XIX Symposium on Condensed Matter Physics SFKM 2015

Book of Abstracts

7 – 11 September 2015
Belgrade, Serbia

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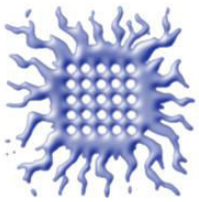

XIX Symposium on Condensed Matter Physics
SFKM 2015

Conference Topics

Conference presentations cover a wide range of research topics within the experimental, theoretical, and computational condensed matter physics, including but not limited to the following:

Semiconductor physics: Electronic structure, Quantum dots and wires, Photonic crystals, High magnetic fields phenomena, Ultra-fast phenomena

Surface, interface, and low-dimensional physics: Graphene, Carbon and other nanotubes, Topological insulators, Complex oxide interfaces, Transport in nanostructures

Magnetism: Magnetic materials and phase transitions, Magneto-electronics and spintronics, Magnetic nanoparticles

Superconductivity: Conventional, high T_c, and heavy-fermion superconductors: Materials and mechanisms, Heterostructures: Proximity effect and transport phenomena

Strongly correlated and disordered systems: Materials with strong correlations and disorder, Dynamical properties from time-resolved experiments, Quantum fluids, Cold atoms and BEC

Phase transitions, phase ordering, and structural ordering of condensed matter: Equilibrium and dynamic phenomena, Ferroelectricity, Multiferroics, Quasi-Crystals, Crystal surface morphology and dynamics, Crystal growth

Soft and biological matter: Polymers, Liquids and gels, Liquid crystals, Elastomers, Membranes, Living cells and living matter

Statistical physics of complex systems: Networks and other structures

Conference venue:
Serbian Academy of Sciences and Arts, Knez Mihailova 35, Belgrade

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Marko J. Rančić, *Department of Physics, University of Konstanz*
Goran Rasic, *North Carolina Central University*
Bojana Višić, *Weizmann Institute of Science, Rehovot*

Invited Talks

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Invited: 1

Spin injection and relaxation in a mesoscopic superconductor

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Abstract. We have investigated out-of-equilibrium spins in conventional superconductors. Injecting spin-polarized electrons or holes into a superconductor and removing Cooper pairs creates both spin and charge imbalances. We have investigated the relaxation of the out-of-equilibrium magnetization induced by spin injection. First, we measured the spin and charge relaxation times (t_S and t_Q) by creating a dynamic equilibrium between continuous injection and relaxation, this leads to constant-in-time spin and charge accumulation proportional to their respective relaxation times. Using a mesoscopic absolute spin-valve, we obtained t_S and t_Q by probing the difference on the chemical potential between quasiparticles and Cooper pairs [1]. We observed that spin (charge) accumulation dominates at low (high) injection current. This artificially generates spin-charge separation as theoretically first predicted by Kivelson and Rokhsar [2]. Second, we directly measured the spin relaxation time in the frequency space and found t_S= 1-10 ns consistently with results from constant current injection [3]. Finally, we measured the spin coherence time of the out-of-equilibrium quasi-particules by performing an electron spin resonance experiment [4]

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Entanglement spectra of interacting fermions from quantum Monte Carlo simulations

F. F. Assaad

Abstract. Entanglement is the defining property of correlated electron systems. For a ground state, $|\Psi_0\rangle$, a measure of entanglement can be obtained by considering a bipartition of the Hilbert space in A and B, and tracing out the degrees of freedom of one partition: $\mathrm{Tr}_B|\Psi_0\rangle\langle\Psi_0| = e^{-\hat{H}_E} \equiv \hat{\rho}_A$. In close analogy to the Unruh effect, the above states that from the perspective of A, the ground state corresponds to a thermal state at temperature $k_BT = 1$. $\hat{H}_E$ is the entanglement Hamiltonian and the entropy associated with the reduced density matrix, $\hat{\rho}_A$, the entropy of entanglement. This talk reports recent progress in auxiliary field quantum Monte Carlo (QMC) simulations for fermionic systems which allow the computation of entanglement entropies [1, 2] and more importantly of the low energy properties of $\hat{H}_E$ [3, 4]. In particular we will demonstrate that correlated topological insulators – as realized in the Kane-Mele model with variable range interactions [5, 6] – can be detected efficiently by studying the entanglement spectrum.

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From Floquet to Dicke: Quantum Spin-Hall Insulator in Quantized Electromagnetic Field

Balázs Dóra[a] and Balázs Gulácsi[a]

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Abstract. Time-periodic perturbations due to classical electromagnetic fields are useful to engineer the topological properties of matter using the Floquet theory. Here we investigate the effect of *quantized* electromagnetic fields by focusing on the quantized light-matter interaction on the edge state of a quantum spin-Hall insulator. A Dicke-type superradiant phase transition occurs at arbitrary weak coupling, and the electronic spectrum acquires a finite gap and the resulting phase is topological with Chern number ± 1. When the total number of excitations is conserved, a photocurrent is generated along the edge, being pseudo-quantized as $\omega \ln(1/\omega)$ in the adiabatic limit, and decaying as $1/\omega$ for high frequencies. The photon spectral function exhibits a clean Goldstone mode, a Higgs like collective mode at the optical gap and the polariton continuum.

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What I Cannot Compute I Do not Understand:
fathoming atomic heat transport from the struggle to simulate it

Stefano Baroni

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Abstract. Modern simulation methods based on electronic-structure theory have long be thought to be unfit to compute heat transport coefficients within the Green-Kubo formalism. This is so because the quantum-mechanical energy density from which the heat flux is derived is inherently ill defined, thus allegedly hampering the use of the Green-Kubo formula. I believe that every property that can be measured can also be computed, at least in principle. If it cannot, it's that the underlying theory is still incomplete. Steered by this conviction, we[1] have derived an expression for the adiabatic energy flux from density-functional theory, that permits the ab initio simulation of atomic thermal transport using equilibrium molecular dynamics. The resulting thermal conductivity is shown to be unaffected by the above-mentioned ill-definedness of quantum mechanical energy densities and currents. Our new methodology is demonstrated by comparing results from ab-initio and classical molecular-dynamics simulations of a model liquid-Argon system, for which accurate inter-atomic potentials are derived by the force-matching method, and finally applied to compute the thermal conductivity of heavy water at ambient conditions.

[1] "We" refers to Aris Marcolongo, Paolo Umari, to whom goes my gratitude for the fruitful and pleasant collaboration, and myself.

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Spin-Dependent Thermoelectric Effects and Spin-Triplet-Supercurrent in Mesoscopic Superconductors

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Abstract. The usually negligibly small thermoelectric effects in superconducting heterostructures can be boosted dramatically due to the simultaneous effect of spin splitting and spin filtering. Building on an idea we published in [1], we propose realistic mesoscopic setups to observe thermoelectric effects in superconductor heterostructures with ferromagnetic interfaces or terminals[2]. We focus on the Seebeck effect being a direct measure of the local thermoelectric response and find that a thermopower of the order of $250\,\mu$V/K can be achieved in a transistor-like structure. A measurement of the thermopower can furthermore be used to determine quantitatively the spin-dependent interface parameters that induce the spin splitting. For applications in nanoscale cooling we discuss the figure of merit for which we find values exceeding 1.5 for temperatures $\lesssim$1K. In the talk I will highlight the quasiclassical circuit theory behind the prediction, which takes into account the usually present diffusive scattering at in-terfaces and surfaces. A crucial ingredient are spin-dependent boundary conditions for the diffusive Greens functions, which need to take into account the microscopic details of the spin-dependent interface scattering. We have recently solved this long-standing problem for the quasiclassical theory [3, 4], which paves the way for a description of novel spintronics phenomena in superconductors. The relevance for possible spin-triplet supercurrents are discussed.

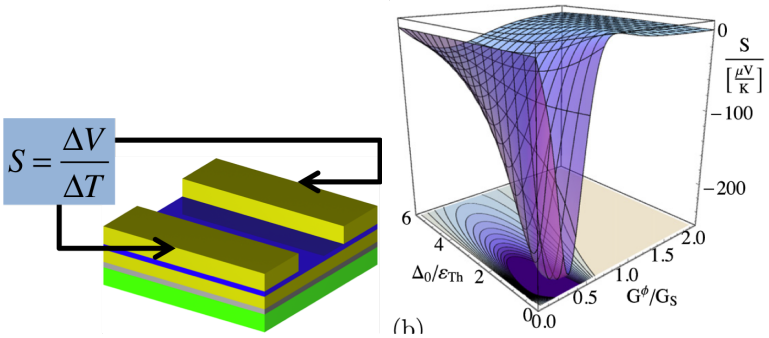

FIGURE 1. The left panel shows a setup to observe the predicted thermoelectric effect. The structure consists of a superconducting substrate (green), coupled to normal metal film (yellow) covered by ferromagnetic insulating film (blue). Current is injected and extracted by two normal contacts on top. By applying a temperature difference ΔT a thermovoltage δV can be measured (at zero current). The resulting Seebeck coefficient $S = \Delta V/\Delta T$ is plotted on the right. [2]

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Ion Beam Induced Modifications of Thin Films/Si bilayers

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Abstract. The modification of the thin films/Si bilayer by ion irradiation is a powerful tool to tailor the structural, optical, electrical, magnetic etc., properties of a wide class of materials. Moreover, the precise control of irradiation parameters along with selection of suitable materials offer advantages in structuring materials on a nanometres scale, nowadays one of the most relevant technological challenge. Changes in structural and magnetic properties in Co/Si and Fe/Si bilayers due to heavy-ion beam irradiation have been investigated as functions of the ion beam mass, energy and fluence as well as substrate temperature and interface morphology. Processes occurring during interface mixing were investigated together with the role of the different above cited parameters. The study focuses on the understanding of atomic transport in the regime of nuclear stopping, the conditions to form specific silicide phase by ion-beam mixing and on ion-induced changes in magnetization of the metal/Si bilayers. Similarities and differences between thermal and ion-induced processes were investigated.

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Evolution of Orthogonally Inequivalent States in Cuprates - Atomic Structure Footprints

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Abstract. Realization that many emerging phenomena, such as colossal magnetoresistance and unconventional superconductivity, may be governed by complex disorder exemplifies the importance of utilization of local probes sensitive to short range correlations. To that effect the knowledge of the local atomic structure may reveal relevant nanometer lengthscale footprints important for more comprehensive understanding of the character of symmetry broken states. Atomic pair distribution function (PDF) is one of the few experimental methods that can speak to this problem. Systematic approach in charting both long and short range structural orders, on an equal footing, across the (x, T) phase diagram of materials emerges as a powerful identification tool for grasping the relevance and hierarchy of length scales reflecting competing and/or coexisting orders. Revealing the nature of the symmetry broken states and fluctuations of short-range order in strongly correlated electron systems in general and in the pseudo-gap (PG) regime of cuprates in particular, remains instrumental in understanding the underlying physical properties. Mounting experimental evidence suggests that the PG in cuprates may represent an electronic state in which the four-fold rotational symmetry (C_4) of the CuO_2 planes is broken (down to at least C_2), pointing to stripe or nematic character. The former is referred to here as orthogonally equivalent (OE), and the later as orthogonally inequivalent (OI) state. I will show recent neutron total scattering based results that extend the systematic approach to the nickelate and cuprate systems. In order to benchmark the sensitivity of powder-based methods for this class of problems, we initially explored T-evolution of structural effects associated with the melting of well-established stripe order in $La_{1.67}Sr_{0.33}NiO_4$ across the charge-order (CO) temperature, T_{CO}. In this model stripe system structural features sensitive to both long and short range stripe order are identified, further suggesting that dynamic charge-stripe correlations survive to T ~$2T_{CO}$[1]. Encouraged by these observations, underdoped $La_{2-x}Ba_xCuO_4$ (LBCO) that hosts stripes was studied next over a range of doping and temperature. Due to presence of two inequivalent oxygen sites in the CuO_2 planes, the average structure in the CO state of LBCO at base temperature is OI. On warming across T_{CO} temperature, our data are consistent with persistence of OI state locally well above T_{CO} and deep into the low temperature orthorhombic (OE) average crystallographic phase within the PG regime. Subsequent T-dependent inelastic neutron scattering measurements (INS) of the x=1/8 LBCO reveal dynamic character of the OI state above Tco. Both INS and PDF assessments suggest that these are correlated on a sub-nanometer length scale. Various measures of OI-ness reveal non-monotonic doping dependence, coincidentally peaking at x=1/8, where the stripe order is the strongest[2]. Time permitting, structural observations of OI-like state in $YBa_2Cu_3O_{6+d}$ will be addressed, where an increased presumably electronic inequivalence of two in-plane oxygens below T_{CO} was observed by NMR.

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The Origin of High-T_c Superconductivity in Cuprates

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ABSTRACT

Superconductivity in cuprates has many mysterious facets, but the central question is why the critical temperature (T_c) is so high. Our experiments target this question.

We use atomic-layer-by-layer molecular beam epitaxy to synthesize atomically perfect thin films, multilayers and superlattices of cuprates and other complex oxides. By atomic-layer engineering, we optimize the samples for the particular experiment. Using a continuous spread in composition we tune the doping level in steps of 0.01%. We use high-throughput measurements on combinatorial libraries to study magneto-resistance and Hall effect in fields up to 90 T and measure accurately the coherence length ξ. We measure the absolute value of penetration depth λ to accuracy better than 1%.

We have shown that HTS films can be quite homogeneous, having a very uniform SC gap. Charge density waves and charge glass are observed in some samples, but none for optimal doping. Phase fluctuations drive the superconducting transition at every doping, but they fade out 10-15 K above T_c, so the pseudogap must have a different origin. *In-plane* charge excitations are strongly coupled to *out-of-plane* lattice vibrations. Superfluid can be confined to a single CuO_2 layer, with T_c equal to that in bulk samples. A large enhancement of T_c is seen in certain heterostructures. Pairs exist on both sides of the superconducting transition, be it induced thermally or by doping.

Here, the results will be revealed of a comprehensive study that took nine years and encompassed thousands of cuprate samples, probably without precedence in the history of Condensed matter physics. The large statistics enables us to identify clear trends and unravel intrinsic properties; this is essential when dealing with complex materials such as cuprates. We have measured the key physical parameters (T_c, λ, and ξ) of the superconducting state and established their precise dependence on doping, temperature, and external fields. The findings bring in some great surprises, challenge the commonly held beliefs, rule out many theoretical models, and hint at the answer to our initial question.

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Quantum Synchronization

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Abstract. Synchronization of classical driven self-sustained oscillators is a universal phenomenon that is important both in fundamental studies and in technical applications. Recent progress in the experimental realization of optomechanical systems has motivated the study of synchronization in quantum systems. I will discuss some approaches to the question of quantum synchronization and how to define and measure it and will then describe our own work. We have analyzed the synchronization behavior of one quantum van der Pol oscillator subject to an external drive, and two dissipatively coupled van der Pol oscillators in the quantum regime.

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Probing and Engineering of Quantum Magnets at Surfaces

Harald Brune

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Abstract. Understanding the magnetic states of individual surface adsorbed atoms and molecules may enable us to realize the ultimate size limit of stable magnets and to create magnetic quantum bits. We combine X-ray magnetic circular dichroism (XMCD) with scanning tunneling microscopy (STM) to address the magnetic properties of individual surface adsorbed atoms and molecules and review the state-of-the-art in that field.

Making magnets smaller increases thermal fluctuations of the magnetization direction, magnetization reversal by tunneling and by electron scattering. For magnetic storage, the spin relaxation time has to be high, and for quantum computing the spin coherence time. The ultimate question is, can a single atom be a magnet in the sense that it exhibits remanence or a significant spin coherence time ? We find exceptionally large magnetic anisotropy energies for single surface adsorbed atoms of 3d elements, with Co on MgO(100) being the record [1]. Nevertheless, these atoms are paramagnetic. Recently published spin-polarized STM results report remanence for single Ho atoms on Pt(111) [2]. However, using XMCD, we find for that system a magnetic ground state that is not compatible with long spin coherence times [3]. Therefore, at present, the smallest stable magnets are ferro-magnetic Fe_5 clusters on Cu(111) [4] and anti-ferromagnetic Fe_8 chains on Cu_2N/Cu(100) [5].

Single molecule magnets exhibit promising properties in powder samples. However, contacting them with metal electrodes, or equivalently, adsorbing them onto a metal surface, results in many cases in their disintegration – or at least in a significant quenching of their spin-relaxation times. One of the most promising exceptions are dysprosium-scandium based endofullerenes. We show that the magnetic moments of $Dy_2ScN@C_{80}$ molecules on Rh(111) are aligned and exhibit spin-relaxation times of half a minute [6].

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Synthetic Magnetic Fields for Atoms and Photons

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Abstract. We will present recent results of our group in the rapidly developing field of synthetic magnetic fields for atoms and photons, in cold atomic gases and photonic structures, respectively. The results can be categorized in three closely related groups. (i) First we present a novel theoretical proposal [1], and the experimental demonstration [2], of synthetic magnetic fields that were for the first time achieved in classical cold atomic gases. The scheme utilizes radiation pressure forces and the Doppler effect [1,2]. The experiment was implemented in the 87Rb Magneto-Optical Trap. (ii) As the second result, we show that a Hamiltonian with Weyl points can be realized for ultracold atoms using laser-assisted tunneling in three-dimensional optical lattices [3]. Weyl points are synthetic magnetic monopoles that exhibit a robust, three-dimensional linear dispersion, identical to the energy-momentum relation for relativistic Weyl fermions [3], which are not yet discovered in particle physics. Weyl semimetals are a promising new avenue in condensed matter physics due to their unusual properties such as the topologically protected 'Fermi arc' surface states. However, experiments on Weyl points are highly elusive. We show that this elusive goal is well-within experimental reach with an extension of techniques recently used in ultracold gases [3]. (iii) Finaly, as a third result, we present a grating assisted tunneling scheme for tunable synthetic magnetic fields in photonic lattices [4]. The synthetic fields emerge from the nontrivial phases of the resulting tunneling matrix elements. The scheme is straightforward to implement at optical frequencies in optically induced one- and two-dimensional dielectric photonic lattices. We propose implementation of the Harper-Hofstadter Hamiltonian in these photonic lattices [4]. Our group (in Zagreb) is funded by the Unity through Knowledge Fund grant 5/13 (www.ukf.hr).

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The emergence of superconducting spintronics

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Abstract. It is generally accepted that the semiconductor electronics scaling road-map will reach its physical limits within the next decade. Different alternative technologies are under active development, in particular the superconducting spintronics, which may be generally described as follows. The Cooper pairs of electrons which carry the current in conventional superconductors consist of electrons with antiparallel spins and so a standard supercurrent is a pure charge current with no spin component. However, these "singlet" pairs can be transformed by a suitable magnetic structure into "triplet" pairs in which the spins are parallel.

Recently it has demonstrated that triplet pairs can penetrate significant distances in ferromagnets and evidence has been reported that triplet pairs can flow from ferromagnets into non-magnetic metals. Since triplet pairs are spin-aligned it is possible for them to carry spin without Ohmic dissipation.

I will review the main mechanisms of the interplay between magnetism and superconductivity and the coexistence between these two different long ranged orders in the bulk magnetic superconductors and superconductor-ferromagnet heterostructures. Special attention will be devoted to the superconductor/ferromagnet/superconductor Josephson junctions. There the noncollinear magnetization of the ferromagnetic layer provides the conditions necessary to generate the triplet superconducting correlations. It leads to the long-range induced magnetic moment, emerging in the superconducting layers and depending on the Josephson phase. By tuning the Josephson current, one may manipulate the long-range induced magnetic moment. The induced magnetic moment controlled by the Josephson current may be used in spintronics devices instead of the spin-torque effect. The proposed mechanism seems to be attractive for superconducting spintronic devices with low dissipation because it provides a direct coupling between the superconducting current and magnetization.

Strain Engineering in Two-Dimensional Transition-Metal Dichalcogenides

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Abstract. Graphene has represented in the past 10 years the most promising new material for a new generation of electronic devices and for the investigation of fundamental physics. The effective employment of graphene-based materials in low-energy electronics is however hindered by the difficulty of opening a bandgap without affecting the mobility and the electronic properties. New actors have however recently entered on the stage, in particular metal-transition dichalcogenides, as MoS_2 and similar compounds. Also these materials, like graphene, can be exfoliated to reach atomically thickness. In advantage, they present an intrinsic bandgap whose nature and size results to be highly sensitive to the number of layers and to external conditions (strain, pressure, electric fields, etc.).

In this talk we demonstrate the possibility to control at a local scale the electronic and optical properties by means of local strain [1]. Lattice corrugations are induced in few-layer MoS_2 samples by means of controlled delamination on an elastic substrate. Local strain is monitored through the phonon resonance energies in Raman spectroscopy, and the local direct bandgap is measured by photoluminescence. The direct correlation between these features proves the feasibility to control the bandgap at a local scale by means a suitable pattern of strain. To understand these results, we generalize a proper tight-binding model [2] for MoS_2 under non-uniform conditions, accounting for the local modulation of the hopping integrals. for the local modulation of the hopping integrals. Such analysis suggests a possible change between direct- to indirect-bandgap upon strain at a local scale, and a possible "funnel" effect in large wrinkles.

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Symmetry In Classical Magnetism: Helical Phases In RKKY ^{13}C Nanotubes

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Abstract. We present general theory of implementing symmetry within quasi classical magnetism. It is based on spin groups generalizing well known magnetic groups, and systematic application of the modified group projector technique [1]. This refers both to determination of the ground state and to low energy dynamics (spin waves). In particular, spin line groups, relevant for the quasi one-dimensional spin systems are classified [2]. Detailed study [3] of nuclear spin order in semiconducting ^{13}C nanotubes reveals subtle interplay of the chemical potential, length, diameter and chirality, resulting in the complex four dimensional phase diagram of the helical ground states. Increase of the chemical potential causes abrupt transitions between different helical spin orderings of three regimes which are interpolated by smooth change of helical angle within each regime: in the middle one helimagnet is deviation from the commensurate order and fully characterizes geometry of nanotube, while outside it ground state is incommensurate helical deviation from ferromagnet. This behaviour of ^{13}C nanotubes manifests long range of RKKY interaction and quasi one-dimensional geometry, thus being universal for all RKKY interaction governed nanowires. Short enough nanotubes are ferromagnetic; the critical length when frustration arises, decreases with the chemical potential, but increases with diameter and chiral angle. The results, verified numerically, show that with nanotubes of the different, but realistic lengths, various scenarios of the helical order response to the gate voltage can be achieved.

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Generalized Bloch theorem and topological characterization

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Abstract. Based on a group theory analysis we present generalization of the Bloch theorem that incorporates all additional symmetries of a crystal. The generalized Bloch theorem constrains the form of the Hamiltonian which becomes manifestly invariant under additional symmetries. In the case of isotropic interactions the generalized Bloch theorem gives a unique Hamiltonian. This Hamiltonian coincides with the Hamiltonian in the periodic gauge. In the case of anisotropic interactions the generalized Bloch theorem allows a family of Hamiltonians. Due to the continuity argument we expect that even in this case the Hamiltonian in the periodic gauge defines observables, such as Berry curvature, in the inverse space. For both cases we present examples and demonstrate that the average of the Berry curvatures of all possible Hamiltonians in the Bloch gauge is the Berry curvature in the periodic gauge.

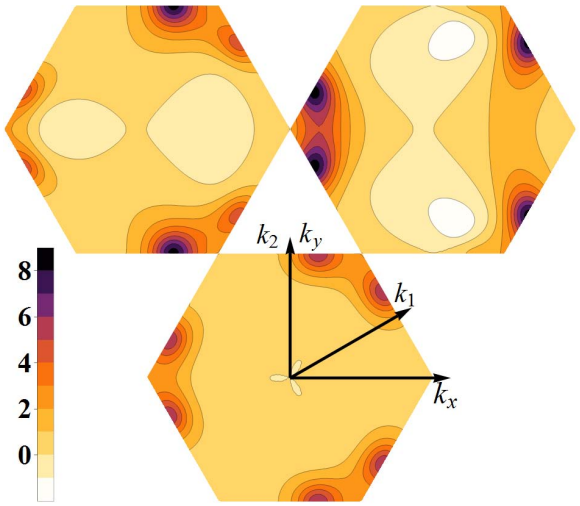

FIGURE 1. Berry curvatures, in the Brillouin zone, of the lowest energy band for the Haldane model.

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Sculpting nanostructures with electrons for nano and biotechnology

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Abstract. In 400 BC, Democritus hypothesized that matter is made of atoms that are miniscule quantities of matter. Today, we have transistors at the size scale of several atoms soon to be integrated into everyday computer chips. Understanding, shaping and manipulating matter at atomic scale remains one of the major contemporary challenges in science and technology. In this respect, electron beams constitute the power tools to shape materials with atomic resolution inside a transmission electron microscope (TEM). I will describe experiments where we push the limits of device size to atomic scale, and expand their function and precision, while addressing fundamental questions about structure and properties at nanometer and atomic scales. Experiments are performed in situ or ex situ TEM. In situ TEM experiments include the study of electrons flow in nanowires in novel two-dimensional materials as a function of their structure as they are nanosculpted down to zero width. We reveal the electrical current scaling with size and atomic structure and develop methods to realize pristine and highly conducting sub-10-nm-wide wires. Ex situ TEM include the ultrafast, all-electronic detection and analysis of biomolecules or nanoparticles by threading them through tiny holes – or nanopores – in thin membranes, including efforts towards mapping a human genome under 10 minutes. As particles are driven through nanopores in solution, they block the current flow resulting in current reductions from which particle's physical and chemical properties are inferred. Measurements of DNA, proteins, microRNA and other biomolecules as well as solid-state particles will be highlighted, where we improved the temporal and spatial resolution and sensitivity. I will also describe alternative uses of nanopores such as electrically controllable chemical nanoreactors, and explore the use of nanopores in two-dimensional nanowires to highly localize and probe molecules.

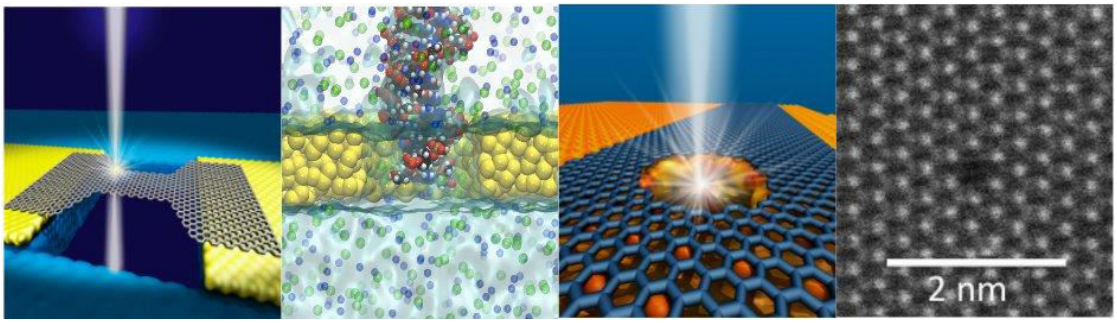

FIGURE 1. From left to right: illustrations of graphene nanoribbon sculpting with the electron beam; passage of a DNA molecule through a silicon nanopore; nanopore drilling through graphene nanoribbon transistor; one-atom-large nanopore in a MoS_2 sheet.

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Fundamental Building Blocks in Nanomaterial Synthesis by Pulsed Laser Vaporization

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Abstract. In this talk I use the octahedrally coordinated TiO_6 atomic structure units as an example for discussing nanomaterial synthesis from fundamental building blocks (FBBs). The distortion of individual octahedral FBBs and their spatial connectivity determines whether a titanium oxide compound will exhibit the properties of anatase, rutile, or some other less common metastable phase. It is even more intriguing that the preference for a particular TiO_2 phase appears to be already present in material that is amorphous. Pulsed laser vaporization (PLV) is well known for its highly non-equilibrium growth capabilities that can be used for creating a variety of initial conditions in nanoparticle (NP) synthesis. Material deposited by PLV at room temperature is already aggregated into 3-5 nm NPs with clearly defined shape. Selected area electron diffraction (SAED) reveals that these NPs are amorphous lacking long range crystalline order. However, using a technique of nanobeam electron diffraction (NBED) to probe diffraction from highly localized nanoscale volume, ordering is observed on the length scale of 1-4nm, known as medium range order. This length scale is particularly intriguing because it is related to the formation of subcritical seeds preceding nucleation of a stable crystalline phase. An intriguing example of the transformation of such amorphous NPs into a special form of TiO_2 known as "black TiO_2"—because of its unexpected dark color—will be described in detail.

Understanding the relationship between atomic structure, chemical composition and catalytic activity of black TiO_2 is of great interest because it produces a dramatic enhancement in photocatalytic efficiency. After annealing in Ar the initially transparent amorphous NPs turn black. We use a combination of high spatial resolution imaging, and high energy resolution electron spectroscopy techniques to characterize the phase evolution produced by annealing. Depth profiling on a scale of single NPs was performed to explore the possible transformation pathways leading to stable phase formation. The known relationship between the configuration of TiO_6 units and the electronic structure was used for interpreting the changes in EELS spectra and NBED patterns observed in the evolution of these structures. These data are consistent in showing that the crystallized NPs contain a perfect stoichiometric rutile core, and a 1-2 nm thin shell of disordered narrow bandgap semiconductor, Ti_2O_3. Our data suggest that annealing in pure argon sets up a dynamic oxygen deficiency gradient directed toward the growing edge of the NPs. Crystallization of Ti^{4+} rutile becomes unsustainable beyond a certain level of oxygen deficiency forcing nucleation of a Ti^{3+} phase of Ti_2O_3 that is responsible for the dark color and the enhanced catalytic activity of black TiO_2 NPs.

Classical And Statistical Mechanics Of Celestial Scale Strings: Rotating Space Elevators

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Abstract. With the advent of ultra-strong materials such as carbon nanotubes and diamond nano-thread structures, the concept of a Space Elevator has propagated from science fiction to real science. We review a new venue in this area: Rotating Space Elevators (RSE) [1, 2]. An RSE is a loopy string reaching deep into outer space. The floppy RSE loop executes a motion which is nearly a superposition of two rotations: geosynchronous rotation around the Earth, and yet another faster rotational motion of the string which goes on around a line perpendicular to the Earth at its equator. Strikingly, objects sliding along the RSE loop spontaneously oscillate between two turning points, one of which is close to the Earth (starting point) whereas the other one is deeply in the outer space. The RSE concept thus solves a major problem in space elevator science which is how to supply energy to the climbers moving along space elevator strings. The floppy RSE strings exhibit interesting nonlinear dynamics and statistical mechanics phenomena discussed in this talk.

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Numerical Models In Analysis Of Morphological Properties Of Oxide Nanopowders

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Abstract. The morphology of nanomaterial mainly determine its physical properties and possible application. In case of nanopowders, the morphology relates not only to particles shape, size and distribution, but also to the porous structure. Some aspects of numerical models related to experimental methods often used in morphological characterization of porous oxide nanopowders (CeO_2 and different polymorphs of TiO_2, pure and doped) are presented. The phonon confinement model (PCM) is used to analyze the influence of nanocrystallite size and distribution on the Raman spectra of oxide nanopowders. The comparison of experimental spectra and those calculated by PCM provides the insight in the nanopowder morphology [1, 2]. The values of some microscopic parameters of nanocrystalline powders may also be deduced from the infrared reflectivity spectra of nanomaterials, which is influenced both by particle size and porous structure. For this purpose the models based on a generalized Bruggeman effective medium approximation, using the factorized form of the dielectric function of different porous oxide nanopowders, have been applied [3-5]. The porous structure of nanopowders is also revealed by the analysis of nitrogen sorption experimental data. Beside usually used models, the corrugated pore structure model (CPSM) was employed to determine not only the pore size distribution, but also the pore structure tortuosity factor, which provides the information on the connectivity among the pores [6].

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Intercalation of Metal Supported Graphene

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Abstract. The coverage-dependent intercalation of oxygen, CO, hydrogen, alkali metals, and halogens between graphene and Ir(111) is investigated using density functional theory with van der Waals corrections [1]. By comparing adsorption on clean Ir to intercalation we show that the presence of the graphene layer shifts the stability of the adsorption structures towards higher coverages, with oxygen as the only exception preferring low-coverage intercalation structures. In general, we find that the preferred adsorption site of the intercalant is important for the stability of intercalation structures, where an atop adsorption site favors higher-coverage structures compared to a hollow adsorption site. Comparisons to experimental information where available will be presented. Some of the structures were determined using a newly developed automated structure optimization technique, which will be described [2].

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Non-Fermi liquids and (Mott) insulators in electronic systems with parabolic band touching

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Abstract. I will review the recent work on the phases and quantum phase transitions in the electronic systems that feature parabolic band touching at the Fermi level, the celebrated and well-studied example of which is the bilayer graphene. In particular, it will be argued that three dimensional such systems are in principle unstable towards the spontaneous formation of the strong topological Mott insulator at weak long-range Coulomb interaction. The mechanism of the instability can be understood as the collision of non-Fermi liquid fixed point, discovered by Abrikosov in the `70s, with another, quantum critical fixed point, which approaches it in the coupling space as the system's dimensionality approaches certain ``critical dimension" from above. Some universal characteristics of this scenario, the width of the non-Fermi liquid crossover regime, and the observability of the topological Mott phase in common gapless semiconductors such as gray tin or mercury tellurude will be discussed.

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SiGeSn Alloys For Silicon-Based Photonics

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Abstract. Monolithic integration of a laser source with silicon photonic integrated circuits is considered as "the Holy Grail" for merging mature Si electronics and photonics. Numerous approaches towards this goal have been reported in the literature. Heterogeneous integration of III-V epitaxial layers by layer transfer and bonding provides high quality III-V films on top of Si waveguides, however this technology faces limitations related to the dense integration problems. The alternative approach, monolithic integration (with CMOS compatibility) of optical and electronic devices based on tin-containing group IV materials (GeSn or SiGeSn), which can have a direct band gap in appropriate range of alloy compositions and/or strain conditions, has attracted a large research interest in recent years. Recent successes in good-quality material growth have led to a successful demonstration of optically pumped laser[1], and give rise to expectation that GeSn will be the basis of Si-compatible injection lasers, emitting in the mid-infrared range, typically 2-4 μm, with a variety of possible applications, including short-range communications, biomedical and environmental sensing, etc. The band structure of the (Si)GeSn material, and its implications on the possibility of optical gain in this system is first discussed. Furthermore, the gain achievable in the binary GeSn alloy, and its limitations, are discussed based on calculations using k.p method to account for interband and inter-valence band transitions, and the second-order perturbation method for indirect interband and various free carrier absorption processes (induced by acoustic and optical phonons, intervalley, ionised impurity and alloy disorder scattering). The regions of the parameter space (alloy composition, doping, strain, carrier injection) are identified where good values of gain can be expected. The ternary SiGeSn alloys are unlikely to be useful as gain media[2], but may be very useful for cladding layers in waveguides and cavities, or for carrier confinement in GeSn, and their properties are also discussed.

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Coherent Optical Phenomena in Superconducting Metamaterials: Self-induced Transparency and Dicke Superradiance

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Abstract. We study the propagation of the electromagnetic waves in quantum metamaterial built up of the one-dimensional array of periodically arranged superconducting charge qubits, regarded as two–level systems. It is demonstrated that the two remarkable, coherent optical phenomena, i.e., self–induced transparency and Dicke-type superradiance, may occur during the coherent light-pulse propagation in these media.

Superconducting qubits are currently preferred for building quantum computers. Thus, in a view of recent discoveries of superradiance in quantum dots arrays and Bose–Einstein condensates, the experimental confirmation of the similar effect in superconducting qubits may open a new pathway to potentially powerful quantum computing.

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Space Group Classification of Topological Band Insulators

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Abstract. Topological band insulators are bulk insulating states of matter, which in the presence of time-reversal symmetry feature metallic states at their edge or surface. This state of quantum matter has been experimentally realized in HgTe/CdTe quantum wells and various (mostly) Bismuth-based compounds.

I will first introduce the concept of topological band insulators and then discuss the role of crystal symmetries in the physics of these states of quantum matter. I will derive the classification of topological band-insulators protected not only by time-reversal, but also by space group symmetries [1] As a result, there are three broad classes of topological states: (a) Gamma-states robust against general time-reversal invariant perturbations; (b) Translationally-active states protected from elastic scattering, but susceptible to topological crystalline disorder; (c) Valley (crystalline) topological insulators sensitive to both elastic and crystalline disorder. I will also discuss probing of the topological states in the bulk by magnetic π-fluxes [2] and lattice dislocations both in two [3] and three dimensions [4]. Finally, some experimental implications of our classification scheme will be considered.

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How to Build a Proportional Cell

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Abstract. The cell, which is the fundamental unit of life, is not a bag of chemicals. Instead its various functions are spatially segregated among micron-sized compartments. For example, the nucleus stores and processes genetic information while the cytoskeleton provides tracks for intracellular transport. The size of these organelles affects their function and is under precise control by the cell. A widely discussed mechanism of size control, for which there is growing experimental evidence, is a limited pool of molecular building blocks. In this talk I will consider the limitations that physics of diffusion imposes on this simple mechanism. In light of these theoretical results I will discuss experiments on actin patches and cables in yeast cells, which provide examples of how nature circumvents these limitations. These experiments and related theory provide general ideas about how cells measure and control the size of their organelles.

Resistive Switching Mechanism In Nanostructural Functional Oxides

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Abstract. Electronic properties of nanostructural functional oxides attract a lot of interest in nanoscience due to their rich physics. Local transport properties (I-V characteristics) exploring NP/perovskite oxide interfaces is of crucial importance for both, the study of the resistive switching mechanism and the development of new resistive memories. Hysteretic I-V curves in $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films [1] can be used to identify the nature of the resistive switching process. We present recent results on iron-oxide/manganite nanostructures (Fe-NP/LSMO), studied using conductive scanning force microcopy. Assembly of nanoparticles, prepared by RF sputtering [2], exhibits at room temperature a voltage-current hysteresis with four different states: initial, electroformed, IN and OFF (Figure 1). Such behaviour could be interpreted in terms of two simultaneous bipolar responses, associated to two existing interfaces (tip/NP and NP/manganite) and their corresponding Schotcky's barrier.

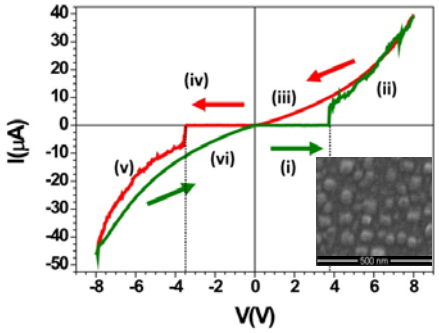

FIGURE 1. Figure illustrating typical I-V characteristics of Pt/Fe-NP/LSMO system presented in linear scales. The voltage sweep direction and current response is indicated by arrows and roman numbering.

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Soft Confotronics

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Abstract. Soft confotronics is an emergent branch of molecular biophysics that investigates collective conformational states of large assemblies of bio-molecules (monomers) forming regular functional superstructures. The interacting conformational states of the monomers give rise to new phenomena, only present in the assembled superstructures and performing tasks that a single unit cannot. After reviewing several biophysical examples, like switchable actin filaments and microtubules, we move towards fully synthetic bio-inspired systems , including switchable, energy storing topological gels and information transmitting "confotronic fibers" that are presently being developed.

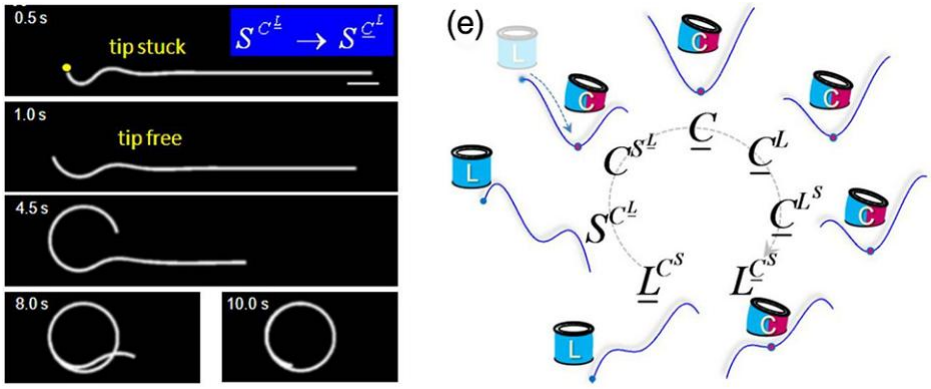

FIGURE 1**.** A microtubule gliding on kinesin motors undergoes a mechanical hysteresis loop due to a mechanical switch of the tubulin dimer conformation [3].

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Raman Scattering in Iron-Based Superconductors and Related Materials

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Abstract. The discovery of superconductivity in F -doped LaFeAsO in 2008 brought a new excitement to the field of superconductivity. In the months following the initial report, numerous superconducting iron-based compounds have been found and categorized into several sub-classes. The class of iron-chalcogenide superconductors shows an exceptional variety of features, such as the existence of the excess Fe atoms or Fe vacancies, different types of magnetic order in the normal state, intrinsic phase separation and, possibly, a novel paring mechanism. We present the results of a comprehensive polarization and temperature dependent Raman scattering study of iron-chalcogenide superconductors and related materials. Special emphasis will be placed on the intrinsic phase separation in the alkali-doped iron-selenides. Clear evidence of phonon modes renormalization due to electron-phonon and spin-phonon interactions is presented.

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Magnetism and Relativistic Effects in Functional Oxides

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Abstract. One of the very lively research fields in condensed-matter physics is focusing on transition-metal oxides (TMO), due to a large variety of interesting physical properties they posses. For example, multiferroic materials, possessing both ferroelectric and ferromagnetic order in the same phase, are interesting both in basic research and in numerous applications, e.g. for data storage and writing. A further topic in the physics of TMO is connected to their conducting properties: what determines whether a TMO will be insulating or metallic is not an easy question, owing to the complexity of physical effects that play a role in such systems. In 3*d* compounds, the enhanced onsite Coulomb repulsion often pushes the system into an insulating state. In 5*d* TMO the Coulomb repulsion is reduced, but its interplay with the spin-orbit coupling can drive the so-called spin-orbital Mott transition, resulting, again, in the insulating behavior. We use first-principles calculations to investigate the various phenomena in TMO in bulk and in the form of thin films [1-4]. In this talk, we will consider the TMO in perovskite structure, containing the heavy 5*d* transition-metal elements. We will discuss their magnetism and the role of the spin-orbit coupling in their physical properties and in possible applications.

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Organic and printed Photovoltaics: Process and in-line optical monitoring

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Abstract. Organic and printed photovoltaics (OPVs) onto plastic substrates have attracted an enormous interest in the modern science & industry, due to their several advantages that include conformability to curved surfaces and potentiality for fabrication by low-cost production processes such as roll-to-roll (r2r) printing. One of the main factors that determines the achievement of high OPV efficiency is the optimization of the morphology of the photoactive layer, which is a blend of a polymer electron donor and a fullerene-based electron acceptor. Also, the optimization of the quality of the OPV printed nanomaterials (organic semiconductors, transparent electrodes, barrier nano-layers etc.) onto flexible polymer substrates is a prerequisite for the achievement of the required performance, efficiency and lifetime of OPVs that will enable their wide market exploitation. In this presentation, we provide an overview of the latest advances on the fabrication of advanced nanomaterials for OPV applications by r2r printing methods, in combination with laser scribing (in both sheet-to-sheet and roll-to-roll configurations) of the different OPV layers (transparent electrodes, photoactive layers, metal electrodes). The methodology for the combination of the different printing and structuring techniques will enable the low-cost fabrication of OE devices for several consumer applications. Also, we present the novel methodology for the combination of in-line Spectroscopic Ellipsometry (SE) working in the near infrared to visible and far ultraviolet spectral region and Raman Spectroscopy (RS) for the robust investigation of the optical properties, morphology and bonding structure of r2r printed OPVs. Finally, we demonstrate the potentiality of SE and RS to be used as standard tools for the in-line robust determination of the thickness, optical and structural properties and the quality of other thin films and nanolayers for many organic and printed electronics applications.

Spectroscopic And Scanning Probe Microscopic Investigations And Characterization Of Graphene

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Abstract. Graphene synthesized by various techniques has different properties. Here we give an overview of several graphene synthesis techniques and device fabrication processes; as micromechanical exfoliation, fabrication of free standing membranes, chemical vapor deposition, liquid phase exfoliation, Langmuir-Blodgett assembly, wet transfer, shadow mask and UV photolithography. We employ various scanning probe and optical spectroscopy techniques to determine how these different fabrication processes affect properties of graphene, and present advantages and drawbacks for various applications.

In particular we focus on optical properties of graphene obtained using spectroscopic ellipsometry, and how these are altered by the interaction with an ambient [1], or various dielectric and metallic substrates [2], or by different fabrication processes [3]. We highlight how transfer residue and sample annealing affect optical properties of graphene [3], as well as how the interaction between graphene and a gold substrate can be observed through spectroscopic ellipsometry and Kelvin probe force microscopy [2]. In addition, we demonstrate how graphene can be manipulated by an atomic force microscope, using dynamic plow lithography [4].

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Potential of helically coiled carbon nanotubes for sensing applications

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Abstract. Carbon nanotubes (CNTs), due to their extraordinary mechanical, electrical, optical and electromechanical properties, are promising candidates for sensitive elements in commercially viable nanodevices.

Depending on the structure, straight CNTs can exhibit either metallic or semiconducting behavior. The high elasticity of the covalent carbon-carbon bond allow single-walled carbon nanotubes (SWCNTs) to return, even from a strong deformation, to its original state. Young modulus of CNTs is in the range of 1 TPa. Apart from being stiff, strong and elastic, CNTs are also extremely light, which promotes them as ideal nano-sized beams for resonant mechanical sensors: tunable CNT resonators as strain/stress sensors or resonant inertial balances for small mass detection. Several percents of strain induces a decrease in conductance of SWCNTs for more than two orders of magnitude. Effective piezo-resistive gauge factor of semi-conducting SWCNTs is reported to be of order of 10^3. SWCNTs are optically active materials which only absorb and emit light linearly polarized along their axes, so that they can be applied in devices such as polarized photo-detectors.

Helically coiled carbon nanotubes (HCCNTs), combining peculiar helical morphology and fascinating properties of nanotubes, exhibit many exceptional properties as well. However, due to the difference in morphology, HCCNTs only to a certain extent retain the properties displayed by the straight CNTs and exhibit several novel properties, specific to the coiled morphology (semi-metallic HCCNTs with high electronic DOS at Fermi level, superelasticity, NanoVelcro, high anisotropy of thermal expansion, etc.)

Here, we explore the potential of HCCNTs for sensing applications: tunable nano-mechanical resonators in mass and strain sensors, sensitive piezo-resistive pressure sensors and piezo-resistive detectors of resonant motion of nanomechanical resonators, photothermal thermoelastic actuators and optically-based tactile sensors with highly sensitive discriminatory abilities. In particular, we calculate sensitivity, gauge factors and quality factors of HCCNT piezo-resistors and examine fundamental modes of vibration and mass detection sensitivity of cantilevered and doubly clamped HCCNT resonators, as well as intrinsic energy dissipation of the latter, comparing it to the dissipation characteristics of the straight CNT nanoresonator counterparts. Finally, we make comparative analysis of the performances of HCCNT-based and straight CNT-based nanosystems. Our calculations predict the utility of HCCNTs for sensing applications.

Emergent Phenomena in Multigap Superconductors

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Abstract. Multiband/gap superconductivity is emerging as a complex quantum coherent phenomenon with physical consequences which are different from or cannot be found at all in single-gap superconductors. This became particularly relevant after the recent discoveries of predominantly multi-band/gap superconducting materials, e.g. transition metal-borides, iron-pnictides and chalcogenides. In these materials the cross-pairing between bands is typically disfavored energetically, hence multiple coupled condensates coexist, hybridize and govern the overall superconducting behavior. The increased number of degrees of freedom allows for novel effects which are unattainable otherwise. For recent Special Issue of Superconductor Science and Technology devoted to this topic, please see [1].

In this talk, I will focus on few such effects, and discuss their theoretical predictions, simulations and experimental evidences. In particular, I will discuss the emergence and stabilization of fractional-flux vortices [2], their dynamics and observation in magnetic and transport measurements, then hidden criticality [3] where length-scales of involved condensates can become radically disparate [4], unusual magnetic behavior that cannot be classified into standard types [5] and can lead to e.g. giant paramagnetic response [6], and the first prediction of type-I behavior in known multigap compounds.

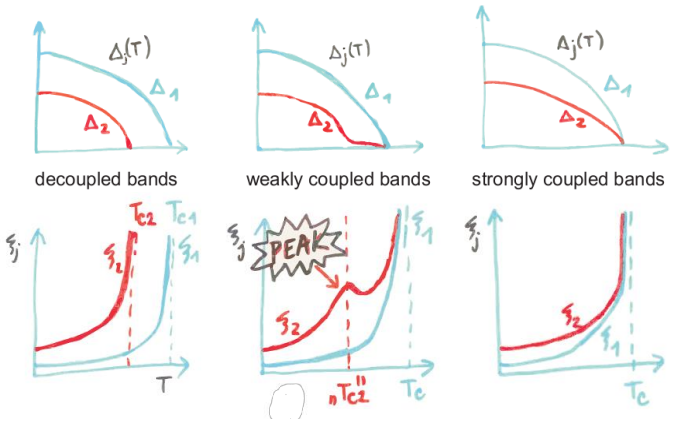

Figure 1. Cartooned illustration of the phenomenon of hidden criticality in two-gap superconductors, and the related behavior of the length-scales.

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The Quantum Hall Bilayer at Intermediate Distances

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Abstract. We will reconsider the description of the quantum Hall bilayer at the filling factor one at intermediate distances. The basic description of the bilayer with respect to the distance between the layers, with a (pseudo)magnetic phase for small distances and Fermi-liquid-like phase for large distances in the phase diagram, parallels the description of many strongly correlated materials. Moreover, there are suggestions to view the intermediate region as a pairing state of composite fermions [1] . We will discuss a possibility that this phase can be also viewed as a critical phase of paired composite bosons, in which still some ordering of the nearby magnetic phase is present.

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Modeling Graphene Interactions With Electrolyte

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Abstract. While the experimental investigation of graphene-based materials for applications in biochemical sensors has been rapidly accelerating over the past few years [1], theoretical modeling in the electrochemistry of graphene is still in its infancy. In those applications graphene typically operates in the configuration of a field-effect transistor (FET) with its surface exposed to an electrolyte containing mobile ions [2,3]. By applying the gate potential through an aqueous solution one can efficiently measure the quantum capacitance of graphene [2] or achieve good control of graphene's conductivity that is extremely sensitive to the presence of adsorbed bio-molecules, ion concentration, or the pH in the electrolyte [3]. However, graphene is usually supported by an insulating substrate, such as SiO_2, which may contain a large density of charged impurities that also affect graphene's conductivity [4]. After reviewing some experimental aspects of the interaction of graphene FETs with electrolyte, we shall present several recent developments in using the continuum electrochemical models [5] to describe the interface of graphene and aqueous electrolyte [6-8]. In particular, we shall discuss the effects of finite size of dissolved ions [6] and dielectric saturation of water on the capacitance of graphene [7], as well as cooperative screening of charged impurities in the underlying oxide by both the charge carriers in graphene and the mobile ions in the solution [3,4,8]. In addition, we shall describe some interesting effects of the nearby aqueous solution on Dirac plasmons in graphene.

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Quantitative Study and Modeling of Collective Knowledge Building via Questions and Answers

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Abstract.
Collective knowledge building is a socio-cultural process which takes place trough self-organized dynamics of interactions among individuals with limited level of expertise. Question and Answers (Q&A) sites are excellent repositories of collective knowledge and provide a proper environment where the dynamics of collective knowledge building can be studied. On these sites individuals engage in collaborative solving of specific problems by asking, answering and commenting questions. By combining the stochastic model with the empirical analysis of data from Q&A, we show that collective knowledge emerges as a collective phenomena in large network of actors and artefacts. We examine this collective behaviour by measuring the information divergence and advance of knowledge over time and by analysing the characteristic self-organisational patterns. We also examine the structure of connections and formation of communities with the respect to the level of expertise in the system, which we vary within the model. Our results show that the dynamics of collective knowledge building is strongly influenced by the distribution of expertise in the system.

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Majorana Fermions in Ferromagnetic Atomic Chains on a Superconductor

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Abstract. Majorana fermions are zero-energy excitations predicted to localize at the edge of a topological superconductor, a state of matter that can form when a ferromagnetic system is placed in proximity to a conventional superconductor with strong spin-orbit interaction. With the goal of realizing a one-dimensional topological superconductor, we have fabricated ferromagnetic iron atomic chains on the surface of superconducting lead [1]. Using high-resolution spectroscopic imaging techniques, we show that the onset of superconductivity, which gaps the electronic density of states in the bulk of the chains, is accompanied by the appearance of zero-energy end-states. This spatially resolved signature provides evidence, corroborated by other observations and theoretical modeling [2], for the formation of a topological phase and edge-bound Majorana states in this system. Our results demonstrates that atomic chains are viable platform for future experiments to manipulate Majorana bound states and to realize other 1D and 2D topological superconducting phases [3].

This work has been performed in collaboration with I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig and A. Yazdani.

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Spin-orbit torques in topological-insulator/ferromagnet heterostructures

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Abstract. Topological insulators (TIs) are recently discovered class of "Dirac materials" which possess an energy gap in the bulk, akin to conventional band insulators, while hosting metallic edge [in two dimensions (2D)] or surface [in three dimensions (3D)] states. Their low-energy quasiparticles behave as massless Dirac fermions whose spins are locked to their momenta due to strong surface spin-orbit coupling (SOC) of the Rashba type, which is effectively orders of magnitude larger than its more familiar counterpart in two-dimensional electron gases. The TIs have attracted considerable attention by the basic research communities, because of offering a platform to probe exotic particles borrowed from high energy physics (such as axions, magnetic monopoles and Majorana fermions), as well as by the applied research communities interested in spintronics, thermoelectrics and quantum computing. This talk will discuss theoretical and computational modeling of *nonequilibrium* phenomena on the surface of current-carrying 3D TIs with and without ferromagnetic (F) overlayer, which are of interest to spintronic applications. In the absence of F overlayer, injected unpolarized charge current drives nonequilibrium spin texture on the surface (the so-called Edelstein effect), as well as within a thin layer underneath due to injection of evanescent wavefunctions from the surface into the bulk. In the presence of F overlayer, nonequilibrium spin accumulation can change its direction due to the coupling to magnetization, as well as cause magnetization dynamics when electrons polarized by the surface SOC flow into the F overlayer to impinge SO torque on it. By decoupling slow magnetization from fast conduction electrons, the classical dynamics of magnetization can be described by the Landau-Lifshitz-Gilbert-type equation whose terms are extracted from nonequilibrium Green functions for electrons. The SO torque can also be generated in vertical TI/F heterostructures where electrons tunnel through a thin TI layer and flow perpendicularly through the TI/F interface.

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Kondo Topological Insulators

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Abstract. Samarium hexaboride (SmB_6), a "heavy fermion" material, appears to be a topological insulator (TI). The latest neutron scattering experiment [1], interpreted by a perturbative slave boson theory [2], reveals both the strong correlations and non-trivial topology of SmB_6. Such heavy-electron correlations could have various novel imprints on the topologically enhanced dynamics. One could view the topologically protected surfaces of heavy fermion TIs as two-dimensional Dirac "heavy fermion" systems. Quantum criticality spanning Fermi and non-Fermi liquid metallic states, magnetic orders, unconventional superconductivity, and exotic algebraic or non-Abelian spin liquids can be anticipated on adequately prepared Kondo TI boundaries [3]. Both perturbative and non-perturbative field theory approaches applied to a Kondo TI surface model provide at least qualitative descriptions of these states. A related interesting system are quantum wells made from Kondo or other correlated TIs [4–6]. These fully gapped two-dimensional systems could additionally host SU(2) vortex lattices [7], as well as non-Abelian incompressible quantum liquids of novel type whose description requires a generalization of the well-known Chern-Simons theory [8].

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Non-Abelian Topological Orders in Quantum Hall Bilayers

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Abstract. Condensed matter systems whose emergent excitations possess the non-Abelian statistics have attracted much interest in recent years. Here we discuss two recent examples of systems that are expected to realize such non-Abelian topological phases. One of them is the zeroth Landau level ("octet") of bilayer graphene, where an incompressible quantum Hall state has recently been observed at filling $\nu = -1/2$. By modeling the effect of screening and Landau level mixing, which play an important role in bilayer graphene, we show that this fractional state is related to the $\nu = 5/2$ "Pfaffian" state in GaAs [1]. As a second example, we consider a semiconductor bilayer heterostructure with filling $\nu = 1/3$ per layer. We find that this system also supports a non-Abelian phase that we identify as the "interlayer Pfaffian" [2]. In addition to the non-Abelian statistics similar to the $\nu = 5/2$ state, the "interlayer Pfaffian" also exhibits a novel form of bilayer-spin charge separation. An important aspect of these two states for future experimental studies is their high degree of tunability, either by varying the interlayer distance and tunneling, or by the perpendicular electric field in bilayer graphene.

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Superconducting and Normal States in Iron Chalcogenides

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Abstract. Iron based superconductors have been attracting considerable attention since their discovery in 2008 [1]. In particular, alkali-doped iron selenide materials have recently emerged to the frontier of research due to critical temperatures (Tc's) that exceed Tc's in iron arsenides [2,3]. In this talk I will discuss the pair breaking mechanism and the normal state above H_{c2} in $K_xFe_{2-y}Se_2$ superconductors in high magnetic fields as T → 0 [4-5]. The discussion will be centered on the peculiarities of the crystal structure [6-10] and on its perturbations by Ni and Co substitution [12].

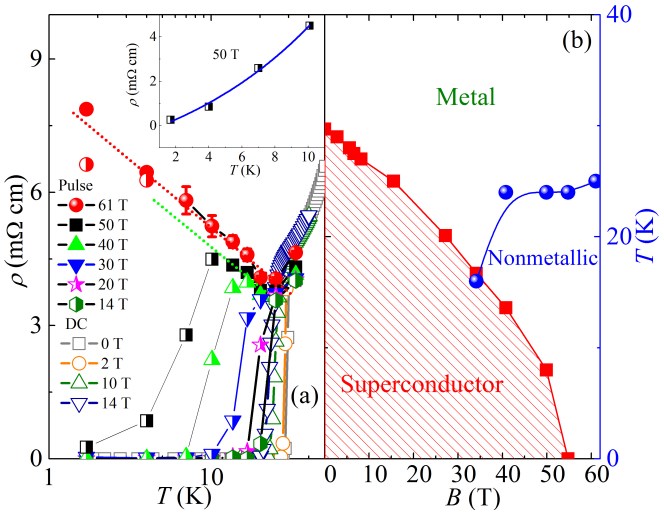

FIGURE 1. (a) Temperature dependence of the in-plane resistivity in several DC (open symbols) and pulsed (filled symbols) magnetic fields for temperatures between 1.75 and 100 K. Pulsed-field data (filled symbols) near Tc are consistent with results in DC and zero fields (open symbols). The two half-filled symbols for 61 T at 1.75 and 4 K denote the extrapolated values of the resistivity after complete suppression of the superconductivity. The red and green dashed lines are the linear fitting result for the 61 T data and 50 T data when using the logarithmic scale, respectively. Inset: Resistivity of the mixed state in a 50-T field. The blue dotted line is an exponential fitting result (see text). (b) The schematic temperature-field phase diagram of $K_{0.70}Fe_{1.46}Se_{1.85}Te_{0.15}$.

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Quantum Criticality and Far-from-Equilibrium Dynamics in Strongly Correlated (Quasi-) Two-Dimensional Electron Systems

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Abstract. Many unusual properties of various strongly correlated materials have been attributed to the proximity of quantum critical points and the presence of several competing degrees of freedom. There is also increasing evidence that far-from-equilibrium (or glassy) behavior may underlie many complex phenomena exhibited by these systems. In fact, glassy dynamics may very well be the smoking gun manifestation of this emerging complexity. For example, there is ample evidence for the emergence of glassy charge dynamics near the 2D metal-insulator transition in semiconductor heterostructures, resulting from the interplay of Coulomb interactions and disorder [1].

This talk will focus on the La-based family of copper-oxide high-temperature superconductors, which are quasi-2D systems, and describe several experiments designed to probe the nature of the ground states, the transitions between them and the associated dynamics. The goal is to elucidate the interplay of charge, magnetism, and crystal structure, as well as roles of disorder, quantum and thermal fluctuations, in these complex materials. Studies include a combination of transport and time-resolved measurements carried out over a wide range of temperatures and magnetic fields. These techniques have been applied to quantum phase transitions, such as doping-driven [2] and magnetic-field-tuned superconductor-insulator transitions [3], as well as to thermally-driven transitions between various phases [4]. In all cases, there is evidence for the emergence of dynamical heterogeneities or far-from-equilibrium dynamics in the critical regions; examples will be discussed as time permits. The particular form of the dynamics that is identified in these materials and the observed critical behavior put strong constraints on the types of theories that can describe La-based cuprates.

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Functional Oxide Nanowires For Thermoelectric Applications

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Recently we discovered a novel method to produce $M_2O_3(ZnO)_n$ polytypoid nanowires (MZO, where M could be In, Ga, Fe, and other tri-valent metals) by a facile solid state diffusion process and to control their microstructure at atomic level. Due to to the decoupling of certain electrical and thermal properties, these polytypoid nanowires, which contain periodic compositional and structural features, typically on the nanometer scale, are promising materials for a variety of applications, including thermoelectrics. The efficiency of energy conversion in thermoelectrics is related to the material-dependent figure of merit, $zT=S2\sigma T/k$, where S, σ, T, and k represent the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity, respectively. The prediction theoretically that low dimensional materials can be increase zT can be attributed to two factors: electronic band structure changes (increasing the Seebeck coefficient) and enhanced interface phonon scattering. Using high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) imaging we performed a detailed structural analysis on the $In_{2-x}Ga_xO_3(ZnO)_n$ nanowires. HAADF imaging of a IGZO nanowire reveled the presence of In-enriched monoatomic layers of indium perpendicular to the [002] direction, separated by wurtzite $MZn_nO_{(n+1)}^+$ slabs of varying thickness. The O atoms on the edges of the MO_2^- octahedral layers are each bonded to three In/Ga atoms and one metal atom within the $MZn_nO_{(n+1)}^+$ layer. This creates an inversion domain boundary (IDB) in the wurtzite lattice since the Zn-O bonds on either side of the octahedral layer point with the O atoms toward the In/Ga layer (tail-to-tail configuration). The MO_2^- inclusion layer is also associated with a stacking fault, and the wurtzite lattice on one side of the In/Ga layer is translated by ⅓<100>. In some of the nanowires, partial In/Ga inclusions were also observed. The ends of these partial inclusions are associated with edge dislocations with the dislocation line lying at the leading edge of the MO_2^- plane. Moiré images taken along the 002 and 102 reflections confirmed the presence of the edge dislocations. The HAADF imaging allowed us to unambiguously determine the location of indium within the structure and enabled us to evaluate lattice strain and the presence of defects. Based on this analysis we propose that the superlattice structure is generated through a defect-assisted process. One of the greatest advantages of this novel synthesis is the ability to tune the nanoscale features of the polytypoid wires by simply adjusting the amount of metal precursor. Using HAADF imaging we were also able to perform a quantitative analysis of the change in superlattice inclusion density and periodicity with metal deposition. In summary, $M_2O_3(ZnO)_n$ polytypoid nanowires were converted from pure ZnO nanowires using a simple diffusion process that can be used to produce a wide range of ZnO alloys with controllable alloy concentration and inclusion layer density. The single layer inclusion growth is originated from the surface and propagates though the nanowire by a defect-assisted process. From this study it is apparent that better control of nanometer-scale features could be the key to developing next-generation thermoelectric materials.

Long Range Spin-Triplet Proximity Effect in Ferromagnetic Bilayers

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Abstract. We have predicted a dominant second harmonic in the current-phase relation, $I(\phi) \propto \sin(2\phi)$, of SFF'S Josephson junctions with conventional (s-wave) superconductors and two highly unequal ferromagnets with noncollinear magnetizations [1], see Fig. 1(a). This is a manifestation of the long range spin-triplet proximity effect in ferromagnetic bilayers where the first harmonic is suppressed [2] and the phase coherent transport of two Cooper pairs becomes dominant [3,4]. Effect is also accompanied by distinctive two-peak structure in energy dependence of electronic density of states [5], see Fig. 1(b), which can be detected in the tunneling spectroscopy. Although we have considered clean and moderately diffusive ferromagnets, the effect persists in diffusive systems as well [6]. It has been observed recently in insulating ferromagnetic bilayer [7]. The half-periodicity of $I(\phi)$, like at 0-π transitions, can be used for "silent" quantum interferometers (SQUIDs) in the absence of an external magnetic field, and for superconducting spintronics [8].

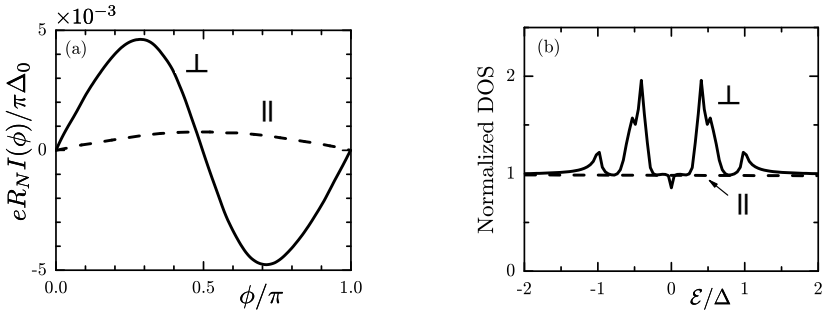

FIGURE 1. (a) The Josephson current – phase relation for an asymmetric (magnetic influence ratio 1:100) SFF'S junction with parallel (∥, dashed line) and orthogonal (⊥, solid line) magnetizations [1]. (b) Normalized electronic density of states in the middle of the thick (strong) F' layer as a function of energy near the Fermi level [5]. Moderately diffusive case is shown (electronic mean free path in ferromagnets $l = 200k_F^{-1}$) at low temperatures ($T/T_c = 0.1$).

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Quantifying Self-Organization and Complexity in Complex Systems

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Abstract. A multifaceted framework for the study of complexity and self-organization in nonlinear systems is developed based on the wavelet Hidden Markov Model [1]. The method uses the concept of statistical complexity which defines complexity as the minimum information necessary for optimal prediction. The optimal wavelet basis is chosen as the one which maximizes complexity while self-organization is defined as the complexity increasing in time (or across scales). This framework simultaneously manages several important issues related to the nonlinear and multiscale phenomena involved, namely it:

- Chooses the optimal template wavelet for the analysis of temporal or spatiotemporal data
- Detects parameter values at which bifurcations occur
- Quantifies complexity and self-organization of the dynamics
- Enables short-term prediction of nonlinear dynamics
- Extracts coherent structures in turbulence by separating them from the incoherent component.
-Removes noise effectively in the data generated by nonlinear processes

In order to illustrate the method we analyze the well known chaotic systems such as the logistic and tent maps, etc.. Further on, the first two aspects, namely determination of the optimal wavelet and the detection of changes in the dynamics of a nonlinear system are illustrated by analyzing the Stimulated Raman Scattering (SRS) in a bounded, weakly dissipative plasma [2]. We also show the advantages of the method by analyzing self-organization in fusion plasmas based on experimental data and also based on the numerical simulations of the Gyrokinetic Vlasov model of plasma dynamics. Additional example of the application includes detection of art forgery and recognition of creative artistic work in paintings. Finally, we present the extension of this method to simplicial networks (simplicial complexes obtained from complex networks).

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Josephson Superconductor/Ferromagnet Systems: From Sandwiches to Planar Structures

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Abstract. Josepson hybrids based on superconductors (S), normal metals (N) and ferromagnets (F) attract increasing attention in the last decade [1-7]. The most interesting and important observations were made mainly on S/F/S sandwiches [3-7]. Among them it should be noted the implementation of π-junction [3-5], observation of the spin-triplet superconductivity [6], realization of SFS switches for ultra-low-power, high-density cryogenic memorie [7]. Modern fundamental and applied researches make the actual implementation and study of planar multiterminal S/F/N structures. Planar Josephson S-(F/N)-S structures with complex bilayered (F/N) barriers were proposed recently in [8] and realized in [9]. The structure, which we studied in [9], included a Cu/Fe bilayer forming a bridge between two superconducting Al electrodes. The appreciable critical current was detected up to 120 nm of the bridge length. It was observed a double-peak peculiarity in differential resistance of the S-(N/F)-S structures at a bias voltage corresponding to the superconducting minigap. The splitting of the minigap was explained by the electron spin polarization in the normal metal which was induced by the neighbouring ferromagnet. Our new observations are related to quasiparticle- and spin-injection to banks and barriers of planar Josephson junctions**.**

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Dissipative Solitons in Cellular Microtubules

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Abstract. Microtubules are the most regular and symmetric polymer protein structure in living cells. They possess quasi–one–dimensional cylindrical geometry and are typical soft matter objects. Softness of interaction leads to non-linearity. All these circumstances provide safe conditions for collective mechanical and electrical oscillations yielding to creation of localized solitary waves which propagate along these biopolymers. The dissipative effect is partly compensated by the action of intrinsic electric fields directed along cylinder.

Summary. Microtubules (MTs) are mayor cytoskeletal protein polymers assembled of identical units called tubulin α–β heterodimers. They have a helical lattice pattern with left–handed chirality forming hollow cylinders, see Fig. 1. The outer and the inner radius of a MT cylinder are 25 nm and 15 nm, respectively. The lengths of MT can span from the order of micrometers to millimeters. MTs form an important part of the cellular scaffold and provide a network of "rails" for active intracellular transport by motor proteins. By possessing the high symmetry and regularity as well as being typical soft matter objects, MTs are the true candidates for sustaining nonlinear excitations and waves. We realized that above properties could be the preconditions for appearance of mechanical, electrical and mechano–electrical localized excitations which could propagate along MTs. These excitations have properties of dissipative solitons due to the viscosity of cytosol in which MTs are immersed. These excitations appear to have very important roles in signaling and transport phenomena in cell's physiology. We will demonstrate the physical basis and the essence of mechano–electrical and electrical solitons generated in MTs.

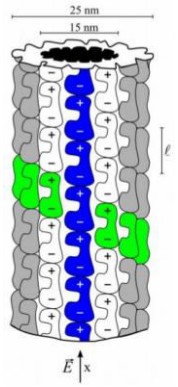

FIGURE 1. The MT's hollow cylinder of 13 parallel protofilaments with denoted characteristics dimension: outer and inner diameters of 25 nm and 15 nm, respectively, and with tubulin heterodimer length of l = 8 nm. The protofilament is blue and left–handed chirality is indicated by green color. E is the intrisic electric field.

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Flocks on a sphere: Effects of curvature on active collective motion

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Abstract. In this talk we show that coupling to curvature has profound effects on collective motion in active systems, leading to patterns not observed in flat space. Biological examples of such active motion in curved environments are numerous: curvature and tissue folding are crucial during gastrulation, epithelial and endothelial cells move on constantly growing, curved crypts and vili in the gut, and the mammalian corneal epithelium grows in a steady-state vortex pattern. Using Brownian dynamics simulations, we study a model of self-propelled particles with polar alignment on a sphere. Hallmarks of these motion patterns are a polar vortex and a circulating band states arising due to the incompatibility between spherical topology and uniform motion - a consequence of the hairy ball theorem. Furthermore, inspired by recent experiments of Baush and Dogic groups on droplets coated with actively driven microtubule bundles, we address active nematic systems confined to the surface of a sphere.

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Spanning Avalanches As Extreme Events In Two-dimensional Random Field Ising Model

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Abstract. A Numerical and a finite-size scaling analysis of the spanning avalanches as extreme events in a two-dimensional (2D) nonequilibrium zero-temperature random field Ising model is presented. The analysis, performed for distributions of various characteristics of spanning avalanches, shows that subcritical 2D-spanning avalanches play a dominant role in model behavior below and at the critical disorder.

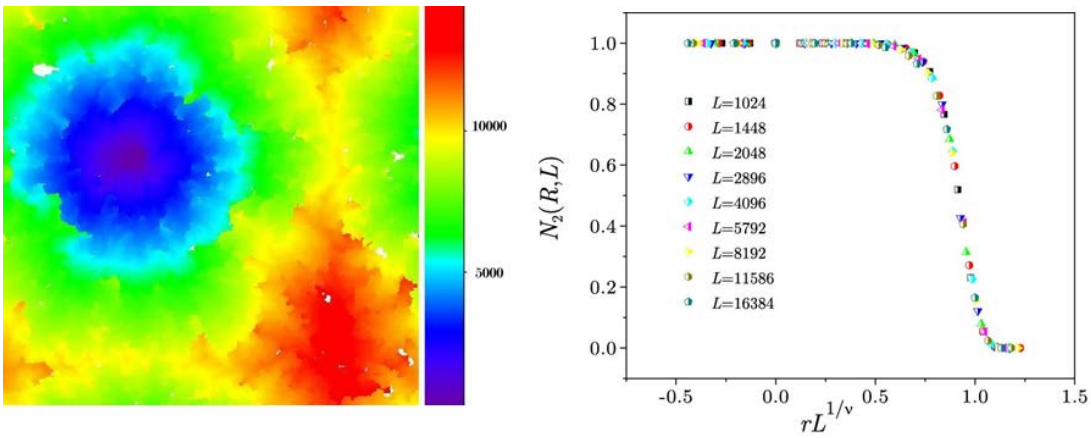

FIGURE 1. Left: time evolution of a subcritical spanning avalanche. Right: scaling collapse of the number $N_2(R,L)$ of 2D-spanning avalanches in the 2D model versus reduced disorder $r=(R-R_c)/R$ scaled by the system size L.

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Spin-electric Coupling in Molecular Magnets

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Abstract. Molecular magnets behave as large spins at low energies. They show hysteresis controlled by quantum tunneling of magnetization, long spin coherence times, and spin texture in the ground state. Coupling of molecular spins to an external electric fields would provide a superior mechanism for their control and manipulation. In triangular low-spin antiferromagnets with broken inversion symmetry it is the chirality of spin texture that couples to electric fields. We show that the chirality has long coherence time, and that it allows for a controllable superradiant phase transition.

Hyperfine-induced decoherence in a triangular spin cluster varies across independent two-level subsystems that encode a qubit. Electrically controllable eigenstates of spin chirality show decoherence times that approach milliseconds, two orders of magnitude longer than those estimated for the eigenstates of the total spin projection and of the partial spin sums. The robustness of chirality is due to its decoupling from components of both the total spin and individual spins in the cluster.

A crystal of triangular molecular antiferromagnets coupled to a resonant cavity shows superradiant phase transition. The critical coupling strength for transition depends on the external magnetic field, in sharp contrast to the standard case of two-level emitters, where the critical coupling was set by the structure of emitter alone. The source of modification is traced to the entanglement of spin and chirality in the low-energy states of the cluster.

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Defect-Induced Magnetism in Graphene

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Abstract. The search for evidence of the magnetic ordering in graphene has been an active field of research for last ten years and has focused primarily on point and line defects as the most promising candidates for engineering magnetism in graphene. Vast majority of the studies where theoretical due to challenges in experimental efforts to control defects in graphene, combined with the problems to capture weak magnetic signals from prepared samples. Here we give an overview of recent experimental and theoretical results, including our studies of magnetism in graphene induced by adsorbates like hydrogen and fluorine. At variance to a weak paramagnetism induced in graphene by mono-vacancies or H atoms, we found a strong interaction between magnetic moments which emerge in graphene upon F adsorption. However, we have not observed any type of long ranged magnetic ordering.

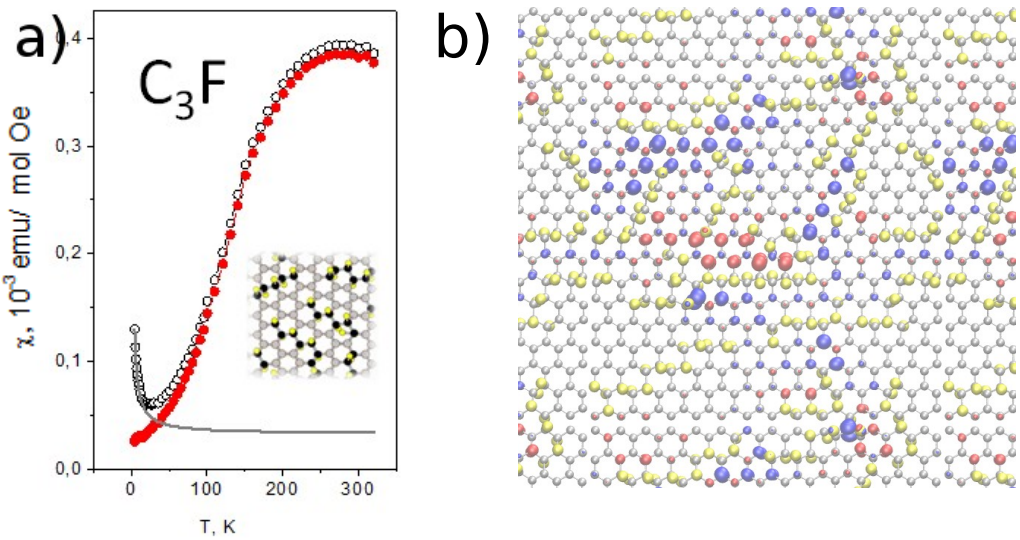

FIGURE 1. a) Magnetic susceptibility of fluorinated graphene and b) the corresponding structural model from density functional theory calculations with iso-surfaces of induced spin density. Regions with opposite spin orientation are painted in blue and red. Carbon and fluorine atoms are shown as gray and yellow spheres, respectively.

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Size And Shape Control In The Synthesis Of Nanosized Particles

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Abstract. Until very recently, the synthesis of nano and micro-sized particles with specific, well-defined properties was an empirical enterprise, resulting in the compilation of a systematic list of practical but incompletely understood protocols and procedures. These procedures have been designed to produce nanocrystals of uniform size and establish experimental control over their mean sizes. Despite impressive experimental advances, little theoretical work was done on quantitative modeling because particle synthesis includes several multi-scale kinetic processes, including transport of matter, nucleation, growth, aggregation, surface restructuring, and detachment. Building on the classical works on nucleation theory, we describe here semi-quantitative microscopic model for nanoparticle growth and identify conditions under which size and shape selection can be achieved. Our calculations should be generally applicable for nanoparticle synthesis from supersaturated solution, when the dynamics follows the two-step development of burst nucleation followed by the diffusive growth. The model includes the qualitative explanation given in the earlier work by LaMer, but for the first time it is formulated in a way that actual calculations and comparisons with experimantal data can be carried out. Within this formulation, it is possible to derive asymptotic expressions for large-time behavior of the growth parameters and compare the results with the experiments: for illustration, we use the representative data and parameters corresponding to the growth of gold nanoparticles, shown in Fig. 1.

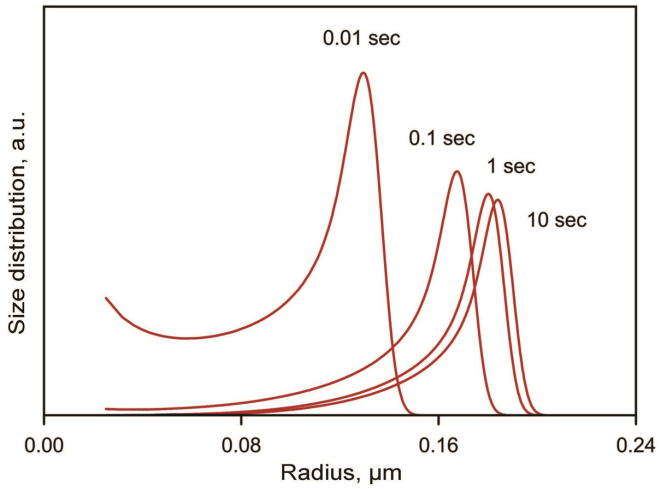

FIGURE 1. Example of a calculated colloid particle size distribution (in arbitrary units) plotted as a function of the colloid particle radius. The parameters used were for a model of formation of spherical Au colloid particles. Note the shift of the peak position with time and the reduction in the tail of distribution.

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Structure of Noise in Complex Systems Revealed by Multifractal and Graph-Theory Techniques

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In complex systems, temporal fluctuations of dynamical variables contain vital information about the fine-grain dynamics yielding the emergent collective behaviors. The collective dynamics is recognized by long-range temporal correlations, clustering of events or avalanching, and (multifractal) scale-invariance [1]. Recently, different prospectives in the understanding of complexity are opened by geometrical characterizations of the dynamical structures, from quantum systems [2] to large-scale social networks [3]. Here, we map time series into mathematical graphs, representing the manifolds in the system's phase space, and use algebraic topology techniques to investigate these graphs. We consider time series of domain-wall motion in disordered media as

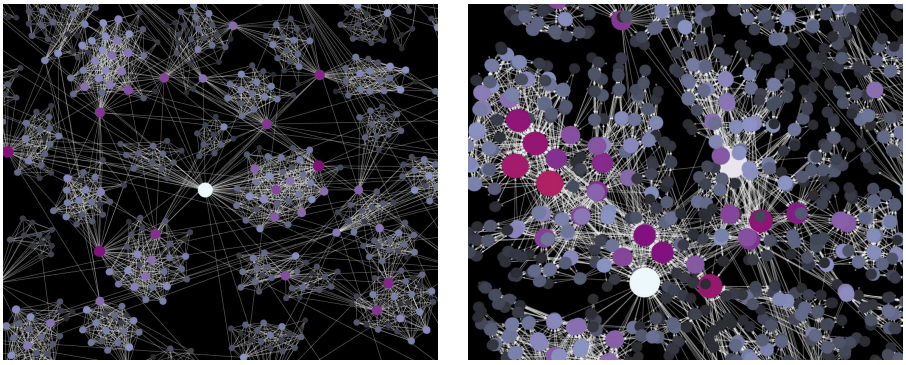

FIGURE 1. Graph presentation of time series for the nucleation (left) and domain wall dynamics (right).

well as stochastic fluctuations superimposed on a cyclic trend, occurring in social systems [4]. The multifractal analysis of time series, sampled for different driving modes, complements the study of topological spaces in the corresponding time series graphs.

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Magnetotransport Properties of Graphene van der Waals Heterostructures

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Abstract. We exploit recent experimental achievements and study transport in graphene with artificially engineered properties. In particular, breaking of inversion symmetry as well as enhancing the intrinsically weak spin-orbit coupling (SOC) was demonstrated by sandwiching graphene with other 2D materials. Although each effect leads to a gap opening in the bulk, the resulting insulating phases are topologically distinct. We demonstrate that this has two interesting implications [1,2]. On the one hand we show that orbital magnetic moments coupled to the spin degree of freedom arise when SOC is nonzero. This is analogous to valley-coupled orbital magnetic moments emerging in systems without inversion symmetry, and will reflect on conductance measurements in the presence of a magnetic field. On the other hand, the interplay of the two insulating phases leads to a spin-valley dependent gap. We show that this feat, in conjunction with a strain-induced pseudomagnetic field, can be employed for filtering pure spin-valley-locked states.

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Mott quantum criticality and bad metal behavior

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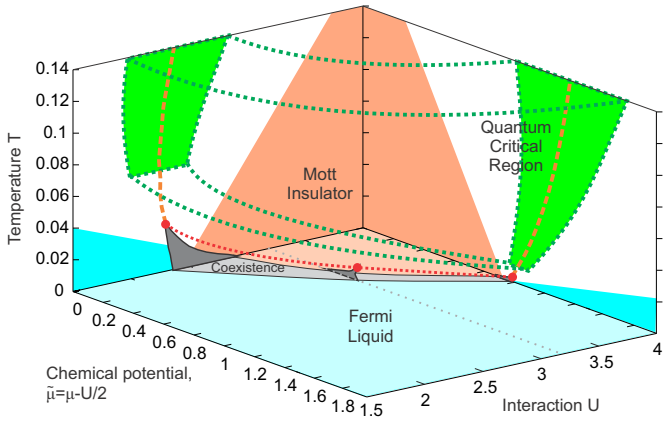
Abstract. "Bad metal" behavior featuring linear temperature dependence of the resistivity extending to well above the Mott-Ioffe-Regel limit is often viewed as one of the key unresolved signatures of strong correlation. Here we associate the bad metal behavior with the Mott quantum criticality by examining a fully frustrated Hubbard model where all long-range magnetic orders are suppressed, and the Mott problem can be rigorously solved through dynamical mean field theory. We show that for the doped Mott insulator regime, the coexistence dome and the associated first-order Mott metal-insulator transition are confined to extremely low temperatures, while clear signatures of Mott quantum criticality emerge across much of the phase diagram. Remarkable scaling behavior is identified for the entire family of resistivity curves, with a quantum critical region covering the entire bad metal regime, providing not only new insight, but also quantitative understanding around the Mott-Ioffe-Regel limit, in agreement with the available experiments.



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Organic thin film growth on various graphene substrates

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Abstract. Crystalline films of small semiconducting organic molecules offer attractive potential for optoelectronic applications on flexible substrates. However, these applications require a transparent and flexible electrode material; and here the novel material graphene (Gr) comes into play. Since small conjugated molecules like the rod-like oligophenylene molecule para-hexaphenyl (6P) fit well to the hexagonal structure of graphene, growth of 6P on Gr can be expected in a lying configuration. As observed in situ by low-energy electron microscopy, 6P grows at 240 K indeed in a layer-by-layer mode with lying molecular orientation on Ir(111) supported graphene [1]. 6P islands nucleate at Gr wrinkles [2]. At higher temperatures, needle-like 6P crystallites - also composed of lying molecules - are observed [3]. On exfoliated, wrinkle-free graphene, such needles develop with discrete orientations defined by the Gr lattice as detected by atomic-force microscopy (AFM) [4]. Interestingly, for few-layer exfoliated Gr the needle length decreases significantly with increasing layer number [5]. Growth of 6P can also be used to sense the cleanliness of large-scale, chemical vapor deposited graphene which is transferred by polymethylmethacrylate (PMMA) to all kinds of supports [6]. There, the increasing length of resulting 6P needles indicates a reduction of PMMA contaminations of the substrate with increased annealing temperature in hydrogen atmosphere. Finally, the mechanical robustness of graphene is demonstrated by AFM based dynamic plowing lithography [7].

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Entropy for Complex Systems

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Abstract. In information theory the so-called 4 Shannon-Khinchin (SK) axioms uniquely determine Boltzmann-Gibbs-Shannon entropy as the one-and-only possible entropy. Physics is different from information in the sense that physical systems can be non-ergodic. Many complex systems in fact are non-ergodic. To describe strongly interacting statistical non-ergodic systems within a thermodynamical framework, it might be reasonable to introduce generalized entropies. A number of such entropies have been proposed in the past. The understanding of the fundamental origin of these entropies and its deeper relations to complex systems has remained unclear. Non-ergodicity explicitly violates the fourth SK axiom. We show that violating this axiom and keeping the other three axioms intact, determines an explicit form of a more general entropy

$$S \sim \sum_i \Gamma(d+1, 1-c\log p_i) \tag{1}$$

All recently proposed entropies appear to be special cases. We next prove that each (!) statistical system is uniquely characterized by the pair of the two scaling exponents (c,d), which define equivalence classes for all (!) interacting and non-interacting systems, and that no other possibilities for entropies exist. The corresponding distribution functions are special forms of so-called Lambert-W exponentials containing - as special cases Boltzmann, stretched exponential and Tsallis distributions (power-laws) - all abundant in nature. We show how the phasespace volume of a system is related to its (generalized) entropy and illustrate this with physical examples of spin systems on constant-connectency networks and accelerating random walks. We are able to show that the Max Ent principle can be extended in a coherent way to certain classes of history dependent complex processes. We present several concrete examples.

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Biophysical and Biochemical Properties of Tubulin and Microtubules, Their Therapeutic Implications and Technological Potential

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Abstract. Tubulin is a mid-size hetero-dimer protein that both in vitro and in vivo forms cylindrical polymeric structures called microtubules[1]. Microtubules perform key functions in all eukaryotic cells, with the formation of mitotic spindles being perhaps the most important role in dividing cells. I will discuss the biophysical and biochemical properties of tubulin and microtubules, including their electrostatic, conductive and mechanical characteristics, which are of cardinal importance to their biological roles[2]. I will also provide a detailed analysis of the binding energy results that explain the unique assembly/disassembly properties of microtubules called dynamic instability. Finally, our atomic-level insights into the structure and function of tubulin and microtubules allow us to design novel cancer therapies and contemplate using these biological structures for nanotechnology applications.

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Electron and Electron-hole Wave Functions in a Driven Quantum Contact

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Abstract. Our work is motivated by recent experimental and theoretical advances in the emerging field of electron quantum optics where coherent electronic states are created and manipulated in mesoscopic devices [1]. We have obtained theoretically the many-body quantum state and the wave functions of electrons and electron-hole pairs in a driven quantum contact. We have checked our results experimentally by performing an electronic analog of the optical Hong-Ou-Mandel correlation experiment, where electrons emitted from the two terminals with a relative time delay collide at the contact [2]. The agreement between theory and experiment corroborates that dynamic control of elementary excitations has been achieved in the experiments at hand [3]. In particular, it has been demonstrated that a harmonic drive with ac amplitude smaller than dc voltage offset can be used to create single-electron states with a small admixture of electron-hole pairs [4]. This opens a way of engineering single-electron states with a required time profile or energy distribution that differs from the exponential distribution which is characteristic of the Lorentzian pulses. This has important applications in mesoscopic electronics and in the field of electron quantum optics.

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Bosonic Phases On The Haldane Honeycomb Lattice

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Abstract. Recent experiments [1] in ultracold atoms have reported the implementation of artificial gauge fields in lattice systems. Motivated by such advances, we investigate the Haldane honeycomb lattice tight-binding model [2], for bosons with local interactions at the average filling of one boson per site. We analyze the ground state phase diagram and uncover three distinct phases: a uniform superfluid, a chiral superfluid and a plaquette Mott insulator with local current loops. We apply bosonic dynamical mean field theory and exact diagonalization to obtain the phase diagram, complementing numerics with calculations of excitation spectra in strong and weak coupling perturbation theory. The characteristic density fluctuations and excitation spectra can be probed in future experiments.

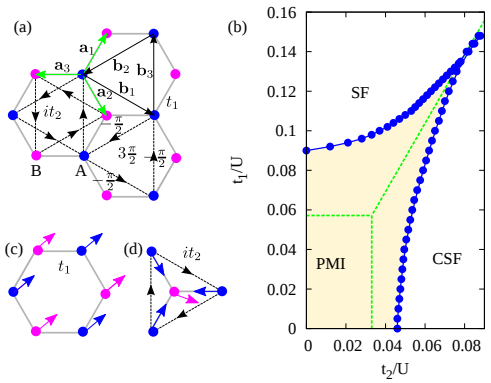

FIGURE 1. a) Lattice vectors and hopping integrals the Haldane model. b) Phase diagram of the model at unit filling, containing plaquette Mott insulator (PMI), uniform superfluid (SF) and chiral superfluid (CSF) phases. c) Local condensate order parameter in the uniform superfluid; d) In CSF the condensate order parameters on sublattices A and B are determined up to a relative phase.

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Entanglement of 3000 Atoms by One Photon

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Abstract. Quantum-mechanically correlated (entangled) states of many particles are of interest in quantum information, quantum computing and quantum metrology. Metrologically useful entangled states of large atomic ensembles (spin squeezed states) have been experimentally realized, but these states display Gaussian spin distribution functions with a non-negative Wigner quasiprobability distribution function [1]. Non-Gaussian entangled states have very recently been produced and characterized in atomic ensembles [2-4]. Here we generate entanglement in a large atomic ensemble via an interaction with a very weak laser pulse; remarkably, the detection of a single photon prepares several thousand atoms in an entangled state. We reconstruct a negative-valued Wigner function, and verify an entanglement depth (the minimum number of mutually entangled atoms) of 2,900(200) out of 3,100 atoms [5]. The achieved purity of the state is slightly below the threshold for entanglement-induced metrological gain, but further technical improvement should allow the generation of states that surpass this threshold, and of more complex Schrödinger cat states.

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Interplay of Dirac Fermions and Structural Deformations in Topological Crystalline Insulators

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Abstract. Topological crystalline insulators (TCIs) are a new class of topological materials which harbor massless Dirac surface states (SS) [1,2]. Theory postulates that these SS are protected by crystalline symmetries, and that SS electrons can acquire a mass if these symmetries are broken. Moreover, this unique crystalline protection has led to a series of intriguing predictions of strain-generated phenomena, such as the appearance of pseudo-magnetic fields and topological phase transitions. In this talk, I will present our recent scanning tunneling microscopy (STM) investigations of two TCI systems: single crystals of $Pb_{1-x}Sn_xSe$ [3,4] and strained thin films of SnTe [5]. Simultaneous imaging of the atomic and electronic structures in TCI single crystals reveals that a fraction of the Dirac electrons acquire mass due to a surface distortion that breaks a crystalline mirror symmetry [4]. Furthermore, we discover that even in the absence of any symmetry breaking, nanoscale strain in TCI heteroepitaxial thin films can induce spatially dependent changes in the SS dispersion associated with the momentum-space shift of the Dirac nodes [5]. Our experiments provide the first direct visualization of the effects of strain on the SS band structure in topological materials and suggest a novel pathway for manipulation of Dirac electrons via structural deformations.

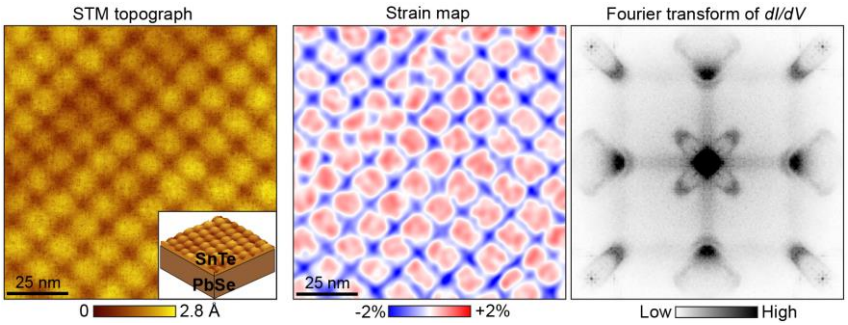

FIGURE 1. STM topograph, strain map and a representative Fourier transform of a dI/dV image of topological crystalline insulator SnTe/PbSe(001) heteroepitaxial thin films

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Contributed Talks

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Contributed: 1

Magnetic Properties of $Ca(Ru,Ti)O_3$ System

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Abstract. Perovskite type transition metal oxides have been the mainstay of condensed matter physics ever since the discovery of high temperature superconductivity in La-Ba-Cu-O system[1]. Here, we focus on peculiar properties of the pseudo-cubic $Ca(Ru,Ti)O_3$ system[2,3,4,5]. Namely, as soon as any concentration of either Ru or Ti is introduced into the pure compounds, a ferromagnetic-like transition occurs at low temperatures. Strangely, $CaTiO_3$ is well known dielectric material with no magnetic order, while $CaRuO_3$ is metallic and does not show ordered magnetic state down to the lowest temperatures. Furthermore, "ferromagnetic" transition temperature does not change throughout the concentration-temperature phase diagram. In order to address these phenomena we performed detailed dc and ac magnetization measurements for varied concentrations of Ru and Ti. Our results show that "ferromagnetic" transition persists even at zero applied dc magnetic field and shows clear frequency dependence with low amplitude applied ac magnetic field, pointing to glassy magnetic behavior.

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Mean-field Dynamics of Systems of Delay-coupled Noisy Excitable Units

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Abstract. Excitability is a dynamical feature of systems whose parameters are set close to bifurcation underlying transition from the fixed point to oscillatory state. Response of excitable units to external perturbation is extremely sensitive to stimulus magnitude within a narrow range of its values. One of the most striking points associated to excitable units lies in their ability to synchronize, which gives rise to a rich variety of self-organization phenomena and complex pattern activities. Appreciating this fact, the coupled excitable systems are now regarded as a distinct class of dynamical systems, which comprises important examples from biophysics (neuronal populations or cardiac tissue), as well as lasers, chemical oscillators and models of climate dynamics.

Given a number of characteristic spatial and temporal scales, modeling systems of excitable units typically involves different forms of noise, whose action in general may be considered as excitability amplification. One is further required to explicitly take into account the interaction delays deriving from finite conduction velocities and/or the latency in the unit's responses.

We focus on assemblies of type II delay-coupled excitable units represented by the canonical Fitzhugh-Nagumo model. Synchronization between the units' activities may give rise to collective mode/modes, whose emergence corresponds to stochastic bifurcation of global variables. Given that the analysis on stability of original system of stochastic delay-coupled differential equations cannot be carried out analytically, we derive the approximate mean-field (MF) model which qualitatively accounts for the stochastic stability of the exact system, the onset and the suppression of the collective mode. In quantitative terms, the model is capable of capturing the frequency of the induced oscillations. The MF model is based on two relevant approximations, referred to as the Gaussian and the quasi-independence approximation. We demonstrate that these approximations are not universal in a sense that one has to adapt them to the considered class of systems. As for validity of introduced approximations, an important point is that the bistable dynamics of the MF model may indicate in a self-consistent fashion the parameter domains where the mean-field approximations fail. It is further illustrated how the application of the MF model may be extended to hierarchical networks involving interacting populations of excitable units. Apart from the analysis of long-term behavior in thermodynamic limit, it is indicated that the appropriate mean-field model with included finite-effects may account for the most probable activation paths of an assembly of excitable units.

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Plasmonic Nanomembranes For Detection And Sensing

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Abstract. Nanomembranes, freestanding quasi-2D structures with thickness of the order of tens of nm and smaller and a giant aspect ratio with lateral dimensions of the order of millimeters, even centimeters, represent an important building blocks in micro and nanosystems [1], corresponding to ubiquitous bilipid membranes in living cells [2]. In this contribution we present our results in theory, design and experimental fabrication of metallic and metal-dielectric nanomembranes with plasmonic properties, intended for the use in the field of sensing. We first consider different approaches to functionalization and nanostructuring of nanomembranes [3]. These include introduction of noble metal or transparent conductive oxides fillers directly into the nanomembrane, lamination (multilayering) and patterning by 2D arrays of subwavelength nanoholes. Within this context we describe our results on nanofabrication of 8 nm thick chromium-based composite nanomembranes. Biomimetic structures utilizing nanochannel-based pores are also considered. We further present our results related to the design of chemical and biological sensors based on nanomembranes with plasmonic metamaterial properties [4]. Such sensors function as refractometric devices utilizing evanescent near fields as optical concentrators and adsorption-desorption mechanism, which ensures their ultra-high sensitivity that reaches single molecule detection [5]. We present some results on chemical sensors utilizing nanomembranes exhibiting extraordinary optical transmission, as well as those based on double-fishnet structures. Finally we consider the enhancement of infrared detectors by nanomembranes [6] utilizing the designer plasmon mechanism [7].

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Electrical Conductivity of Nanocrystalline Y-doped Nickel Ferrites

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Abstract. This paper presents results concerning on dielectric behavior and conductivity of the nanosized $NiY_xFe_{2-x}O_4$ powders (x = 0, 0.05, 0.2, and 0.3), obtained by coprecipitation method. The frequency dependance of the dielectric permittivity and the conductivity of the samples are determined in the frequency range (1-10^6) Hz, at temperatures from 300 to 450 K. The variation of dielectric constant ε', as well as electrical conductivity σ, as a function of frequency reveals that the dispersion is due to Maxvell-Wagner type of polarization and the hopping of electrons between Fe^{2+} and Fe^{3+} ions at octahedral B-sites. The reciprocal behaviour of conductivity with respect to permittivity confirms the semiconductor properties of the investigated ferrites. The AC conductivity was found to follow universal dielectric response $\sigma_{ac}(\omega,T) = A(T)\cdot\omega^{n}(T)$. Analyzing the variation of the parameter *n* with the temperatures we discuss the possible conduction mechanism in investigated samples. Qualitatively, non-overlapping small polarons (NSPT) are usually associated with increase in *n* with increasing temperature, while correlated barrier hopping (CBH) shows a decrease in *n* with increasing *T*.

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Light-responsive liquid-crystal elastomers for solar energy harvesting

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Abstract. Liquid-crystal elastomers are rubbers with liquid-crystal order. They contract along their nematic director when heated or illuminated. The shape changes are large and occur in a relatively narrow temperature interval or at low illumination around the nematic-isotropic transition. We describe the complex time dependence of the buildup of force exerted by a clamped nematic photoelastomer under illumination. Nonlinear (non-Beer) absorption leads to a bleaching wave of a significant cis isomer dye concentration deeply penetrating the solid with a highly characteristic dynamics. We fit the experimental response at one temperature to obtain material parameters; force-time data can be matched at all other temperatures with no fitting required.

We also present a conceptual design of a mechanical, turbine-based engine using photoactive liquid-crystal elastomers to extract mechanical work from light. By exposing one part of an elastic band to light and keeping the other in shadow, we develop both fundamental understanding and practical designs for turbines, and show that in principle realistic systems can directly convert light to mechanical energy at up to 40% efficiency.

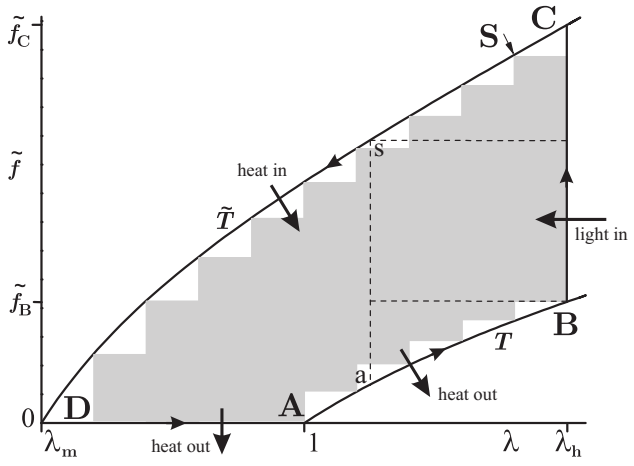

FIGURE 1. The opto-thermal cycle of the engine.

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Effective interactions between steric fluid membranes

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Abstract. A self-consistent theory is proposed for the general problem of interacting undulating fluid membranes subject to the constraint that they do not interpenetrate. The steric constraint is implemented via a certain representation of the Heaviside function, which enables one to transform the constraint into a novel effective steric potential. The steric potential is found to consist of two contributions: one generated by zero mode fluctuations of the membranes, and the other by thermal bending fluctuations. For membranes of cross-sectional area S, we find that the bending fluctuation-dependent part scales with the inter-membrane separation d as d^{-2} for $d \ll \sqrt{S}$, but crosses over to d^{-4} scaling for $d \gg \sqrt{S}$, whereas the zero mode-dependent part of the steric potential always scales as d^{-2}. For membranes interacting exclusively via the steric potential, we obtain exact nonlinear expressions for the effective interaction potential and for the rms undulation amplitude σ, which becomes small at low temperatures T and/or large bending stiffnesses κ. Moreover, σ scales as d for $d \ll \sqrt{S}$, but saturates at $\sqrt{k_{\mathrm{B}}TS/\kappa}$ for $d \gg \sqrt{S}$. In addition, using variational Gaussian theory, we apply our self-consistent treatment to study inter-membrane interactions subject to three different types of potential: (i) an attractive square well, (ii) the Morse potential, and (iii) the Moreira-Netz potential for a pair of strongly charged membranes with an intervening solution of polyvalent counterions.

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Electronic states at the interface between crystalline and amorphous domains in conjugated polymers

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Abstract. Materials based on conjugated polymers exhibit complex structure with interlaced crystalline and amorphous domains [1]. In this work, microscopic insight into the electronic states at the interface between amorphous and crystalline domains in poly(3-hexylthiophene) (P3HT) is given for the first time. We have considered two types of the interface: (1) sharp interface, where polymer chains belong to ideal crystalline or amorphous domain (type A) and (2) interface that consists of extended chains, where chains are extended out from crystalline domain and have the end in amorphous domain (type B). Type B interface is generally believed to be more representative of interfaces that occur in real interfaces. Atomic structures were generated using Monte Carlo simulations, while electronic structures were calculated using density functional theory-based charge patching method [2] and overlapping fragments method [3]. Results show that wave functions of highest states in the valence band are delocalized and belong to the crystalline domain (Fig. 1a), regardless of the interface type. On the other hand, highest states in amorphous regions are localized on one or two chains (Fig. 1b). In the case of type A interface, we also find the states localized at the interface with the energy between the band edge energies of the crystalline and amorphous region. HOMO offset in the case of type B interface is around 0.5 eV, while in the case of type A interface it is even larger. These offsets present high barriers for holes, which implies that hole transport dominantly goes across crystalline regions.

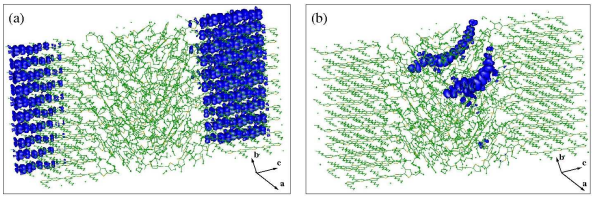

FIGURE 1. Wave function moduli of the (a) highest electronic state in the valence band in the crystalline domain and (b) highest electronic state in the valence band in the amorphous domain in the case of type B interface.

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Contributed: 8

Fermionic quantum criticality in honeycomb and π-flux Hubbard models

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Abstract. We numerically investigate the critical behavior of the Hubbard model on the honeycomb and the π-flux lattice, which exhibits a direct transition from a Dirac semimetal to an antiferromagnetically ordered Mott insulator. We use projective auxiliary-field quantum Monte Carlo simulations and a careful finite-size scaling analysis that exploits approximately improved renormalization-group-invariant observables. This approach, which is successfully verified for the three-dimensional XY transition of the Kane-Mele-Hubbard model, allows us to extract estimates for the critical couplings and the critical exponents. The results confirm that the critical behavior for the semimetal to Mott insulator transition in the Hubbard model belongs to the Gross-Neveu-Heisenberg universality class on both lattices.

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Sensitivity of A Multi-State Atom Interferometer

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Abstract. In this paper, we estimate the sensitivity of a multi-state atom interferometer using the Fisher-information (FI) formalism. The ultimate sensitivity is obtained in the Cramer-Rao bound, $CRB=1/\sqrt{FI_{max}}$ [1]. Our theoretical model describes an atom-chip interferometer realized with five states from the Zeeman $|F=2, m_F>$ manifold [2]. Coherence of the states is secured by Bose-Einstein condensation of atoms and a short delay between the radio-frequency pulses that act as input and output couplers. During evolution in a constant magnetic field Zeeman states accumulate the relative phases proportional to their energy separations, which results in oscillations in state populations measured at the output of the interferometer. We study dependence of the ultimate sensitivity (CRB) of such an interferometer on energy of the coupling radio-frequency pulses. The maximum fringe narrowing is detected for $\pi/2$ Rabi pulses. The interferometer in this configuration is further investigated as a non-directional magnetometer.

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Quasiparticle Transport Properties of SFS and DFD Junctions

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Abstract. We develop a quantitative theory describing the behavior of current/voltage characteristics (CVC) and conductances (G) for both s-wave (S) and d-wave (D) type of clean superconductor/ferromagnet (F)/superconductor (SFS or DFD) junctions. The calculation is based on the nonequilibrium microscopic theory of transport in isotropic s-wave superconductor/normal metal (SNS) junctions by Kümmel, Gunsenheimer and Nikolsky [1] in the relaxation time approximation using the time-dependent Bogoliubov-de Gennes equations [1–3]. The model operates for different barrier thicknesses d, the mean free path in the barrier $l > d$, and different temperatures $T < T_c$. For given exchange energy h the shape of CVCs depends, first, on the barrier thickness, while the presence and number of nonlinear structures are determined by h. For SFS junctions we find that rich nonlinear structures in CVCs, as well as h-dependent position of the peaks, are obtained for weak h lower than or comparable to the superconducting energy gap $\Delta = \Delta(T)$. They are interpreted to be induced by multiple Andreev reflections (AR), modified in the presence of h in ferromagnets. For DFD junctions, the AR suppression due to the presence of order parameter nodes in D, and the presence of h in the F barrier leads to relatively smooth CVC for any value of h and of d in contrast to the SFS case. This striking difference in shape and in the amplitude of CVC between the case of isotropic pairing in superconducting electrodes and the anisotropic case in general provides an indication of the superconductor order parameter symmetry.

We find that conductance curves $G(V)$ have a rich nonlinear structure in low-voltage multiple AR region, while at higher voltages, the curves are almoust flat, with characteristic dips located at $neV = 2\Delta(T) \mp h$, with $n = 0, 1, .., \Delta(T)$ being the maximum order parameter at the temperature T. We suggest that from observed dip's locations at given temperature one could determine experimentally the value of the exchange field in the barrier, independently of the superconducting anisotropy and misorientation of superconducting electrodes.

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The effect of the trigonal warping on the energy and the entanglement spectrum of graphene bilayers

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Abstract. We present an analytical study of the entanglement spectrum of graphene bilayers. We mainly focus on the influence of the skew parameter, which causes the trigonal warping in the energy spectrum, on the topology of the entanglement spectrum. Furthermore, we explore a connection between two characteristics: the entanglement spectrum of a bilayer structure, given by tracing out one of the layer, and the energy of the resulting monolayer structure, which is shown in many previous analytical and numerical studies. An explicit relation between the entanglement spectrum and the energy spectrum of remaining monolayer graphene is shown when the skew tight binding parameter, which causes the trigonal warping is neglected. However, the trigonal warping of the graphene bilayers is reflected to the topology of the entanglement spectrum and a similarity between the entanglement spectrum of graphene bilayers and the energy spectrum of the monolayer graphene is broken.

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Equilibrium Charge Transport in Nanocrystal Solids: Polaron Effects

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Abstract. Nanocrystal solids, also known as colloidal quantum dot supercrystals, are novel type of structures with colloidal quantum dots self-arranged into a lattice. It was suggested that these artificial solids may exhibit band-like transport paving the way for new cheap optoelectronic technologies [1]. However, it seems that many physical effects are preventing band-like transport such as disorder, weak electronic coupling of adjacent dots, dielectric response of ligand matrix and electron-phonon interaction [2]. We studied the effects of electron-phonon interaction on transport properties of these structures. We have modeled these structures using the generalization of the Holstein model with multiple localized phonon modes per each site/dot. Phonon energies and electron-phonon coupling constants were obtained by employing the elastic and dielectric continuum models. The model was then analyzed using a variational approach which gives exact solutions in two limiting cases, strong electron-phonon coupling regime and weak electron-phonon coupling regime. By minimizing the upper bound of free energy, we have identified that recently fabricated structures are in strong coupling regime. Using linear response theory we calculated the mobility of carriers and identified the small polaron hopping nature of transport. Even though mobility decreases by increasing the temperature, we show that band-like transport is still not achieved in these structures [3].

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Electric Dipole Spin Resonance In The Presence Of Valley Degeneracy

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Abstract. We theoretically investigate the electric dipole spin resonance (EDSR) in a single Si/SiGe quantum dot in the presence of a magnetic field gradient, e.g., produced by a micomagnet. The control of electron spin states can be achieved by applying an oscillatory electric field, which induces periodic back and forth motion of the electron spin inside the quantum dot. This motion inside a magnetic field gradient, produces an effective periodic in-plane magnetic field, and allows for driven spin rotations near resonance [1]. By solving a Lindblad master equation, we discuss possible electron spin relaxation and decoherence mechanisms relevant to EDSR. In Si there is 5% of naturally occurring nuclear spin $1/2$ isotope, which causes the electron spin to decohere. Nuclear spins are included in our model through the additional random Overhauser magnetic field. Furthermore, a valley dependent g-factor, combined with intervalley scattering gives rise to another electron spin decoherence mechanism. The goal of our study is to describe the efficiency of a spin echo sequence in the presence of all mentioned relaxation and decoherence mechanisms.

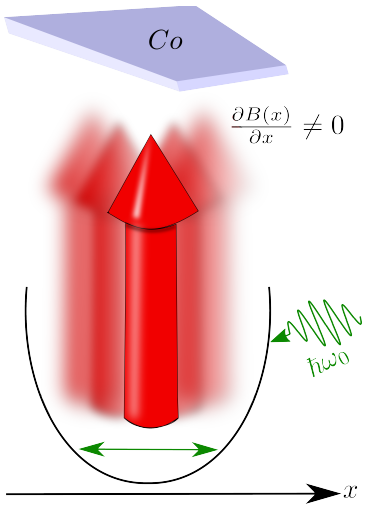

FIGURE 1. Visualisation of EDSR in the presence of a micromagnet (Co)

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Contributed: 14

Reducing Coercivity In Magnetic Thin Films Through Surface Nanostructuring

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Abstract. Spinel nickel ferrite ($NiFe_2O_4$) is a promising material for next generation high-frequency sensors, antennae and microwave devices. A key issue to be addressed is the magnetic loss, which is proportional to frequency and becomes substantial at frequencies above 1 MHz. Recently, we reported on a method to reduce coercivity in $NiFe_2O_4$ through surface patterning[1,2,3]. Here, the effects of varying the feature size on magnetic behavior, including loss will be presented. Nickel ferrite thin films were deposited on *c*-plane sapphire substrates using chemical solution deposition and patterned via nanoimprint lithography with patterning masters having feature sizes varying from 500 to 1500 nm in 200 nm increments. Atomic force microscopy showed good feature transfer for all samples. X-ray diffraction images showed all samples to be single-phase inverse spinel nickel ferrite with similar texture. All patterned samples showed coercivity reductions relative to the unpatterned samples. Magnetic force microscopy images (shown in Figure 1.) confirmed the origin of coercivity reduction to be shape-anisotropy-forced alternating domain formation. Finally, the new domain structure in patterned $NiFe_2O_4$ films was explained within micromagnetism theory.

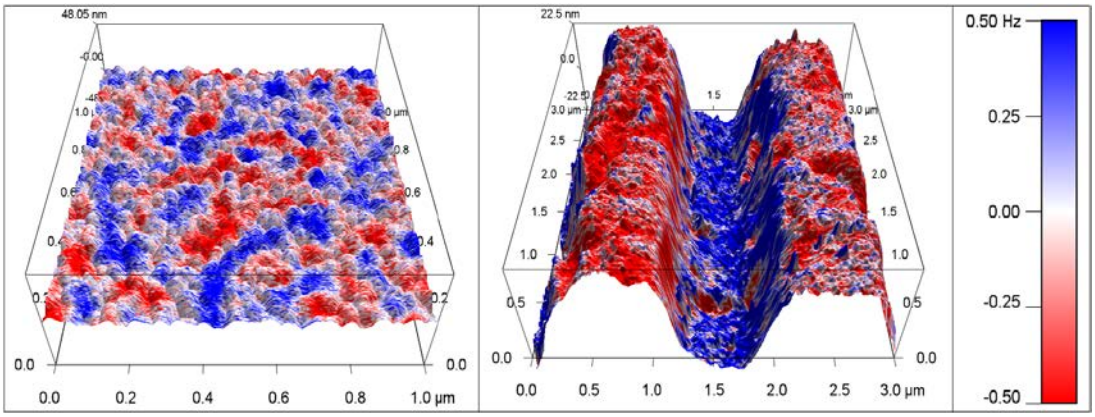

FIGURE 1. Magnetic force microscopy images showing magnetic domain distribution in (a) flat and (b) surface patterned $NiFe_2O_4$ thin film.

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Optical Properties Of WS_2 Nanotubes And Their Decoration With Au And Pd Nanoparticles

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Abstract. The recent discovery of localized surface plasmon resonances in inorganic nanotubes and fullerene-like nanoparticles of WS_2 and MoS_2 opened up new interest in their optical properties[1]. The coexistence of plasmons and excitons in the WS_2 nanotubes leads to their strong coupling and hybridization into plexitons. Addition of metallic nanoparticles with their own inherent plasmon resonance to the WS_2 nanotubes can influence their optical behavior. The morphology of the new systems obtained by decorating WS_2 nanotubes with gold and palladium nanoparticles is studied, as well as their optical properties. For the latter, techniques such as total extinction, decoupled and transient absorption are used.

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Poster Presentations

Phenomenology Of Charge-Regulation Interaction In The Protein World

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Abstract. In the world of proteins one can find exotic electrostatic phenomena such as long-ranged attraction between two electro-neutral proteins in an aqueous solution, stemming from thermal charge fluctuations of dissociable charge groups on their surface, known as the Kirkwood-Schumaker (KS) interaction [1]. We present here an extension of KS theory, formulating it in a field-theoretical framework. Our model takes two small spherical macro-ions with dissociable charge groups, which are immersed in a monovalent salt solution. Fluctuating charge on a macro-ion's surface is regulated by local variables such as pH, salt concentration and local electrostatic potential. Charge regulation is described with the proper free energy function [2] for each of the macro-ions, while the coupling between the charges is evaluated at the approximate Debye-Hückel level. Strong attraction between like-charged particles is found close to the point of zero charge, specifically due to asymmetric and anticorrelated charge fluctuations of the macroion charges. The general theory is then implemented for a system of two protein-like macro-ions with known amino acid composition, generalizing the form and magnitude of the Kirkwood-Schumaker interaction. Results show that the strength of protein electrostatic interactions depends on the rate of change of the charge of the macro-ion with respect to the solution pH, i.e. the molecular capacitance of the macro-ion, which is protein specific [3, 4].

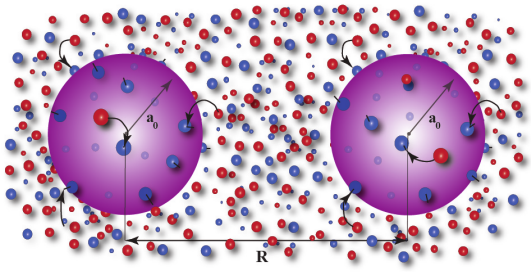

FIGURE 1. Two charge-regulated macro-ions, immersed in a solution composed of monovalent salt ions that can be exchanged with the surface sites.

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Transport properties of graphene bilayer on substrate from exact electronic Green's function

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Abstract. Graphene bilayer since its discovery [1] presents a unique representative of two-dimensional system in the condensed matter physics possessing outstanding mechanical and transport properties. The problem of constructing a theoretical model describing an energy spectrum and optical- and magneto-optical conductivities of graphene bilayer with disorder generated by interaction with different substrates both without and with an external electromagnetic fields for non-zero temperature and densities of charged carriers is not yet completely solved [2]. We present the results of a theoretical study of an influence of the substrate on the ground state energy gap at the Dirac K and K' points in the quasiparticle spectrum on longitudinal and transverse (Hall) optical conductivities of graphene AB-stacked bilayer on the substrate on the base of quantum field theory tools in (2+1)-dimensional space-time. To do this we use, first, both 2-band and 4-band low-energy microscopic Hamiltonians (see Fig. 1 for energy spectrum) and corresponding exact electronic Green's functions [3], second, an interaction of bilayer with substrate which leads to appearance of structural inhomogenities (destroying hexagonal structure). We calculate the influence of such defects both on the density of states and on electronic conductivities. We discuss the influence of the interaction of bilayer with substrate on the ground state gap in electric (5-20 meV) and magnetic fields (3-10 Tesla) in order to find application to optoelectronic devices on bilayer ground.

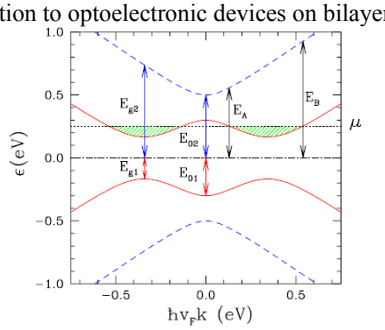

FIGURE 1. Band structure around the Fermi level in the presence of the gap Δ for values Δ=0.3 eV, γ_1=0.4 eV and fiite chemical potential μ = 0.25 eV [2]. line.

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Symmetry Based Analysis of Gap Plasmons in Fishnet Metamaterials

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Abstract. Like photonic crystals, metamaterials are periodic structures whose symmetry is described by (usually symmorphic) diperiodic groups. In this contribution we used a theory [1] developed for two dimensional photonic crystals, to analyze the symmetries of electromagnetic fields associated with gap plasmon polaritons propagating through the thin dielectric gap of fishnet metamaterials belonging to TC_{2v} and TC_{4v} symmetries. The group-theory-based prediction of field transformation properties is confirmed experimentally by far-field spectroscopy and numerically by direct calculation of plasmonic near-fields of the several relevant normal modes in fishnet metamaterials containing rectangular [2] and square [3] holes.

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Theoretical and Experimental Study of Helices Composed of Spherical Dipoles

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Abstract. Tubular and cylindrical lattices are principal structural elements in biological systems. They give rise to structures, such as bacterial flagella and microtubules, which are essential building blocks of cells. The complexity of the structures formed by the particles with dipole-dipole interaction is a result of the interplay between anisotropic near-field interaction and long-range influence of the global geometry of the structure. Subject of this paper is the investigation of infinite 3D structures, i. e. tubes and helices. We will show that tubes are in terms of structure, actually a subset of helices. There is an endless number of different helical configurations. Nevertheless, densely packed structures exist in a number of well defined points in parameter space. We observe a structural similarity of, so called, Z-tubes, with the structures in typical experimental images of microtubules. These tubes can be decomposed into chains which are analogous to biological filaments, of which microtubules are made of. We present a way of geometric generation of densely packed helical structures composed of hard spheres. Later on, we show how to assign dipole moments to the particles making up those structures, in order to obtain dipole orientations which follow the geometry. Experimental study has proved that structures with such dipole orientations are stable.

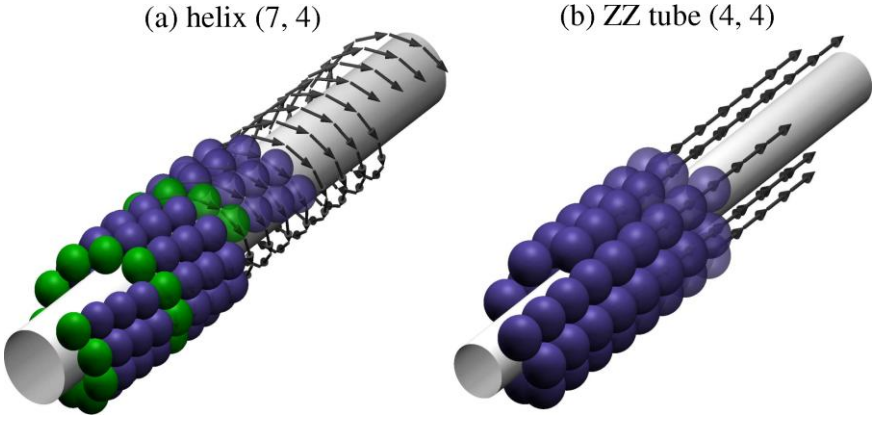

FIGURE 1. Ilustration of one representative four-stranded helix (i. e. having ST dipole orientation) (a) and one representative ZZ tube (b).

Analyte Recognition And Quantification Based On Fluctuation Phenomena On The Active Surface Of Biochemical Sensors

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Abstract. Experimental data obtained for a graphene-based gas sensor [1,2] show that adsorption of different analytes has a different influence on the spectrum of fluctuations of the sensor signal, i.e. that the spectrum contains a unique adsorbate signature. A theoretical model of the fluctuations of the sensor signal, derived in [3,4], shows that the specific features in the spectrum, which contain information about the adsorbed analyte, originate from the fluctuations in the number of adsorbed analyte particles (described by the spectrum $S(f)$), caused by surface diffusion, adsorption-desorption process and bulk mass transfer. In this work, by using the mentioned theoretical model, we analyze (Fig. 1) the possibility for quantification of analyte concentration based on the measured fluctuations spectrum.

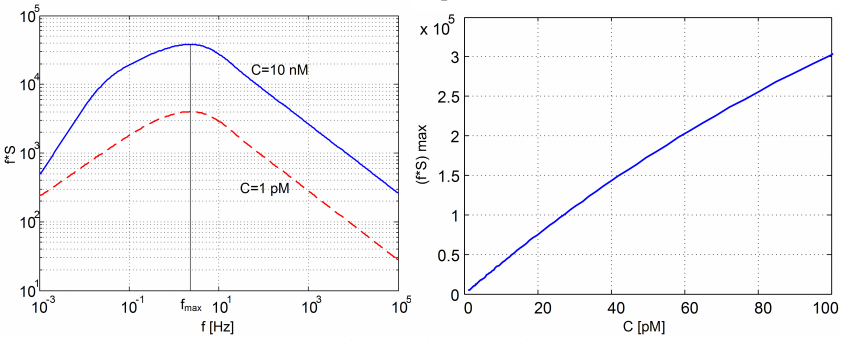

FIGURE 1. The fluctuations spectrum multiplied by f, for the same analyte present in two different concentrations (left). Dependence of the maximum of the curve $f \cdot S$ on the analyte concentration (right).

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Surface Hypermodes In Photonic Hypercrystals

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Abstract. Photon-electron coupling at metal-dielectric interfaces and formation of conventional surface plasmon polaritons allows for light confinement beyond subdiffraction-limit. This fact has been one of the guiding forces for the whole field of plasmonics during the past two decades. However, the subwavelength localization of light is also the mode of operation with the highest surface-plasmon propagation losses. Therefore, finding a way to enhance localization and reduce losses represents a goal of the highest priority. Hyperbolic metamaterials, where the dielectric permittivity tensor components have the opposite signs in two orthogonal directions, leading to the TM-polarized wave propagation with the unlimited wave numbers k, have recently attracted a lot of attention [1]. These high-k waves necessarily cause Bragg reflection and scattering when a periodic variation of the dielectric permittivity is present. This leads to the formation of photonic band gaps in both the wave number and the frequency domain. Namely, optical surface states are formed due to the Bragg reflection in the band gap of a photonic crystal. This effect is responsible for the optical Tamm or Shockley surface states, but it normally does not lead to subwavelength localization. In hyperbolic metamaterials, however, there are no longer limitations on localization, since the surface states can be formed with high-k that are localized at a scale much shorter than the free-space wavelength. Hyperbolic metamaterial supports a broad spectrum of high-k waves that leads to the very high [2], or even singular photonic density of states [3]. Topological transitions in metamaterials have been studied in [4].

In order to avoid both localization limitations and high losses, the hypercrystal composed of unit cells that consist of alternating hyperbolic material (either artificial or natural), and isotropic material have been recently proposed [5, 6]. We have studied both analytically and numerically, the formation of photonic band gaps that allow for photonic surface "hyperplasmons" and surface "hyperstates" for both doped semiconductor and metal-dielectric hyperbolic metamaterial components of the hypercrystal. Both forward and backward surface "hyperplasmons" are found that are highly localized with significantly lower losses compared to the conventional surface plasmons polaritons.

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Nonequilibrium High-frequency Conductivity in Materials with Localized Electronic States

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Abstract. A broad range of disordered materials contain electronic states that are spatially well localized. These include amorphous inorganic semiconductors, inorganic crystals doped with randomly positioned impurities and organic semiconductors based on conjugated polymers or small molecules. Usual approaches to simulation of ac conductivity of these materials rely on Kubo's formula which expresses the ac conductivity in terms of the mean square displacement of a diffusing carrier. Such approaches therefore assume that carriers are in equilibrium and that they are only slightly perturbed by external alternating electric field. However, in many realistic situations, the carriers are not in equilibrium; a typical example concerns the carriers created by external optical excitation across the band gap of a semiconductor.

In this work we obtain the expression for the optical conductivity in a material with localized electronic states and weak electron-phonon or electron-impurity interaction [1]. The expression is valid for any nonequilibirum state of the electronic subsystem prior to the action of electric field. It gives nonequilibirum optical conductivity in terms of microscopic material parameters and contains both coherences and populations of the initial electronic subsystem's density matrix. Particularly, in the case of incoherent nonequilibrium state of the electronic subsystem, the optical conductivity is entirely expressed in terms of the positions of electronic states, their nonequilibrium populations, and Fermi's golden rule transition probabilities between the states. The same mathematical form of the expression is valid both in the case of electron-phonon and electron-impurity interaction. Moreover, our result for the nonequilibrium optical conductivity has the same form as the expressions previously obtained for the case of equilibrium. The derivation was performed by expanding the general expression for ac conductivity in powers of small electron-phonon or electron-impurity interaction parameter. Our results are expected to be valid at sufficiently high frequencies, such that the period of the electric field is much smaller than the carrier relaxation time. We apply the derived expressions to two model systems, a simple one-dimensional Gaussian disorder model and the model of a realistic three-dimensional organic polymer material obtained using previously developed multiscale methodology [2]. We note that the simple one-dimensional model captures the essential features of the mobility spectrum of a more realistic system. Furthermore, our simulations of the polymer material yield the same order of magnitude of the terahertz mobility as previously reported in experiments.

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Stroboscopic Phenomena In Superconductors With Dynamic Pinning Landscape

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Abstract. With recent achievements in (ultrafast) optics and nanoengineered plasmonics it has become possible to exploit the interaction of light with superconductivity, and create not only spatially periodic imprints on the superconducting condensate, but also temporally periodic ones. Here we show that in the latter case, temporal matching phenomena develop, caused by stroboscopic commensurability between the characteristic frequency of the vortex motion under applied current and the frequency of the dynamic pinning. The matching resonances persist in a broad parameter space, including magnetic field, driving current, or material purity, giving rise to unusual features such as externally variable resistance/impedance and Shapiro steps in current-voltage characteristics. All features are tunable by the frequency of the dynamic pinning landscape. These findings open further exploration avenues for using flashing, spatially engineered, and/or mobile excitations on superconductors, permitting us to achieve advanced functionalities.

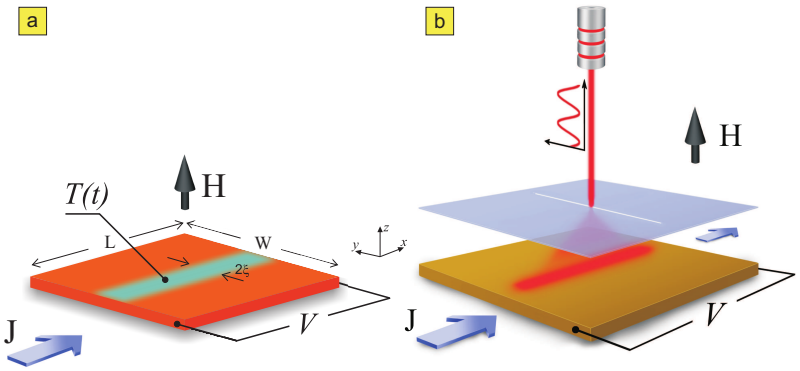

FIGURE 1. Layout of the studied system. (a) A superconducting stripe of width $W = 24\xi$ (ξ is the superconducting coherence length) with a central, time-dependent, pinning line of width comparable to the vortex size, and an applied *dc* current (with density J), and measured voltage (V, at contacts separated by distance L). A depletion region is simulated as sinusoidally oscillating local heating up to the critical temperature T_c and back to working temperature, with frequency ω. (b) Possible experimental setup corresponding to (a), by using a laser light at the far field passing through a metallic mask to create time-dependent and spatially modulated depletion of the superconducting condensate.

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Mott-insulator to superfluid transition by multiple bound dark-state polaritons in Jayne's-Cummings-Hubbard lattices

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Abstract. Strongly correlated many-body systems, which are composed of one particle species e.g. pure bosons or fermions, have been attracted a lot of attention for the past few years. Bose-Hubbard model describes quantum phase transitions (QPT) of ultra-cold atoms in periodic potentials with two atoms on site, interacting and hopping between adjacent sites in optical lattices[1,2]. Moreover, systems of coupled cavities filled with atoms have captured the physics of strongly correlated many-body systems with a corresponding Bose-Hubbard like model, called Jayne's-Cummings-Hubbard model (JCH model)[3]. Essential feature of these systems is the existence of polaritons – excitations composed of both photonic and atomic degrees of freedom. Here, QPT appear due to the conversion of excitations between polaritonic and photonic types rather than among different phases of bosons or fermions in the one particle species case[4]. Both models depend on the competition between the local interaction and the nonlocal tunnelling[5].
In this work we will examine a solid light system which is represented by an array of coupled micro-cavities, each containing a single atom. The field of a cavity mode couples one ground and an excited state, while the classical control field (with Rabi-frequency Ω) drives the transition between another ground and the excited state. In this system of an atom and two fields, in so called Λ-configuration, there exists a superposition of atomic ground states that cannot be excited by either fields – dark state. When the fields are in two-photon Raman resonance with a large single-photon detuning, the excited state can be adiabatically eliminated. We discuss the formation of multiple dark-state polaritons (DSPs) which can be bound. Further, we distinguish two cases of solid light systems with constant (no disorder) and periodically changing (disordered) non-local tunnelling between the cavities. We show that the DSPs undergo a Mott-insulator to superfluid QPT and we calculate the Mott lobes at T=0 in case of lacking and present disorder. As we tune Ω, we get a reduction in the number of DSPs while undergoing the Mott-insulator to superfluid transition. We argue that such a behaviour might be related to a glassy phase[4,6] that divides the Mott-insulating and superfluid phases.

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Probing the Plasmon-Phonon Hybridization in Supported Graphene by Externally Moving Charged Particles

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Abstract. We study the effects of variation in the doping density of graphene on hybridization taking place between its Dirac plasmon and the surface optical phonon modes in a SiO_2 substrate, and show that this hybridization may be probed by a point charge that moves over graphene at a speed comparable to graphene's Fermi speed. Using the dielectric-response formalism within the random phase approximation, we show that the plasmon-phonon hybridization exerts strong effects on the wake pattern in the induced potential in the plane of graphene, as well as on the stopping and image forces on the incident charge, in a manner that may be controlled by changing the doping density of graphene.

A Theoretical Study On The 60K Plateau In $YBa_2Cu_3O_{6+x}$ Superconductor

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Abstract. The horizontal section, the so called 60K plateau, in the $T_c(x)$ characteristic of $YBa_2Cu_3O_{6+x}$ superconductor is known to be related to the orthorhombic order in the chain planes of this compound. However, this part of the $T_c(x)$ curve in the improved, high quality superconducting $YBa_2Cu_3O_{6+x}$ samples appears to be, not a flat horizontal section of almost constant T_c, but rather a section where $T_c(x)$ continues to rise but at somewhat reduced rate. In the present study we propose a theoretical model of charge transfer from chain planes to the superconducting planes which assumes that only CuO chains longer than, or equal to, some critical chain length l_{cr} can provide superconducting holes. This model explains in a natural way, how the well defined 60K plateau transforms into a less pronounced "quasi" 60K plateau due to improved orthorhombicity of the crystal sample. The calculated $T_c(x)$ dependences, obtained for appropriate values of l_{cr}, are found to be in a very good agreement with corresponding $T_c(x)$ values obtained experimentally.

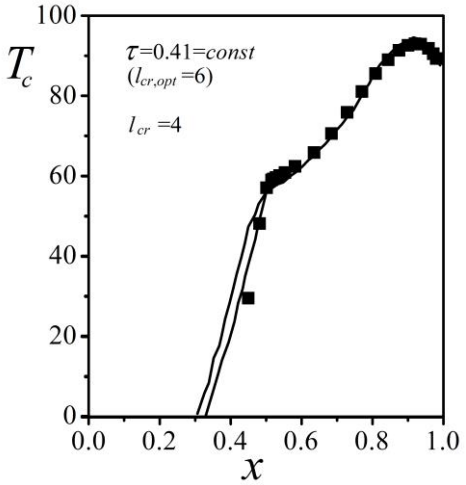

FIGURE 1. Calculated values of T_c(x) dependence (black squares) at τ = const = 0.41 for l_{cr} = 4 (τ is the scaled temperature). Also shown (solid line) is the experimental $T_c(x)$ from Ref. [1]. At τ=const=0.41 the value of l_{cr} for which 60K plateau is almost flat, $l_{cr,opt}(\tau)$, is approximately equal to 6, so that the calculated $T_c(x)$ (for l_{cr} = 4) falls into the $l_{cr} < l_{cr,opt}(\tau)$ regime.

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Chemical Doping Of Langmuir-Blodgett Assembled Graphene Films For Flexible Transparent Conductive Electrodes

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Abstract. We demonstrate how chemical doping can be used to enhance properties of liquid-phase exfoliated (LPE) graphene films. Langmuir-Blodgett assembly (LBA) on a water-air interface was used to fabricate multi-layer graphene films several square centimeters in size (Fig. 1(a)). Sheet conductivity of these films is enhanced through doping with nitric acid, leading to a fivefold improvement while retaining the same transparency as un-doped films (Fig. 1(b)). In addition, chemical doping increases the work function by 0.75 eV, to a value of 4.95 eV, making these films a promising candidate for anode electrodes in hybrid solar cells and organic electronics.

Acknowledgement: This work is supported by the Serbian MPNTR through Projects OI 171005, III 45018, 451-03-2802-IP/1/167 and by the Qatar National Research Foundation through Project NPRP 7-665-1-125.

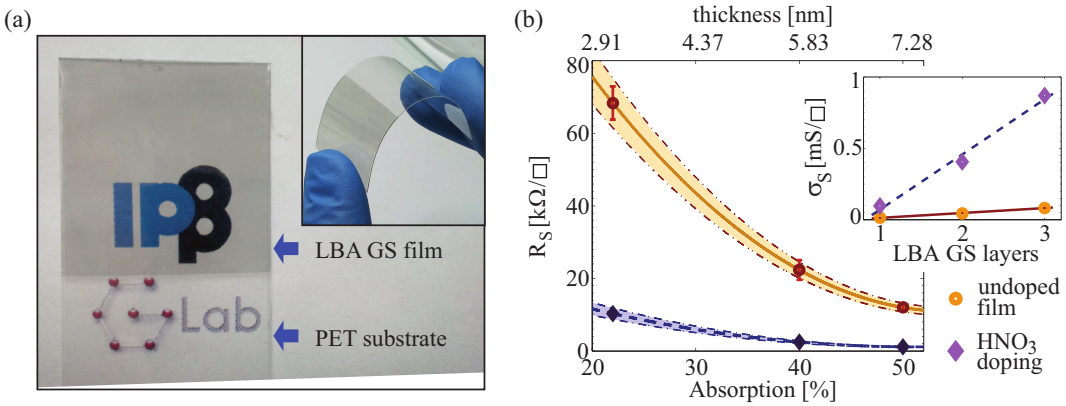

FIGURE 1. (a) 2×2 cm^2 LBA graphene sheet (GS) film on a polyethylene terephthalate (PET) substrate. (b) The sheet resistance (R_S) and sheet conductivity (σ_S) (inset) of stacked LBA GS layers, prior and after chemical doping.

Interplay Between Snake And Quantum Edge States In a Graphene Hall Bar With a PN-junction

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Abstract. Snake states in graphene appear in the presence of a pn-junction and a perpendicular magnetic field that were observed experimentally [1]. We investigate the influence of quantum effects on this classical phenomena. The magneto- and Hall resistance of a locally gated cross shaped graphene Hall bar was calculated in the quantum regime. The edge of the top gate is placed diagonally across the center of the Hall cross. Four-probe resistance was calculated using the Landauer-Büttiker formalism, while the transmission coefficients are obtained using the Kwant package [2]. Simulations showed that the position of the peaks in the resistance are in disagreement with the ones predicted for the snake states by classical simulations [3] (see Fig. 1(a)). We show that these peaks are a consequence of the interference between snake states that were injected from edge channels. The interplay between transport due to edge channels and snake states is further investigated. When two edge channels are occupied we predict oscillations in the Hall and the bend resistance as function of the magnetic field (see Fig. 1(b)). The effect of disorder on the oscillations observed in the resistance are also investigated. We examine cases of edge disorder as well as random vacancies.

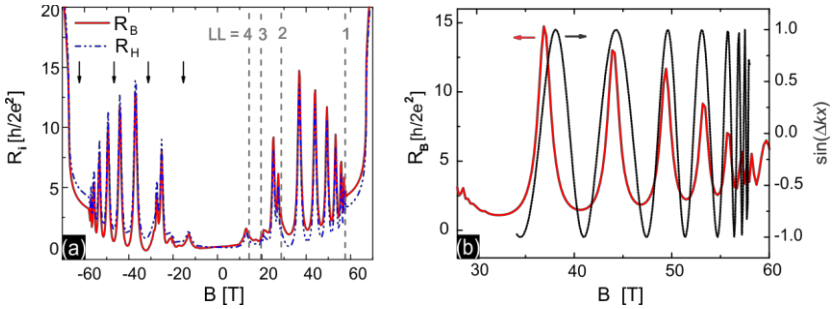

FIGURE 1. (a) Resistances R_B and R_H versus the applied magnetic field. The arrows indicate the position of the resistance peaks due to the snake states as obtained from a semiclassical calculation. (b) R_B and sin(Δkx) for $\Delta k = k_1 - k_0$ and $x = L_{pn}$, where k_n is the wave vector of the n-th edge state and L_{pn} is the length of the pn-interface.

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Optically Generated Nonlinear Temperature Variations On Sample Surfaces

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Abstract. This paper investigates two models of surface temperature variations of a laser-excited sample, inside which the heat sources, dependant on the current sample temperature, are generated. The fixed points are located and the solutions' stability and convergence are examined. The differences of these two models' predictions are discussed.

Nonlocal Effects In Periodic Plasmonic Nanostructures With Deep Subwavelength Perturbations

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Abstract. The possibility to tailor electromagnetic near fields and evanescent waves in the optical range using plasmonics promises a plethora of applications. Maybe the most important among them is the possibility to bridge a gap between electronics and photonics and merge them into a single field by creating structures with the packaging densities of contemporary integrated circuits and simultaneously with extreme speeds of all-optical circuits [1]. Other applications include ultrasensitive chemical and biological sensors [2], where structures like optical antennas can ensure single-molecule detection (e.g. [3]). Here we consider a class of plasmonic metamaterials based on ultra-thin (membrane-based) metal-dielectric slabs with 2D arrays of subwavelength nanoapertures [4]. We introduce modifications of the geometry of such subwavelength apertures by adding structures that are small compared to the apertures themselves, thus being in the deep subwavelength range. The conventional effective medium theory does not make a difference between a modified and unmodified structure and furnishes identical effective optical parameters for both. However, strong spatial nonlocality caused by the spatial dispersion of relative dielectric permittivity and introduced by deep subwavelength structuring of the nanoapertures results in deviations from the unperturbed case and is reflected in modified spectral response [5]. In our consideration we use an *ab-initio* approach to simulate the response of the modified structures using the finite element method. We perform our analysis for two classes of plasmonic structures, one utilizing patch-like sub-elements superposed on the corners of rectangular subwavelength holes in metallic membrane (or, alternatively, in a metal-dielectric-metal sandwich), and the other consisting of the same hole pattern in the same material that is shifted in-plane along its diagonal, thus forming complex apertures with sharp corners and narrow gaps between elements where extreme field localizations may occur. We show that strong modifications of the overall response are possible when using such supercell-based plasmonic metamaterials. The choice of the geometry ensures a novel degree of design freedom and gives the possibility to tune the spectral response. We finally describe the application of this concept to single-element, multi-analyte plasmonic chemical sensors.

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New Ordered Magnetic Phase in Frustrated spin-1/2 Heisenberg Antiferromagnet in RPA

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Abstract. Frustrated spin-1/2 Heisenberg antiferromagnetic model is investigated using double time temperature Green function method. We analyze thermodynamic properties and examine existence of several ordered phases, depending on ratios of exchange integrals. Finally, we compare our results with those obtained by cluster mean-field theory.

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Oscillator Strengths In An Off-Center Spherically Confined Hydrogen Atom

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Abstract. Semiconductor quantum dots have attracted considerable attention as mesoscopic light emitters. Efficient emitters can be realized by enhancing the interaction strength between QDs and light which is given by oscillator strength [1-2]. We have investigated model of hydrogen atom which is confined in a spherical quantum dot. This kind of model can be used for describing impurity states in the mesoscopic heterostructures, which is important problem in semiconductor physics [3]. The exact solution of hydrogenic donor located at the center of spherical quantum dot is known, and this problem is analytically solved [4]. However, if the impurity is located elsewhere numerical or variational methods are required. In this paper we investigate how absorption oscillator strength of the dipole transitions in hydrogen impurity varies with changes in the radius of the dot and distance of hydrogen atom from the center of the quantum dot.

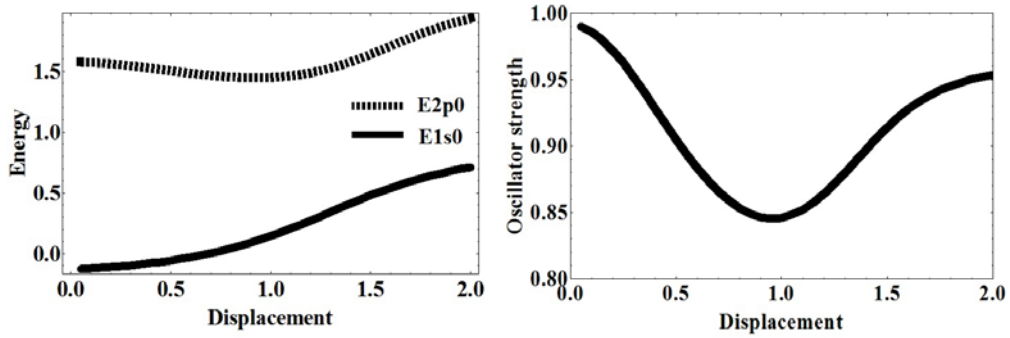

FIGURE 1. The first two energy levels and oscillator strength for different displacements of impurity from the center of QD when the dot radius is R=2.0 a.u.

From the figure 1. it can be seen that oscillator strength at given radius of quantum dot is non-monotonic function of impurity displacement. By changing the displacement of the impurity, the oscillator strength value can be changed, which is important for practical applications in optical devices.

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Density Functional Theory Study of Li and Ti-Intercalated Graphene

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Abstract. Graphene, a single atomic layer of carbon atoms arranged in a honeycomb lattice, has been attracting remarkable attention for its unique properties ever since it was successfully isolated in 2004. [1] Intercalation of atoms into layered materials is known method for providing new properties that are usually distinctly different from those of pristine materials. Intercalated graphene shows various fascinating physical properties which pristine graphene lacks [2,3] and this offers new possibilities for both applications and fundamental research.

When intercalated with lithium, graphene becomes superconductive and this effect can be additionally enhanced with application of strain.[3] Titanium adsorbed on surface of graphene has been studied for energy applications [4,5] and it is known adsorbed Ti adatoms provide strong n-type doping. In this paper, using Density Functional Theory formalism, ab-initio calculations are performed to investigate properties of lithium and titanium intercalated graphene. Using density functional perturbation theory formalism implemented in Quantum Espresso software package[6] we described phonon properties of those structures.

This work is supported by the Serbian MPNTR through Project OI 171005 and by Qatar National Research Foundation through Projects NPRP 7-665-1-125

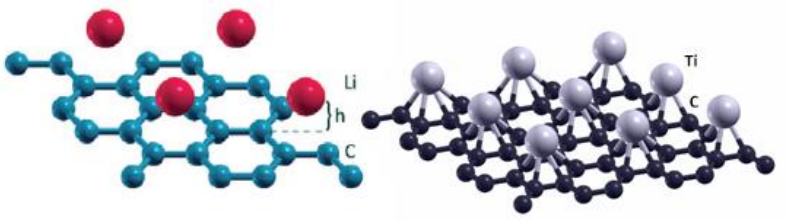

FIGURE 1. Li (left) and Ti (right) adatoms adsorbed on graphene

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Fano Resonances In The Conductance Of Graphene Nanoribbons With Side Gates

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Abstract. Quantum electron transport in narrow graphene ribbons of different widths and edge types (armchair and zigzag) is investigated. The graphene nanoribbon (see Fig. 1(a)) has two side gates that create an electrostatic potential constriction. We found that this system exhibits a series of conductance peaks when the side gate potential is varied (Fig. 1(b)). By comparing these peaks with eigenenergies of a closed system (a ribbon detached from the leads), we are able to interpret them as Fano resonances. The local properties, such as the local density of states (LDOS) and the electron current, show very specific behavior at these resonances. For example, the LDOS in zigzag ribbons peaks at the pn interfaces near the ribbon edges, while it spreads in high potential regions in the armchair ribbons (Fig. 1(c)). Similarly, the electron current in armchair ribbons tends to flow in the high potential regions, while in zigzag ribbons it can flow uniformly or even create vortices. We found other interesting physical effects, such as a valley valve effect in zigzag ribbons that is caused by intervalley scattering.

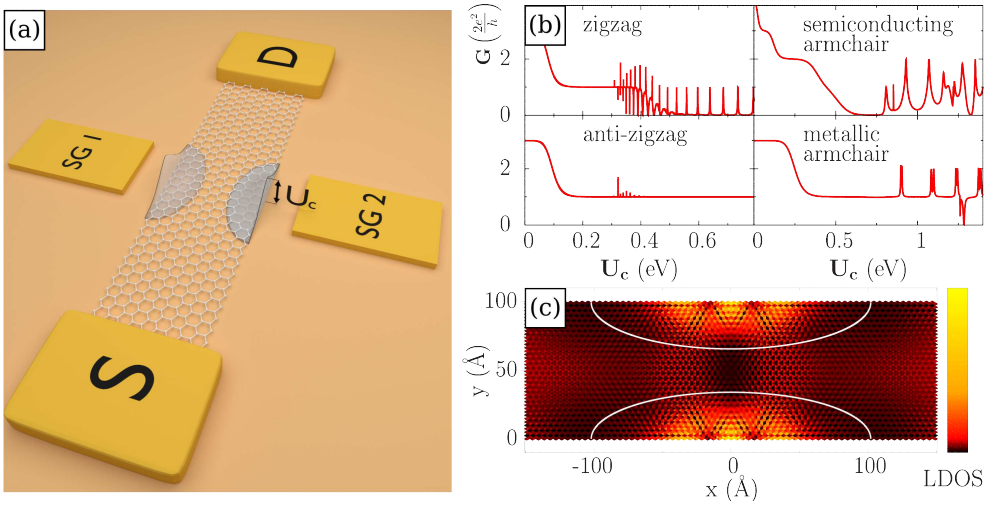

FIGURE 1. (a) Device setup: a graphene nanoribbon gated with two side-gates (SG1 and SG2) creating a potential constriction of height U_c. (b) Fano resonances in the conductance of armchair and zigzag ribbons at constant back-gate voltage. (c) LDOS in the armchair ribbon at one of the resonance peaks.

Electro-acoustic Analogy Of An Open, Minimum Volume, Photoacoustic Cell

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Abstract. In this work, the electro-acoustic analogy is derived, which models the influence of an open, minimum volume, photoacoustic (PA) cell on the acoustic response. Using the analogous electrical circuit, a transfer function of the described cell is derived. It is shown that the influence of the PA cell can be described by a 4^{th} order real rational function, which, under certain conditions, predicts the appearance of resonant peaks in both amplitude and phase PA characteristics. A discussion, based on the derived transfer function, about the influence of the geometry of the microphone chamber and its hole on the position and the shape of the resonant peaks is presented. Additionally, the characteristics of polymer microphone diaphragm are considered.

Charge Density Wave in $CeTe_3$ – A Scanning Tunneling Microscopy Study

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Abstract. Charge density waves (CDW) are a type of coupled electronic-lattice instability found in quasi-low dimensional materials. The rare-earth tritellurides, $ReTe_3$, represent an excellent model system for systematic study of CDW physics. They are layered quasi-2D materials with a weakly orthorhombic crystal structure of the *Cmcm* space group.[1] The layers are composed of a corrugated ReTe slab sandwiched between two planar Te layers and connected together along the crystalline b axis via weak van der Waals forces. The planar Te atomic layers (*ac* plane) are weakly hybridized with the ReTe slab atoms. Hence, the physical properties of $ReTe_3$ are dominantly determined by the Te planes and consequently the CDW state is formed in Te atomic layers.[2] Here we present a scanning tunneling microscopy study of CDW in $CeTe_3$ at room temperature. We demonstrate that $CeTe_3$ hosts an unidirectional incommensurate CDW with a characteristic wave vector, k_{cdw}=3.9 nm^{-1}, which is in a good agreement with theoretically predicted value, $k_{cdw}=2/7\cdot 2\pi/c=4.1$ nm^{-1}. Using scanning tunneling spectroscopy we estimate the CDW gap to be approximately 380 meV, which is in good agreement with previously reported values.[3]

We are grateful to the Serbian Ministry of Education, Science and Technological Development for financial support through projects Nos. OI 171005, III45018.

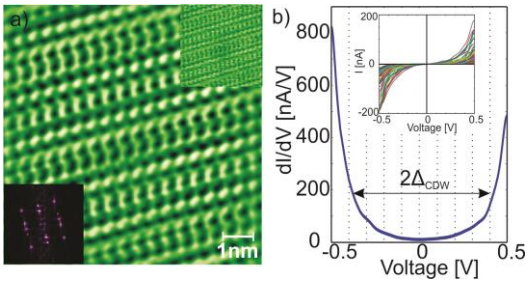

FIGURE 1. (a) STM topography of CDW in CeTe3. (b) dI/dV curve showing 380 meV CDW gap

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Conference attendance patterns

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Abstract. Patterns of scientific publications, collaborations and citations in scientific journals have been extensively studied in last decade while conference attendance patterns remain mostly unexplored from the perspective of statistical physics. In this work we study the conference attendance of scientists on the six conference series in different fields of science. The gathered data contain detailed information about papers/abstracts presented at the conferences for the period of 30 years, which enables us to analyse the total number of participations, number of successive participations and the time lag between two consecutive conference participations for each author. All these properties exhibit broad distributions with exponential cut-off. In order to further investigate the mechanism behind conference attendance patterns, we propose a stochastic model based on two key ingredients, 2-bin generalized Polya process and random termination time of a career. We demonstrate that this model, with positive feedback, can successively reproduce the empirically observed results.

Specifics in Optical Properties of Molecular Crystalline Nanofilms

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[c] *University of Banja Luka, Faculty of Sciences, Physics, Republic of Srpska, B&H*

Abstract. The changes of optical properties under boundary presence in molecular crystal nanofilm were theoretically investigated in this work. The dispersion law and states of excitons [1] as well as their space distribution along boundary direction have been determined using adjusted Green's function method [2] and also by combined analytical and numerical calculations, which were carried out using its own software package. We study the basic micro and macroscopic physical characteristics of ultrathin molecular crystalline films and one can see that essential optical properties of these systems arise with perturbation conditions, which appear at their surface layers [3,4]. On the basis of real and imaginary part of relative permittivity, the absorption, refraction, reflection and transparency indices were determined, and the influences of boundary parameters on occurrence of a very selective and strictly discrete absorption, refraction and transparency were analyzed. What we have found particularly interesting is the significant percentage of reflected and transparent electromagnetic IR radiation in the nanofilm, although bulk samples of the same crystallographic structure are complete absorbers of this spectrum.
In the course of this work, we encountered the very important question for optical engineering (manipulating the optical properties of the sample), regarding the environment effects: environment and substrate – (bio)materials that are above and below the nanofilm, or how the interaction of environment molecules with molecules from the boundary area of film affect the redefinition of exciton states in the film, and thus all other relevant characteristics of the whole nanosamples!

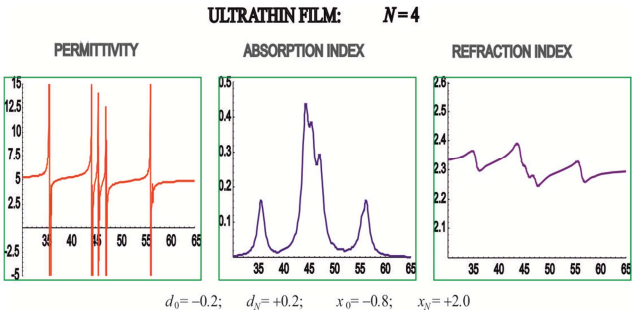

Figure 1. *Dielectric and some optical characteristics of four-layered nanofilm*

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Electrical and mechanical properties of CVD graphene studied by scanning probe microscopy

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Abstract. Chemical vapor deposition (CVD) on various metal substrates is an inexpensive method for the fabrication of a large-area graphene. CVD graphene is a polycristalline two-dimensional material, consisting of single-crystalline domains connected by domain boundaries. These boundaries strongly influence the graphene electrical and mechanical properties. Here we use scanning probe microscopy in order to investigate the effect of the domain boundaries on graphene grown on Cu (Fig. 1(a)) and then transferred on SiO_2 (Fig. 1(b)). Using conductive atomic force microscopy (C-AFM), it is shown that the graphene conductivity drops along the domain boundaries (Figs. 1(c) and 1(d)), while Kelvin probe force microscopy reveals that the difference in the local surface potential of neighboring domains might be on the order of 10 mV (Figs. 1(e) and 1(f)). Regarding the mechanical properties, force modulation microscopy gives a map of the local elasticity which drops exactly across domain boundaries. Using the method of the AFM manipulation, by the scanning graphene in the contact AFM mode and by continuously increasing normal load, we show that graphene cutting is initiated when AFM probe scans across a domain boundary (Figs. 1(j) and 1(k)).

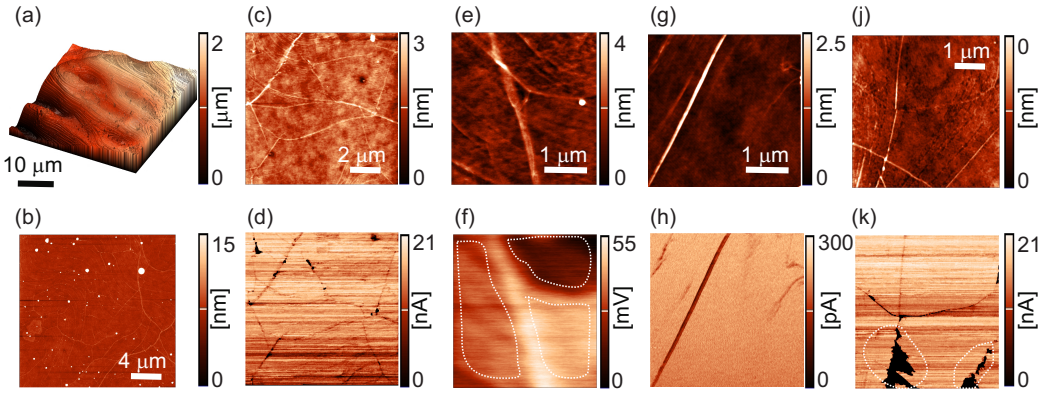

FIGURE 1. (a) Topography of the CVD graphene grown on Cu and (b) the CVD graphene transferred on SiO_2 (graphene samples were supplied by Graphenea). (c) Graphene topography and (d) the corresponding current map. As can be seen, the current drops (dark lines in part (d)) exactly along domain boundaries (bright lines in part (c)). (e) Graphene topography and (f) the corresponding surface potential distribution. Three neighboring domains are denoted with white dotted lines and all of them have different surface potential. (g) Graphene topography and (h) the corresponding elasticity map. The local elasticity drops (dark lines in part (h)) along domain boundaries (bright lines in part (g)). (j) Topography of the graphene before and (k) the current map after the AFM manipulation. Normal load is increased from top to the bottom of the images. At sufficiently high load, AFM probe can hook graphene and pull or cut it thus making holes in the graphene with zero current (denoted with white dotted lines in part (k)).

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Collective Modes of Dipolar Fermi Gas from Collisionless to Hydrodynamic Regime

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Abstract. We study the low-lying collective excitations of a Fermi gas at zero temperature confined to a triaxial harmonic trap, featuring the anisotropic long-range dipole-dipole interaction. In order to analyze the collective modes of this system, we follow Ref. [1] and solve analytically the underlying Boltzmann-Vlasov equation by using the relaxation-time approximation and by performing a suitable rescaling of the equilibrium distribution [2]. The resulting ordinary differential equations for the dynamics of the scaling parameters are linearized around equilibrium in order to determine both eigenvectors and eigenfrequencies of the collective modes. Due to the smallness of the dipolar interaction strength, the collisionless regime corresponds to the case of a noninteracting Fermi gas, i.e., the three low-lying modes represent one-dimensional cloud elongations along only one of the respective trap directions [3, 4]. In contrast to that, we get in the hydrodynamic regime the usual breathing, quadrupole, and radial quadrupole mode, where the cloud elongations are truly three- and two-dimensional, respectivley [5, 6]. We investigate in detail how the eigenvectors change when decreasing the relaxation time all the way from the collisionless to the hydrodynamic regime. We also analyze the quench dynamics, which is induced by a sudden rotation of the polarization of the atomic magnetic moments by 90°, and show that it can be understood by a superposition of the low-lying collective modes. These analytical and numerical calculations are relevant for understanding quantitatively the current Innsbruck experiment with ultracold fermionic erbium atoms, which interact via their magnetic dipole moments [7].

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Faraday Waves in Dipolar Bose-Einstein Condensates

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Abstract. We study the emergence of Faraday waves in quasi-one-dimensional dipolar Bose-Einstein condensates of ^{52}Cr and ^{164}Dy subject to periodic modulation of the radial confinement. We investigate through extensive numerical simulations and detailed variational treatment the effects of the strong dipolar interaction on the spatial and time-period of the Faraday waves. Unlike in the case of homogeneous [1] or inhomogeneous contact interactions [2], the emergence of Faraday waves is found to further destabilize the condensate in the presence of strong dipolar interaction. The interesting effect of spatial period variation of generated density patterns is observed numerically and studied within the Gaussian variational approach.

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Simulations of Optical Properties of III-Nitride Quantum Dots and Nanowires

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Abstract. Nanostructures based on III-nitride semiconductors offer certain advantages for realization of single-photon sources and classical light emitters. Larger band offsets and effective masses lead to strong quantum-confinement effects which enable the operation of devices at higher temperatures. Wide band gap of III-nitrides leads to the emission in the blue and ultraviolet spectral range, which is not accessible with most of the other materials. In this work, simulation insights into the light emitting properties of III-nitride quantum dots and nanowires will be presented.

We performed the calculations of excitonic and biexcitonic states in self-assembled GaN/AlN quantum dots with special emphasis on the use of these dots for single-photon source applications [1]. Theoretical methodology for calculation of single-particle states was based on 8-band strain-dependent envelope function Hamiltonian, with the effects of spin-orbit interaction, crystal-field splitting, and piezoelectric and spontaneous polarizations taken into account. Exciton and biexciton states were found using the configuration-interaction method. Optimal dot heights for their use in single-photon emitters were determined for various diameter-to-height ratios.

Next, we investigated the electronic properties of InGaN quantum structures embedded in site controlled GaN nanowires [2]. The InGaN structures under consideration consist of two sections: the middle one, which is formed on the polar c-facet, and the side one, which is formed on the semi-polar r-facets. These structures exhibit two-color emission at 384 nm and 488 nm. We identified that the main origin of two-color emission is higher In incorporation on the nanowire polar c-facet, while the influences of internal electric field and strain are less significant.

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Post-deadline Poster Presentations

Enhanced performance of organic solar cells with the addition of molecular $Mo_6S_{9-x}I_x$ nanowires and factors determining it

Nevena Celic[a*], Egon Pavlica[b], Miloš Borovšak[a], Jure Strle[a], Gvido Bratina[b], Patrick Denk[c], Markus Scharber[c], Niyazi Serdar Sariciftci[c], Dragan Mihailovic[a]

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Abstract. Here we present the improvement of performance of canonical P3HT:PCBM solar cells by embedding highly dispersed $Mo_6S_{9-x}I_x$ nanowires within the active layer or to the top of it. Adding $Mo_6S_{9-x}I_x$ nanowires increases the hole mobility ~2.5 times, resulting in 52% higher power conversion efficiency compared to control devices, suggesting that the hole mobility is the main factor that influences the performance of the cells with $Mo_6S_{9-x}I_x$ nanowires. We additionally explore the influence of regioregularity of P3HT on the incorporation of $Mo_6S_{9-x}I_x$ nanowires into the P3HT:PCBM blend. We introduce Raman and photocurrent imaging to find the spatial distribution of solar cell parameters and determine the influence of $Mo_6S_{9-x}I_x$ nanowires on short circuit current distribution over the solar cell area. We attribute moderately increased absorbance of the active layer of the devices with $Mo_6S_{9-x}I_x$ nanowires on the top of it to the scattering properties of $Mo_6S_{9-x}I_x$ nanowires.

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Quantum Transport Through Molecular Magnets

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Abstract. One of the goals of nanoscience is to manipulate molecular spins using electrical currents [1], in view of their possible applications as memory devices [2]. We study spin transport through an orbital of a molecular magnet with spin precessing in a constant magnetic field, connected to two metallic leads [3]. The molecular and electronic spins are coupled via exchange interaction. Expressions for spin currents are derived by means of the Keldysh Green's function technique [4]. The coupling between the electronic and molecular spins creates inelastic tunneling processes which contribute to the spin currents. The inelastic spin currents, in turn, generate a spin-transfer torque acting on the molecular spin [5, 6]. This back-action includes a contribution to the Gilbert damping [7] and a component that changes the precession frequency. The Gilbert damping coefficient, can be controlled by changing the bias and gate voltages, and has a non-monotonic dependence on the tunneling rates. Later, we apply oscillating voltages in the leads and treat them as a perturbation [8]. In the low ac-frequency regime the junction can be mapped onto a classical electric circuit. The time-dependent voltages allow to reveal the internal precession time scale by a conductance measurement if the ac frequency matches the Larmor frequency. Moreover, we show that the setup can be used to generate dc-spin currents with arbitrary magnetization direction.

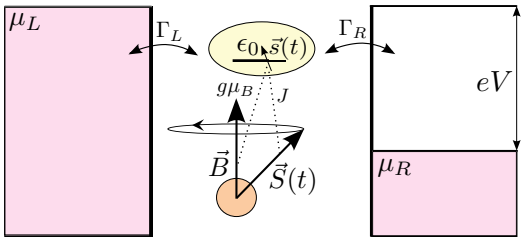

FIGURE 1. Tunneling through a single molecular orbital with energy ϵ_0 coupled to the spin $\vec{S}$ of the molecular magnet via exchange interaction with the coupling constant J, in the presence of a constant magnetic field $\vec{B}$.

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