATION OF NORMAL SURFACE PLASMON MODES IN SMALL SODIUM NANOPARTICLES

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Formation of surface plasmon modes in sodium nanoclusters containing 20-300 atoms was studied using the GW method. It is shown that in the small Na nanoparticles up to 2 nm in size, the loss function $\mathrm{Im}[\varepsilon^{-1}]$ is dominated by a single peak corresponding to localized surface plasmon resonance (LSPR). For particles of 2 nm and more, a resonance corresponding to surface plasmon polariton (SPP) oscillations begins to form, as well as a resonance corresponding to volume plasmon (VP) excitations. Considering the above, the linear size of a particle in the range of 0.7-3.7 nm can be estimated as the lower limit for metal nanodevices operating with SPP. On the example of spherical nanoparticles consisting of a silicon core coated with sodium atoms, it is shown that the LSPR mode is selectively suppressed while the SPP mode is not. Such composite structures can be considered as an example of nanoplasmonic devices with selectively tuned characteristics.

CONTROLLABLE 0−Π PHASE SHIFTER BASED ON INDUCED TRIPLET SUPERCONDUCTIVITY

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It has been shown in Ref. [1] that the combination of the condensate motion, the exchange field and the Rashba spin-orbit coupling (SOC) induces generation of the spin-triplet superconducting correlations, which can be detected via the unusual behavior of Josephson effect and local density of states in superconductor/ferromagnet structures. In this work we predict that such generation is a more general phenomenon, which takes place not only for intrinsic SOC, like Rashba SOC, but also for extrinsic SOC made by impurities. We propose a controllable 0−π phase shifter based on induced correlations. This shifter is controlled by relative directions of the condensate momentum in superconducting leads.

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SECOND HARMONICS OF MAGNETIC QUANTUM OSCILLATIONS IN LAYERED METALS

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We find expressions for the second harmonics of magentic quantum oscillations of interlayer magnetoconductivity and magnetization in quasi-two-dimensional metals. The expressions obtained are useful, since in some experiments with quasi-twodimensional metals, the second harmonic of magnetic quantum oscillations is also observed. We analyze the effect of magnetic oscillations of the real part of electron self-energy part $\mathrm{Re}\Sigma$ on the shape of the quantum magnetization oscillations and on the magnetoresistance of quasi-two-dimensional conductors. In the limit of strong quantum oscillations, which is possible only in two-dimensional or quasi-twodimensional metals, the real part of electron self-energy function $\mathrm{Re}\Sigma$ also oscillates strongly. Usually it is neglected, taking into account only its imaginary part $\mathrm{Im}\Sigma$, since it is assumed that $\mathrm{Re}\Sigma$ only shifts the chemical potential and does not affect the observed properties. However, $\mathrm{Re}\Sigma$ cannot be neglected if it also oscillates. As our calculations show, $\mathrm{Re}\Sigma$ oscillations affect the observed properties, since they shift the chemical potential relative to the Landau level even on average over the period of quantum oscillations. Oscillations of $\mathrm{Re}\Sigma$ affect the shape of the quantum magnetization oscillations [1], which is used to experimentally determine the regime of quantum oscillations: constant chemical potential or a constant electron density [2]. This question is not only of great practical importance for the analysis of numerous experiments, but also of substantial interest for the development of the theory of magnetic quantum oscillations. T. I. M. acknowledges the RFBR grants 19-02-01000, 21-52-12027.

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COMPUTATIONAL MODELLING OF THE SYNTHESIS OF MOS_2 MONOLAYERS

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The emergence of atomically thin 2D materials of semiconducting (transition metal dichalcogenides, TMDs, e.g. MoS_2, WS_2) layers has opened new avenues for scientific and technological advancement in the area of ultrathin electronic and optoelectronic devices [1]. Chemical vapor deposition (CVD) is known as effective method to synthesize monolayers of TMDs by using solid precursors [2] or metal-organic CVD (MOCVD) [3]. One of the most important open questions of the synthesis of different TMDs monolayers is the reaction mechanism, which can be studied by computational modelling of the synthesis process. While the other research efforts were targeted at the development of the thermodynamic models, here we concentrate on both thermodynamic and kinetic approaches of modelling of synthesis processes of MoS_2 monolayers.

We study CVD with solid precursors (S and MoO_3) and MOCVD with H_2S and $Mo(CO)_6$ precursors. Thermodynamic modeling provides analysis of the influence of chemical composition of the reactants, carrier gas (pure Ar or Ar/H_2 mixture), temperature and pressure of the reaction products. Kinetic approach allows us to estimate the reaction rate and to optimize the gas flow rate, which especially relevant for MOCVD cold-wall reactor. In this way we analyze optimal parameters for the synthesis of MoS_2 by CVD and MOCVD. The reported study was funded by the DAAD, program «Mikhail Lomonosov II», project № 16.13419.2019/13.2.

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HYDRODYNAMIC APPROACH TO ELECTRONIC TRANSPORT

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The last few years have seen an explosion of interest in hydrodynamic effects in interacting electron systems in ultra-pure materials. One such material, graphene, is not only an excellent platform for the experimental realization of the hydrodynamic flow of electrons, but also allows for a controlled derivation of the hydrodynamic equations on the basis of kinetic theory. The resulting hydrodynamic theory of electronic transport in graphene yields quantitative predictions for experimentally relevant quantities, e.g. viscosity, electrical conductivity, etc. In this talk I will review recent theoretical advances in the field, compare the hydrodynamic theory of charge carriers in graphene with relativistic hydrodynamics and recent experiments, and discuss applications of hydrodynamic approach to novel materials beyond graphene.

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STRUCTURAL AND ELECTRIC PROPERTIES OF CVD-GRAPHENE FILMS TRANSFERRED ONTO DIFFERENT SUBSTRATES

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Currently, there is an active development of electronics based on graphene and other 2D materials. One of the important issues for this direction is the study of the mutual influence of layers of different materials on heterostructures properties. The wide-spreaded example is vertical van der Waals heterostructures, in which layers of different materials are stacked on top of each other. However, others variants of the layers stacking are possible. In this work, we have created and studied structures based on CVD graphene films and a number of different substrates (films of partial fluorinated graphene, printed graphene oxide layers, oxidized silicon substrates). For substrates with a relief of more than 10 nm, some parts of the film regions were locally suspended. The aim of the work was to create and study the effect of the substrate material on the structure and electrical properties of the created heterostructures. The created structures are of interest from the point of view of the development of such a new direction in nanoelectronics as streintronics.

We used multigraphene films grown by CVD vapor deposition with a thickness of 1-3 nm. AFM images of the surface of the created structures indicate that the multigraphene films are indeed locally suspended or shrinked. The sheet resistance of the films was ~ 1.3-3 kΩ/sq, the films exhibit p-type doping, the mobility of charge carriers is ~ 70-300 $cm^2/V*s$. The rather high value of the sheet resistance and the low value of the mobility of charge carriers can be associated with the presence of mechanical stresses in the multigraphene films. Data on the temperature dependence of the conductivity of multigraphene films supplement information on the structural properties of the films. Further studies of the created heterostructures are planned to study the process of their nanostructuring by irradiation with high-energy heavy ions.

The work was founded by the Russian Science Foundation grant 19-72-10046.

CHARGE DYNAMICS IN STRONGLY-CORRELATED ELECTRONIC SYSTEMS

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We consider the dynamic charge susceptibility and charge density waves in strongly-correlated electronic systems within the two-dimensional t-J-V model. Using the equation of motion method for the relaxation functions in terms of the Hubbard operators we calculate the static susceptibility and the spectrum of charge fluctuations as functions of doped hole concentrations and temperature. Charge density waves emerges for a sufficiently strong intersite Coulomb interaction.

MOLECULAR DYNAMICS STUDY OF MECHANICAL AND THERMAL PROPERTIES OF FLUORINATED GRAPHENE

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It is well-known that the modification of carbon lattice of graphene can tuned up a number of mechanical and thermal and electronic properties of such materials. In particular, fluorine atoms adding has the prospects application in different fields, such as superhydrophobic materials, organic electronics, sensors, gas separation and storage storage, lubricants, etc. It was reported that fluorination by various synthesis methods produces graphene with different fluorine patterns, what may lead to different properties at the same fluorine percentage. Many theoretical studies confirm this. Unfortunately, in most of them, the above properties were calculated either for random distribution of fluorine or for specific fluorine patterns and concentrations, which does not correspond to the actual fluorine distribution.

For generating structures of fluorinated graphene we use statistical model, which fits more realistic fluorine distribution [1]. Molecular dynamics simulations have been performed to investigate mechanical and thermal properties of fluorinated graphene for a wide range of F-coverage. To determine mechanical properties (Young's modulus, tensile strength, fracture strain) we carry out a set of stretching simulations, with varying applied force. To determine thermal conductivity we use the non-equilibrium molecular dynamics approach. We found that structural ordering impact the mechanical and thermal properties and their anisotropy.

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SPIN-ORBIT TORQUE IN VAN DER WAALS HETEROSTRUCTURES OF MAGNETIC TWO-DIMENSIONAL MATERIALS

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The bilayer heterostructures composed of an ultrathin ferromagnetic metal (FM) and a nonmagnetic material hosting strong spin-orbit coupling (SOC) are a principal resource for spin-orbit torque (SOT) [1] and spin-to-charge conversion [2] effects in next generation spintronics. The key to understand SOT is current-driven nonequilibrium spin density [3], which generates SOT when it is noncolliner to the direction of local magnetization and can arise due to variety of microscopic mechanisms (including spin-orbit proximity effect, spin Hall effect and interfacial scattering mechanisms). The recently discovered two-dimensional (2D) magnetic materials [4] offer new avenue for highly efficient and tunable SOT in van der Waals (vdW) heterostructures composed of few monolayers of atomically thin materials. Using first-principles quantum transport calculations, which combine nonequilibrium Green functions with noncollinear density functional theory, we predict [5] that injecting unpolarized charge current parallel to the interface of bilayer-CrI3/monolayer-TaSe2 vdW heterostructure will induce SOT driven dynamics of magnetization on the first monolayer of CrI3 that is in direct contact with metallic transition metal dichalcogenide (TMD) TaSe2. By combining calculated complex angular dependence of SOT with the Landau-Lifshitz-Gilbert equation for classical dynamics of magnetization, we find that this can reverse the direction of magnetization on the first monolayer to become parallel to that of the second monolayer, thereby converting bilayer CrI3 from antiferromagnet to ferromagnet (AFM-FM) while not requiring any external magnetic field that was crucial in recent experiments [6] inducing AFM-FM transition via electric field or electrostatic doping. We explain the mechanism of such current-driven nonequilibrium phase transition by showing that first monolayer of CrI3 becomes conducting due to doping by evanescent wavefunctions injected by metallic TaSe2, while concurrently acquiring strong SOC via this proximity effect. Another vdW heterostructure exhibiting SOT is doubly proximitized graphene, which is neither magnetic nor hosts SOC in isolated form, but proximity induced magnetic moments will exhibit SOT in Cr2Ge2Te6/graphene/WS2 vdW heterostructure which can be tuned by two orders of magnitude via the gate voltage [7]. I will also illustrate fundamentals of spin-orbit proximity effect using examples of conventional ferromagnets (such as cobalt) in contact with TMDs (such as MoS2, WSe2 and metallic TaSe2) or topological insulators (such as Bi2Se3) [8].

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Biosketch

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SPIN FILTERING BY HELICAL EDGE STATES OF TOPOLOGICAL INSULATOR

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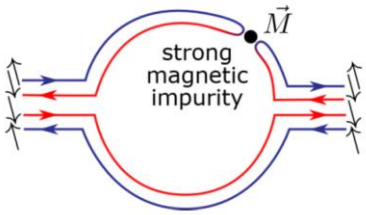

The quantum interferometry is a rapidly growing area of fundamental research with a huge potential for applications in optics, electronics, and spintronics [1].

We study spin filtering properties of interferometer formed by helical edge states of two dimensional topological insulator. We find that unpolarized incoming electron beam entering interferometer through one of the metallic leads acquires a finite polarization after transmission through the setup provided that interferometer contains magnetic impurities. The finite polarization appears even in the fully classical regime and therefore robust to dephasing. There also exists quantum contribution to polarization which survives at relatively large temperature and is tunable by magnetic flux piercing the interferometer. Specifically, the quantum contribution shows sharp identical resonances as a function of magnetic flux with maxima (in the absolute value) at integer and half-integer values of the flux. For interferometer containing a single strong magnetic impurity, which blocks the transmission in one shoulder of interferometer, the spin polarization of transmitted electrons can achieve 100%. The obtained results open wide avenue for applications in the area of quantum networking.

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HYBRID MATERIALS BASED ON LOW-DIMENSIONAL FORMS OF CARBON AND MOS_2 AND THEIR ELECTROCHEMICAL PROPERTIES

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Two-dimensional (2D) materials such as graphene and layered transition metal disulfides (TMD) have a high specific surface and are capable of intercalation with alkali metal ions. The theoretical specific electrochemical capacity of TMD materials is much higher than that of graphite. For low-dimensional 2D structures consisting of one or more monolayers, interaction with alkali metals leads to an even greater effective capacity. In this case, the real surface structure, the presence of vacancy, topological defects, the doping by heteroatoms with electron-donor or electron-acceptor properties into the two-dimensional structure begins to play a significant role Particularly interesting are hybrid materials consisting of layers MoS_2 and graphene. The poor electrical conductivity and high agglomerate risk of pure TMD electrodes can be overcome by interspersing nanocarbon phases within the composite material. The synergetic interactions of TMD and graphene nanohybrid materials for superior electrochemical performance in lithium and sodium ion batteries have been demonstrated in scientific publications in recent years. Using the modern methods of soft X-ray spectroscopy and X-ray photoelectron spectroscopy, NMR spectroscopy and a theoretical quantum chemistry approach, we investigated the process of alkali ions intercalation into composite and hybrid nanomaterials. Based on the results obtained, we determined how the size and morphology of MoS_2 layers and flakes, their imperfection and doping with other metals, as well as the chemical bond with graphene layers will affect the interaction with lithium and sodium atoms and ions and the stability of the electrode material in the processes of electrochemical intercalation/deintercalation.

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CHEMICAL AND STRUCTURAL TRANSFORMATIONS IN SWIFT HEAVY ION-IRRADIATED GRAPHENE OXIDE PREPARED BY DIFFERENT METHODS

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Since the breakthrough paper by Hummers and Offeman [1], published as early as 1958, several modifications of their procedure for graphite oxidation have been developed. Because of this, graphene oxide (GO) obtained by different routes can significantly differ in flake sizes, distributions of oxygen functional groups, and amounts of structural defects.

Here, we investigate the influence of the initial composition of GO on the efficiency of recovering and damaging processes occurring under swift heavy ion (SHI) irradiation.

As starting materials, we used two GO films denoted GO-Z and GO-M. GO-Z was obtained by a procedure employing the same key reagents as the Hummers method. GO-M was prepared without using $NaNO_3$ and under conditions facilitating the exfoliation. The oxidation degree was closely similar for both films (C/O ratio of ~2.5); however, GO-Z was characterized by a higher content of edge groups, smaller average flake size, and possibly more defected carbon lattice.

We found that, in the case of SHI-irradiated GO-M films, the amorphization was suppressed, and the improvement in the electrical conductivity was more significant (5 orders of magnitude for 40 MeV Ar ions). In contrast, the lattice damaging and formation of the nanoholes prevailed for ion-irradiated GO-Z. These results were explained by simulations carried out with a multiscale approach consisting of Monte-Carlo code for excitation of the electron subsystem and reactive molecular dynamics for subsequent lattice relaxation.

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NONLINEAR RESPONSE OF GRAPHENE TO AN ULTRASHORT PULSE OF DIFFERENT POLARIZATION

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The report presents the results of using the nonperturbative kinetic approach to describe the excitation of plasma oscillations in a graphene monolayer under the influence of an electric field of short infrared pulses [1]. The dependence of the process characteristics on the polarization of the pulse and its other parameters is demonstrated.
Using the results of [2], the characteristics of secondary electromagnetic radiation far from the graphene plane are determined. Its spectrum and the nonlinearity coefficient of graphene as an active medium are investigated.
The possibility of generalizing the approach for modeling similar processes in other two-dimensional materials considered.

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EFFECT OF DEFECTS IN GRAPHENE ON THE HETEROGENEOUS ELECTRON TRANSFER KINETICS

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The relevance of this work is since the search for cheap and stable catalysts for various redox systems is a significant challenge today. One of the most promising directions in this field is the use of carbon nanomaterials as electrocatalysts. Various defects in such materials can create local electronic states with energies close to the Fermi level, accelerating electron transport across the interface.

Based on the Marcus and Landau-Zener theories and Density Functional Theory (DFT) calculations, we have obtained the rate constant of heterogeneous electron transfer (HET) with a 3D spatial resolution over the graphene surfaces containing different types of linear [1] and point defects [2, 3]. A fast method for HET estimation based on Tersoff-Hamann approximation was proposed [3].

It was shown that defects could lead to catalysis of the HET strongly depending on the standard potentials of particular redox pair. The most significant effect was found for single vacancies, their presence enhances the electron transfer by order of magnitude at the standard potential from -1V to 0V vs. standard hydrogen electrode (SHE).

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MOLECULAR DYNAMICS STUDY OF SMALL MOLECULES AND IONS DIFFUSION IN A VICINITY OF GRAPHENE OXIDE MATERIALS

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Graphene oxide (GO) is one of the most studied and easiest to obtain two-dimensional nanomaterial. It has potential in catalysis, filtration, electrical equipment (fuel cells, capacitors, accumulators, etc.). In this research, we study the diffusion of water and small molecules and ions through GO using the ReaxFF molecular modeling method. The GO structure was obtained by annealing of graphene sheet with randomly disposed hydroxyl and epoxy groups [1]. Obtained structure correspond to GO obtained by the Hammers method (in terms of the C / O ratio, the proportion of hydroxyl, carbonyl and carboxyl groups, and the size of lattice defects).

The main purpose of this research is to study the diffusion of water, small molecules and ions dissolved in water in a vicinity of GO materials. The results obtained were analyzed to compare the isotropic diffusion in solutions and in various selected directions in GO materials and allowed to simulate the response of the GO-based electrode in aqueous solution. We believe that the results obtained will be useful in the development of GO-based electrochemical devices

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CARBOXYLATED GRAPHENES: SYNTHESIS, ELECTRONIC PROPERTIES AND APPLICATION FOR THE GRAPHENE-BASED APTASENSORS MANUFACTURING

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Rapid developments in the manufacturing of graphene-based devices have facilitated advances in the synthesis of chemically modified graphenes (CMGs). The presence of a certain type of organic groups with the desired concentration in CMGs allows to precisely tune the materials' properties, making them perfectly fitting for the graphene performance in a chosen application.

Hereby we present our results on a long-term study concerned on the carboxylated (C-xy) graphene synthesized via photochemical modification of graphene oxide (GO) [1]. Core-level spectroscopies data revealed that depending on the GO oxidation degree the proposed approach allows to controllably vary the carboxyl groups concentration from 3 at.% to 10 at.%. Using electron microscopy, we found out that carboxylation is accompanied by the perforation of the graphene layer, forming holey graphene. Surprisingly, despite these materials' features, the conductivity and absorbance spectrum of the C-xy graphene are almost the same as in the pristine graphene. At the same time, significant changes in the C-xy graphene valence band spectra were uncovered, correlating with the performed theoretical calculations. Owing to the presence of chemically reactive carboxyl groups, covalent grafting of C-xy graphene with aptamers was performed, resulting in the manufacturing of the graphene-based viral electrochemical biosensor.

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PECULIARITIES OF SHAPIRO STEPS ON THE IV-CHARACTERISTIC OF ANNULAR JOSEPHSON JUNCTIONS

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We have investigated the dynamics of the annular system of underdamped Josephson junctions in the presence of external radiation. It is shown that the ability of the system to lock with some external radiation was determined by the number of trapped fluxons [1]. Shapiro steps can be observed in the current-voltage characteristic only in the system with trapped fluxons or in the system with fluxon-antifluxon pairs. If the trapped fluxons circulate simultaneously with fluxon-antifluxon pairs, there are no Shapiro steps regardless of the amplitude or frequency of the applied external radiation.

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NEMATIC SUPERCONDUCTIVITY IN DOPED TOPOLOGICAL INSULATORS: EFFECT OF HEXAGONAL WARPING

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There is a numerous experimental evidence for the nematic superconductivity with the *Eu* pairing in doped topological insulators. Recent experiments give a direct evidence for this in high-quality single crystals of doped Sr*x*Bi2Se3 [1]. It was observed that the upper critical magnetic field *Hc*2 has a twofold rotational symmetry and depends on the sign of the crystal strain: in the stretched samples the maximum of *Hc*2 is achieved when the in-plane field is transverse to the strain axis, while in the compressed samples this maximum is observed when the field is along the strain direction. This result is naturally explained within a framework of the odd-parity nematic superconductivity. However, from the first theoretical alert, the origin of the nematic superconductivity in the doped topological insulators is a mystery. In their seminal work [2], Fu and Berg show that the triplet superconducting order parameter with *A*1*u* representation is always favorable in comparison with the nematic *Eu* order. We study the superconducting properties of the bulk states of a doped topological insulator with taking into account the hexagonal warping of the Fermi surface that was ignored in [2]. We obtain that this effect stabilizes the observed nematic spin-triplet superconducting phase with *Eu* pairing. The nematic order parameter opens a full gap in the spectrum. This gap demonstrates a non-BCS behavior and strongly depends on doping.

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COULOMB-ENGINEERED 2D HETEROJUNCTIONS

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The band structure and the band gap of semicondcuting layered materials are strongly affected by the Coulomb interaction between carriers within the layer. At the same time we can externally modify this interaction by means of dielectric substrates or dielectric coating. This Coulomb-engineering can thus be used to tailor the fundamental electronic properties of of layered materials.

Here we use a combination of the GdW [1] and WFCE [2] approaches to systematically study the environmental-screening effects to monolayers of semiconducting transition metal dichalcogenides on a material-realistic level. We compare static and dynamic screening effects of homogeneous substrates and derive an effective modeling scheme for spatially-varying heterogeneous substrates [3]. The latter allows for the external and non-invasive induction of heterojunctions within the otherwise homogeneous mononalyer. Our calculations show that spatial band gap modulations on the length scale of a few lattice constants are possible and just limited by the heterogeneous substrate. In the case of WS2 we find a band-gap reduction of about 140 meV on a graphite substrate as compared to a hexagonal boron nitride substrate, while the electronic dispersion of WS2 remains unchanged within the experimental precision of 17 meV [4].

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MANY-BODY EFFECTS IN THE TWISTED BILAYER GRAPHENE

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Zero-temperature many-body properties of twisted bilayer graphene with a twist angle equal to the so-called "first magic angle" are investigated. For the system under study the low-energy quasiparticle spectrum consists of four weakly dispersing partially degenerate bands. Accounting for spin degeneracy, one can say that each band accommodates one electron per Moiré cell per spin projection. Weak dispersion of the single-particle bands make them susceptible to the effects of interactions. We introduce several order parameters with spin-density-wave-like structure and study their stability within the framework of the numerical mean-field theory. The calculations are performed for different doping levels. It is found that the interaction partially lifts the band degeneracy. Furthermore, the details of the low-energy spectrum become doping dependent. For example, at or near the undoped state, interactions separate the eight bands into two quartets (one quartet is almost filled; the other is almost empty), while for two electrons per Moiré cell, the quartets are pulled apart, and doublets emerge. When the doping is equal to one or three electrons per cell, the doublets split into singlets. Similar spectral rearrangements are produced by hole doping. As a result, electronic properties (e.g., the density of states at the Fermi energy) demonstrate oscillating dependence on the doping concentration. Our findings allows us to interpret the behavior of the conductance of the twisted bilayer samples observed recently in experiments [1]. Near half-filling, the electronic spectrum loses hexagonal symmetry indicating the appearance of a many-body nematic state.

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CARBONYLATED GRAPHENE AS A NEW GRAPHENE CHEMICAL DERIVATIVE AND ITS APPLICATION IN GAS SENSING

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Progress in the study of graphenes has led to appearance of a new subclass of nanocarbon materials - chemically modified graphenes (CMG). CMGs, decorated with certain types of functional groups, demonstrate new electronic, optical and chemical properties, thus opening up new possibilities for the use of graphene-based materials in electrochemical and sensing applications.

We present our results on the synthesis, analysis of physical properties and application of one of these derivatives - carbonylated (C-ny) graphene. Carbonylated graphene was obtained by a liquid-phase treatment of graphene oxide using sodium silicate under moderate heating. As a result of this process, the material structure became represented by holey graphene layers with a high density of small-sized holes. Functional composition has also changed. Most of the basal and edge-located groups were eliminated. At the same time, the concentration of carbonyl groups increased. Presented synthesis method allows to control the concentration of carbonyl groups, reaching concentrations from 3 up to 9 at.%.

Detailed study of C-ny graphene using various synchrotron techniques and revealed that functionalization led to significant changes in the C-ny graphene's electronic structure. Particularly, only partial restoration of the π-conjugated network is revealed, while new local states appeared in the graphene valence band near the Fermi level related to the molecular orbitals of the covalently attached carbonyls. This results in the changes of the materials work function value and high resistance of the material of several hundreds of MΩ. This value is too high for the application in electronic devices. However, it was found that C-ny graphene can be used as base-material for gas-sensitive chips, which can operate and regenerate at room temperature with a sensitivity up to hudreds ppm. Moreover, chemoresistive biosensors for viral detection can be further formed using C-ny graphene owing to both its electrical properties and chemical reactivity through non-covalent bonding of the presented carbonyls with organic species.

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UNRAVELING THE INTRODUCTION AND CONVERSION OF NITROGEN SPECIES IN THE GRAPHENE OXIDE UPON ITS SYNTHESIS AND THERMAL TREATMENT

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In recent years, the issue of graphene modification has become one of the central topics in the study of nanocarbon materials. Significant efforts have been made to produce graphene derivatives that have been modified by different functional groups or heteroatoms, improving the performance of graphene-based materials in various practical applications

Hereby we for the first time report that the use of nitrate salts in the conventional Hummer's method leads to the introduction of up to 4.9 at.% of nitrogen into graphene oxide (GO) during its synthesis. It has been shown that the dominant type of doped nitrogen is graphitic nitrogen. A dopant mechanism has also been proposed in terms of GO nitration and transformation of nitrate groups, giving a hint of the processes, underlying graphite oxidation into graphene oxide.

It is further shown that the subsequent thermal reduction of GO leads to almost complete transformation of graphite nitrogen into pyridines and pyrrole, which makes the obtained material a promising platform for use in catalysis. The effect of the introduced nitrogen atoms on the electroconductivity value has been complexly studied by means of electrical studies in combination with the carried out plane-wave density functional theory (DFT) calculations. It is found out that N-doping of rGO results in about doubling of the material conductivity with the Mott variable range hopping (VRH) mechanism of conductivity in the material

As a net result, an easy method for obtaining N-doped GO and rGO layers with the desired type of nitrogen was proposed, and new details of GO synthesis using the Hummer's method were revealed. The obtained N-doped rGO films with the enhanced conductivity are of high interest for the formation of biosensor transducers, improving their performance in the designed devices.

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NEW GRAPHENE STORY OF OLD AMORPHOUS CARBON

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Recent purposeful studies [1–5] have completed the gradually nascent change in the view of sp^2 amorphous carbon as a well-known, familiar physicochemical subject, transferring it to the rank of *high-tech* material of modern nanotechnology. We are talking about material known to humankind since the first decomposed bonfire, which left behind black soot and charcoal. Today, this applies to billions (anthracite coal) - millions (shungite carbon) - thousands (anthraxolite and blackcarbon coatings, which are present everywhere and accompany almost all minerals in nature) tons of only discovered natural deposits and hundreds of millions of tons of synthetic black carbon produced industrially. All this black carbon wealth is amorphous carbon, or a monoatomic solid without long-range order, the atoms of which form sp^2 configured valence bonds with each other. Because of studies [1-5], it was finally established that the black carbon richness described above has a unique common basis, namely, nanoscale molecular compositions of hexagonal honeycomb structures of carbon atoms framed by various necklaces formed by oxygen, hydrogen, nitrogen, sulfur, halogen and other atoms. These framed graphene molecules are basic structural elements (BSUs), varying in size and shape, as well as differing in the chemical composition of the necklaces depending on the history or method of origin and/or production of the black carbon described above. The open and today experimentally confirmed many times, graphene nature of this black gold leads to a revolutionary revision of the theory, modeling and interpretation of the experiment related to this class of solids. In the report, I will focus on the main points that led to a paradigm shift:

Experiment: multilevel fractal structure, accompanied by pronounced porosity; BSU graphene structure; the chemical composition of the framing necklaces - the nature of their occurrences and functions.

Theory: amorphization as enforced fragmentation; class of amorphous solids - amorphics with a molecular structure; BSU with variable sizes as a carrier of size-sensitive effects; molecular crystalline dualism with respect to the spectra of electronic and vibrational (phonon) states; molecular and solid-state quasiparticle approximations as research methods (by the example of phonon spectra).

Modeling: nanoscale framed graphene molecules (real BSU) as an object of modeling; the radical nature of BSU; size-kinetic nature of stabilization of BSU molecular radicals; a manifestation of the radical nature of BSU (carbocatalysis, spin tribology, spin geochemistry, and spin medicine).

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DISCOVERY OF THE MOLECULAR-LIKE STRUCTURE OF ATOMS (ON THE EXAMPLE OF A CARBON ATOM)

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Considering elementary particles as wave formations, as pulsating energy bunches of the primary physical vortex field-space (physical vacuum or the so-called ether), we came to the equation describing pulsations of their wave shells, Based on this equation, we have arrived at the discovery of the fundamental frequency of atomic and subatomic levels, which is responsible for the electromagnetic and strong interactions.

Applying further for the description of such particles the standard wave equation, , we found that atoms have a shell-nodal (molecular-like) structure identical with the structure of disposition of the nodes of standing waves in a spherical field-space. We show this on the example of a carbon atom.

Generally, following the wave approach, we came to a whole series of key discoveries. One of them is the anisotropy of the unstrained hexagonal lattice of graphene confirmed experimentally. We consider this issue here in more details.

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PECULIARITIES OF ANOUMALOUS JOSEPHSON EFFECT IN SUPERCONDUCTING NANOSTRUCTURES

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The Josephson junctions with the current-phase relation Is = Ic sin(φ-φ_0), where the phase shift φ_0 is proportional to the magnetic moment perpendicular to the gradient of the asymmetric spin-orbit potential, demonstrate a number of unique features important for superconducting spintronics and modern informational technologies [1, 2, 3, 4]. This feature of the current-phase relation allows one to manipulate the internal magnetic moment using the Josephson current. Here we present our recent results on phase dynamics, IV-characteristics and magnetization precessions of superconductor-ferromagnet-superconductor φ_0 Josephson junction. We show that along with very complex magnetization precessions appear very regular dynamics with a series of specific phase trajectories in different parts of IV-characteristic. Possible applications of the obtained results in superconductive spintronics are discussed.

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KINETICS OF EHΓ EXCITATIONS GENERATED IN GRAPHENE BY TIME-DEPENDENT ELECTRIC FIELDS

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The kinetics of ehγ excitations in graphene generated by time-dependent electric fields is studied. To do this, following the work [1] and using methods of kinetic theory in QED with strong electromagnetic fields [2], we construct a consistent system of kinetic equations (KE), which nonperturbatively describes the generation and evolution of eh subsystem under the influence of an external electric field and takes into account interaction between eh and photon subsystems in the second order of the perturbation theory.

The constructed KE system takes into account all single-photon processes: the stimulated photoproduction and annihilation of eh pairs and carrier redistribution over momenta. The corresponding single-photon channels open in the presence of an external time-dependent electric field, which is consistent with the general theory of the influence of external fields on elementary processes of interaction in multiparticle systems [3,4]. Maxwell's equations for the internal plasma field complement the system of KE.

In the framework of this approach, electromagnetic radiation from graphene, which accompanies ehγ excitation, is considered. The latter results are compared with the radiation of plasma oscillations in graphene studied earlier in [5].

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ON THE EDGE OF BILAYERED GRAPHENE: UNEXPECTED ATOMIC GEOMETRY AND SPECIFIC ELECTRONIC PROPERTIES

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Intensive investigation of graphene yields a lot of exciting properties of this material which can be used in the various fields of science and technology. The idea of open a band gap in graphene monolayer by formation of periodically arranged holes (antidots) got a second wind in the bilayered graphene (BG) case. Indeed, whereas open edges of holes in graphene single layer are reactive and requires passivation, edges of bigraphene holes are naturally self-passivated [1]. BG with holes can couple together highest conducting properties of carbon nanotubes and controllable electronic properties of graphene ribbons which makes possible the fabrication of ideal two-dimensional quantized conductor for future nanoelectronics. However, the establishing of the method of formation of the holes in bigraphene in controllable manner is attractive but still not realized task.

Here we presented data which may be considered as a first step towards to controllable fabrication of perforated BG with closed edges. We show that monolayered graphene grain boundary theory can well describe the energy of BG closed edges. It allowed us to establish the general behavior of closed edges energy for twisted BG for any Moiré angle and any edge orientation. This data allowed to predict what edges will be in the holes located at different points in BG [2]. It was shown that holes edges change the properties of the material by variation of flexoelectric dipole moment induced by graphene bending at the edge [3].

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EMERGING 2D FERROMAGNETISM AND CHARGE TRANSPORT IN SILICENE, GERMANENE AND GRAPHENE COMPOUNDS

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Recent years have witnessed remarkable progress in engineering two-dimensional (2D) magnetism via defects, edges, adatoms or magnetic proximity. However, intrinsic 2D ferromagnetism remained elusive until recent discovery of magneto-optical response in Cr-based layers, stimulating the search for novel 2D magnets with tunable properties. We discovered a class of 2D ferromagnets based on 2D-Xenes, elemental analogues of graphene – layered structures of silicene [1] or germanene [2] functionalized by rare-earth atoms. We track the evolution from the antiferromagnetism of the bulk to intrinsic 2D ferromagnetism of a few monolayers of MSi_2 [1,3] and MGe_2 [2,3]. The magnets are compatible with the mature Si and Ge technologies, which is instrumental for engineering new spintronic devices. The lateral charge transport is found to be layer-dependent once the MSi_2 structures are scaled down to a few monolayers limit [4].

A similar approach is applied to graphene: By analogy with MSi_2 and MGe_2, we synthesized a monolayer of EuC_6.The system demonstrates the anomalous Hall effect and negative magnetoresistance [5]. EuC_6 monolayer exhibits ferromagnetism: its magnetic transition temperature is controlled by low magnetic fields – a fingerprint of 2D ferromagnetism [5]. In proximity with EuO, graphene becomes ferromagnetic at 220 K, well above the Curie temperature of EuO [6].

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BETHE-SALPETER EQUATION AND EXCITON SPECTRUM OF THE TRANSITION METAL DICHALCOGENIDES

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Using the Bethe-Salpeter equation we derive the equation for the four component wave function of the interacting electron and hole in the transition metal dichalcogenides. We investigate the solutions of the equation for different potentials and different dimensionless interaction constants. For small interaction constant we obtain in the leading and next-to-leading order in the interaction constant the hamiltonian of the interacting electron and hole. We demonstrate that the obtained hamiltonian does not coincides with naive expansion of the hamiltonian of the two interacting Dirac particles. For the small interacting constant we found the energy of the excitons in the leading and next-to-leading orders in the interaction constant.

We also investigate the dependence of the binding energies of the electron and hole on the interaction constant value for different types of the potentials. We found the critical values of the interaction constant for which the lowest binding energy reaches the valence band. We found the critical values of the interaction constant for the Coulomb potential and for the exponentially decreasing potential which does not contain a singularities.

ANISOTROPY OF INTERACTIONS AND UNIVERSAL MAGNETIZATION DYNAMICS IN 2D RASHBA MAGNETS

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In this talk I overview our recent progress in understanding the role of strong spin-orbit interactions of conduction electrons in 2D magnetic systems. First, I present a general point group classification of linear-in-gradient terms in micromagnetic energy that is designed to revise the seminal work of Bogdanov and Yablonskii. In particular, I will demonstrate that, apart from Dzyaloshinskii-Moria interactions represented by Lifshitz invariants (LI), there exists non-LI contributions in micromagnetic energy. Such contributions are shown to be highly relevant in stabilizing non-collinear magnetic order at least in some crystals. I will also demonstrate that in crystals defined by the point groups Td, Dh3, and Ch3, the Lifshitz-Invariant terms are forbidden and non-LI terms become most important. I will present a new model for a chiral magnet in Td point group symmetry. I will present a microscopic analysis of non-LI terms in a generalized 2D Rashba ferromagnet. In the second part of my talk, I present a detailed study of current induced phenomena in 2D Rashba ferromagnet. In particular I will show how Gilbert damping and in-plane spin-transfer torques acquire strong anisotropy due to spin-orbit interaction. I will also derive a general relation between these quantities that make the speed of magnetic textures universally equal to the drift velocity of conduction electrons in the Rashba model. At the end of my talk I will compare our microscopic results to the standard phenomenological equations on magnetization dynamics to make some further insights.

OPTICAL PROPERTIES OF TRICARBOXYLIC ACIDS AND ETHYLENEDIAMINE DERIVED CARBON DOTS

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Carbon dots (CDs) are a new type of nanoparticles characterized by small dimensions (<10 nm). Since their discovery, CDs have received increasing attention due to their unique properties, such as photoluminescence (PL) with high quantum yield, tunable emission wavelength, excellent water solubility and low cytotoxicity, good biocompatibility, high photostability, resistance to photobleaching, chemical inertness, possibility of surface passivation or functionalization and others [1]. CDs find application in different areas, including drug delivery, biological imaging and medical diagnosis, fluorescent ink, chemical sensing of organic species and metal ions, catalysis, optoelectronics, security applications. CDs are environmental friendly and low-cost alternative to semiconductor quantum dots constituted by heavy metals because of simple synthesis methods from organic raw materials.

CDs synthesized from citric acid and ethylenediamine show intense PL, that has been explained by the presence of isolated sp^2 domains (mainly a fluorophore molecule which is covalently bound to CDs and pyridine derivatives) and defect states (dangling carbon bonds).

In this work, we studied four types of nitrogen doped CDs. The combination of citric acid, as a carbon source, and nitrogen-containing molecules as dopants is the most well studied approach to investigate N-doped CDs. Here, N-doped CDs were prepared hydrothermally using ethylenediamine (as the nitrogen precursor) and both citric and trans-aconitic acids (as carbon precursors). Our results imply that the CDs can be considered as hybrid particles in which the carbon core contains aggregated fluorophores.

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STUDY OF PROPERTIES OF MOS2, WS2 FILMS GROWN BY CVD METHOD

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Currently, transition metal dichalcogenides, such as MoS2 and WS2, have attracted the attention of scientists with their unique properties [1]. They are often compared with graphene, but MoS2 and WS2 are semiconductors, unlike graphene, which exhibits semi-metallic properties. Two-dimensional MoS2 and WS2 are direct-gap semiconductors, which is promising for use in various optical and electronic devices.

In this paper, we studied MoS2 and WS2 films grown by chemical vapor deposition (CVD) method. For the synthesis of the MoS2 films, powder precursors MoO3 and S were used. And for the growth of WS2, an aqueous suspension of WO3 deposited on the surface of substrate. The dependences of film growth on various synthesis parameters were revealed: temperature, time, and the number of precursors. Raman spectra showed the presence of single-layer, two-layer, and multilayer regions on the grown films. Two most intense peaks are observed in the Raman spectra of MoS2: the vibrational mode in the E2g plane is about 386 cm–1 and the vibrational mode outside the A1g plane is about 405 cm–1. With an increase the number of layers, an increase in the frequency of the vertical mode E2g mode is observed, while the frequency for the A1g mode will decrease. Photoluminescence of single-layer and two-layer MoS2 films at 670 nm and single-layer WS2 films at 630 nm was detected. The current–voltage characteristics of the synthesized films are photosensitive in the visible region of the spectrum.

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STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF FLUORINATED GRAPHENE

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Fluorinated graphene is the one of a number of possible chemical derivatives of graphene. An additional chemical bound with carbon atom turns it into sp3 hybridization state, which leads to a significant change in material properties. One of the unresolved issue of the theoretical study of such materials is the lack of a good approach to describing the distribution of functional groups.

Here we wont to describe our Boltzmann-like model of fluorine distribution in partially fluorinated graphene. Our approach based on a simple machine learning technique with DFT fluorine-carbon binding energies for different surroundings as an training data. Such model allows us to generate fluorinated graphene structures with desirable functionalization percentage and structure ordering degree.

Using described approach for structure generation we study the electronic and transport properties (were we reproduce the experimentally observable features in fluorinated graphene conductance) [1], thermal, mechanical and other properties of fluorinated graphene.

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NOVEL STRUCTURAL AND ELECTRONIC PHASES OF 2D TRANSITION METAL DICHALCOGENIDES

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Layered transition metal dichalcogenides (TMDs) of chemical composition MX_2 (M = transition metal; X = S, Se, or Te) represent a broad family of materials with diverse electronic properties, including metals, insulators, as well as more complex states such as the charge-density-wave (CDW) and superconducting phases. More recently, the possibility of realizing single- and few-layer TMDs has brought the two-dimensional (2D) forms of these materials into the spotlight of prospective application in electronics, optoelectronics and beyond [1]. In my talk, I will review the "periodic table" of TMDs attempting to reveal systematic trends and develop chemical intuition across this family of 2D materials. Using a Wannier function approach, I will address the relevance of the crystal and ligand fields in determining the relative stability of 1T and 1H polymorphs as a function of the filling of the d-shell in 2D TMDs [2]. Then, I will present a unified picture of lattice instabilities in metallic TMDs that describes both the CDW phases and the strong-coupling scenario resulting in the formation of metal-metal bonds (as e.g. in the dimerized 1T' phases) [3]. In the rest of my talk, I will focus on topological and magnetic phases of TMDs in connection with the Kane-Mele model [4] and the defect-induced magnetism in graphene [5,6,7]. The 1T'-phase of Mo and W TMDs that have recently been shown to host the topologically non-trivial quantum spin Hall (QSH) insulator phase. The robustness of the QSH phase as well as the topological edge states [8] and interface states at the well-ordered 1T'-1H lateral heterojunctions will be discussed in conjunction with recent experiments on 1T'-WSe_2 [9]. I will also cover our recent discovery of magnetic ordering and magnetoresistive switching in few-layer films of metallic $PtSe_2$ [10].

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MAGNETOPLASMON-POLARITONS IN GATED TWO-DIMENSIONAL ELECTRON SYSTEM

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Plasma oscillations or plasmons in two-dimensional (2D) electron systems (ESs) have been studied for more than half a century. Recently, more and more new experimental information has been accumulating on the importance of electromagnetic retardation effects (i.e. the ”finiteness” of the speed of light) for 2D plasmons; see, for example, the review [1]. When electromagnetic retardation effects are taken into account, plasmons are called 2D plasmon polaritons, and, if 2DES is placed in perpendicular constant magnetic field, 2D magnetoplasmon polaritons. The properties of 2D magnetoplasmon polaritons in ”clean” (when electron relaxation time is infinite) 2DES embedded in dielectric medium were theoretically studied in [2]. However, to the best of our knowledge, magnetoplasmon polaritons in gated 2DES, i.e. when the ideal metal electrode (gate) is situated in the vicinity of 2DES, never have been studied.

In this work we consider the properties of magnetoplasmon polaritons in gated 2DES. We find that at zero wave vector (in 2DES plane) the frequency of magnetoplasmon polaritons does not equal the cyclotron frequency of 2D electrons. We also find that, even in ”clean” 2DES, magnetoplasmon polaritons have finite lifetime at small wave vectors due to the radiative decay. Finally, we find that the absorption of electromagnetic wave by gated 2DES correlates with magnetoplasmon polariton properties.

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RETARDATION EFFECT ON ABSORPTION OF MICROWAVE RADIATION IN DISK WITH 2D ELECTRON GAS

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Plasmons in 2D disk have been studied since 1985 [1] and recently were intensively discussed in graphene structures. However most works were done in quasielectrostatic or non-retarded regime, when the size of the sample is much smaller than the wavelength of the exciting electromagnetic field. Here we develop a theory of resonant absorption of microwave radiation in two-dimensional electronic systems in the form of a disk when the radiation wavelength is less than or comparable to the radius of the disk. The problem is solved in a self-consistent approximation. We use the Drude model for conductivity of the system. The absorption peak in the dependence of the absorption power on the frequency corresponds to the excitation of plasma waves, while the linewidth of the peak corresponds to the plasmon damping. We find analytical corrections due to retardation for the fundamental (dipole) and the axisymmetric (quadrupole) modes. The frequency of the axisymmetric mode depends on the electromagnetic retardation rather weakly since the plasma oscillations have zero dipole moment [2]. The damping of the modes strongly depend on the ratio between the radiative and collisional decay. In the absence of collisions, the radiative decay rate of axisymmetric mode is mainly determined by the quadrupole moment for the mode. However, even for small retardation the linewidth of the resonances is not merely the sum of two decays since it contain additional terms.

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1D AND 2D EDGE SPECIFIC GRAPHENE NANORIBBONS

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High-quality graphene nanoribbons (GNR) epitaxially grown on the sidewalls of silicon carbide (SiC) mesa structures stand as key building blocks for graphene-based nanoelectronics. Such ribbons can be successfully grown along both [1-100] and [11-20] SiC crystallographic directions with very well defined zig-zag (ZZ) and arm-chair (AC) edges, correspondingly [1]. The properties of the ZZ and AC GNRs have been studied by using plethora of experimental microscopic techniques: angle resolved photoemission spectroscopy (micro-ARPES), low energy electron microscopy (LEEM), spatially resolved in-situ transport experiments in the STM/SEM system. It was shown that ZZ nanoribbons display 1D single channel ballistic transport at room temperature with exceptionally long mean free path [2]. They also show protected and spin-polarized transport channel which is the hallmark of topological insulators [3]. In turn, AC GNRs reveal the development of a width-dependent semiconducting gap driven by quantum confinement effects [4]. Micro-ARPES demonstrates an ideal one-dimensional electronic behavior consisting of well resolved subbands non-dispersing across the ribbons. These experimental findings coupled with theoretical tight-binding calculations set the grounds for a deeper exploration of quantum confinement phenomena and open intriguing avenues for new low-power electronics.

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COMPARATIVE STUDY OF FIELD ELECTRON EMISSION FROM DISORDERED AND HIGHLY ORIENTED CARBON STRUCTURES

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The results of experimental studies of field emission from glassy carbon and highly oriented pyrolytic graphite (HOPG) are presented. It has been shown that multilayered graphene-like structures (GLS) such as HOPG, nanotubes and GLS obtained by detonation synthesis confirm the phenomenon of low-threshold (LT) field electron emission, as was shown earlier [1-3]. In the case of glassy carbon, which is a typical carbon material with a disordered structure, the observation of the effect of LT emission is difficult. The result allows us to conclude that the phenomenon of LT emission, as well as the effect of high-current field emission from graphene-like structures, is associated with an ordered layered structure and deformation perturbations of this structure by the electric field [3].

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