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Localized Pairs And Pseudogap Near The Superconductor-Insulator Transition In Amorphous Superconductors

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Abstract. Physical meaning of the concept of localized superconducting pairs is discussed basing on analysis of behavior of granular superconductors and of superconductors with low electron density, and the parity effect. Experimental evidence of the existence of localized pairs relies on measurements of the magnetoresistance and on STM measurements of the density of states. Transformation of superconductor into insulator is not necessarily accompanied by appearance of localized pairs. Some factors should favor their appearance. In particular, these may be proximity of metal-insulator transition which leads to fractal dimensionality of electron wave functions, or certain correlations in the random potential.

The talk is based on two recent publications [1,2].

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Deciphering the enigma of high-T_c superconductivity in cuprates - one atomic layer at a time

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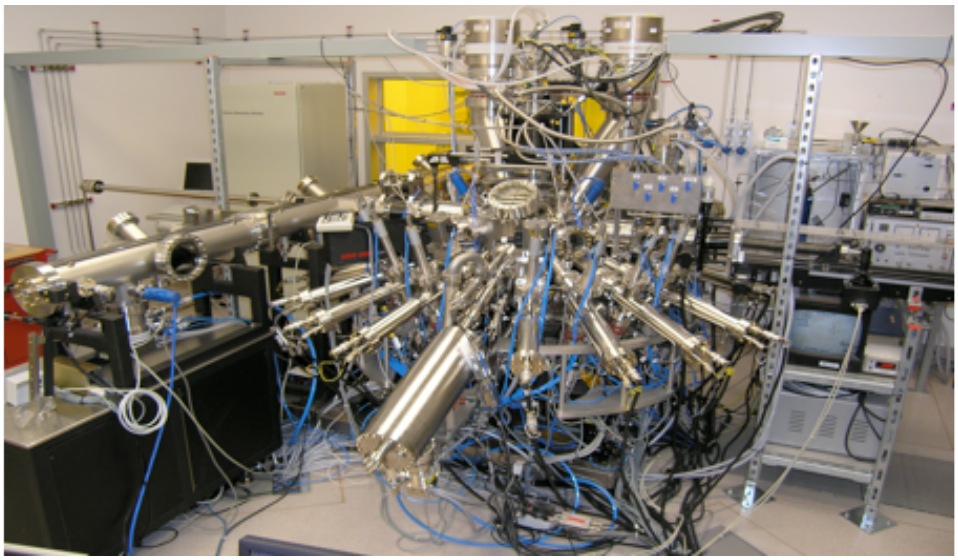
Abstract. Using a unique molecular beam epitaxy system we synthesize digitally - atomic layer by layer - thin films, multilayers and superlattices of cuprates and other complex oxides. The constituent layers can be just one-unit-cell thick and the interfaces atomically perfect. Various heterostructures are designed to enable novel experiments that probe the basic physics of high-temperature superconductivity (HTS).



In this talk, I will review our recent experiments on such films and superlattices, some of which involved advanced research tools such as synchrotron-based Resonant soft X-ray scattering and COBRA surface crystallography, Angle-resolved time-of-flight ion scattering, Ultrafast electron diffraction, Low-energy muon spin resonance, THz spectroscopy, etc. Some key questions in HTS physics - about the dimensionality, relevant interactions, the roles of (in)homogeneity and fluctuations – are answered as follows:

(i) In an isolated single CuO_2 plane without holes, quantum spin liquid forms.[1]
(ii) In an isolated CuO_2 plane doped with holes, HTS can occur with T_c even higher than in the bulk.[2]
(iii) HTS cuprate samples can be quite homogeneous (have a very sharp and uniform SC gap, etc.)[3]
(iv) HTS and anti-ferromagnetic phases separate on the scale of 1 Å in space and 1 eV in energy.[4]
(v) Pseudo-gap state mixes with the SC state on the 1,000 Å length scale ("Giant Proximity Effect")[5]
(vi) *In-plane* charge excitations are strongly coupled to *out-of-plane* lattice vibrations.[6]
(vii) Strong *phase* fluctuations drive the SC transition, but 10-15 K above T_c they fade out.[7]

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Phase and DOS Inversion in Superconductor/Ferromagnet Structures.

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The talk reviews recent fundamental and applied investigations of superconductor/ferromagnet structures carried out by Chernogolovka experimentalists in collaboration with different scientific groups. Nb/CuNi bilayers and Nb/CuNi/Nb Josephson sandwiches were investigated in detail to study different effects related to the order parameter spatial oscillations. Reentrant and double-extinct behavior of superconductivity of S/F bilayers was demonstrated [1,2]. The oscillations of the critical temperature of S/F bilayers are a consequence of interference between the part of the incoming pair amplitude reflected at the S/F interface and the pair amplitude reflected at the outer surface of the ferromagnetic layer. The double extinction of superconductivity was observed giving evidence for the multiple reentrant behavior predicted by theory. Moreover, successful experiment on DOS inversion in S/F(Nb/CuNi) bilayers was carried out in collaboration with Paris group [3]. Clean ("juvenile") surface of ferromagnetic CuNi layer was prepared directly in ultra-high-vacuum STM chamber. Recently, the fabrication technology of the superconductor-ferromagnet-superconductor (SFS) π-junctions based on Nb/CuNi/Nb sandwiches was substantially improved and offered the basis for realization of integrated logic circuits including both conventional and π-type Nb-based Josephson junctions. Use of the complementary elements ensuring the well-defined phase shift in the single flux quantum (SFQ) circuits is particularly favourable for reliable storing and processing signals. I will report on successful integration of the SFS π-junction in the Toggle Flip-Flop (TFF) circuit [4]. A quantum Josephson circuit, a π-biased phase qubit, was also realized [5]. Coherent qubit operation (Rabi oscillation of the excited qubit state population probability) was demonstrated. We find no degradation of the measured coherence time compared to that of a reference qubit without a π-junction.

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Zero-field quantum Hall effect in two-dimensional toroics

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Abstract. Crystals with toroidal magnetic order (toroics) are discussed as topologically nontrivial systems that exhibit fundamental feature similar to observed in the quantum Hall effect (QHE). A chiral edge Hall current with quantized conductance has a topological origin [1]. 2D lattice in periodic internal magnetic field, introduced by Haldane [2], directly predicts a new state of matter similar to the integer QHE state without external magnetic field. Quasiparticle spectrum with edge chiral fermion excitations without partners of opposite chirality turns out to be nonsymmetric with respect to inversion of quasi-momentum. In the excitonic insulator [3] with coinciding band extrema, we discuss electron-hole pairing in 2D system that breaks time-reversal symmetry due to toroidal magnetic order with imaginary order parameter [4]. We show this order results in an asymmetry of the quasiparticle spectrum and corresponds to topologically nontrivial insulator similar to zero-field QHE state. We prove the equivalence between Haldane's model and two-band excitonic insulator. Also, we show that magnetoelectricity is a generic feature of systems with toroidal magnetic order. We discuss the conditions under which the state with toroidal magnetic order could be the ground state of the system. When the positions of the extrema of nested valence and conduction bands do not coincide, there is a rise of density-wave states with broken translational symmetry. We discuss a nodal charge or spin-density-wave state such as toroics (toroidal moment density waves). When an additional order parameter with opposite reflection symmetry is introduced to a nodal density-wave state, the system turns out to be fully gapped [5]. We consider topological properties of such insulators in which gapping nodal points transforms the system from nodal density-wave state to topological density-wave insulator.

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Magnetism and Superconductivity in Iron Chalcogenide Superconductors

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Abstract. I will outline recent developments in synthesis and characterization of iron based chalcogenide superconductors. This will include binary anti - PbO type (11) as well as recently discovered ThCr2Si2 – type (122) superconductors. Selected single crystal thermodynamic, transport and magnetic characterization results will be presented as well as their connection with some key structural parameters that have significant influence on magnetic and superconducting states.

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Evidence for Dynamic Charge Inhomogeneities in $La_{2-x}Sr_xCuO_4$ in the Pseudogap Regime

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Abstract. The role of nanoscale inhomogeneities in the pseudogap regime in cuprates remains one of the key questions of high-T_c superconductor (HTSC) research. Inhomogeneities arise due to the existence of several competing degrees of freedom, such as orbital, spin, charge, and lattice. In particular, general arguments suggest that, in a lightly doped material, the system will undergo a nanoscale phase separation, leading to the possibility for the emergence of the associated glassy or out-of-equilibrium dynamics. The nature of the ground state is of great interest, because it is from this state that the HTSC emerges with hole doping. While spin glass (SG) behavior has been well established over a wide range of dopings, studies of charge dynamics have been relatively scarce. Here we review a set of experiments specially designed to probe the charge dynamics and its evolution as a function of doping near the transition to a HTSC.

The resistance (R) noise spectroscopy employed at low temperatures (T) is a technique that is well suited for probing the charge dynamics in these materials. Measurements of the R noise were performed on the insulating $La_{1.97}Sr_{0.03}CuO_4$ single crystals at low T, deep inside the SG phase, in both out-of-plane [1,2] and in-plane [3] configurations, and also in the presence of the in-plane and out-of-plane magnetic fields (B). The results indicate that the charge dynamics becomes increasingly slow and correlated as $T \to 0$. The analysis of the higher order noise statistics provides evidence for the existence of a collective ground state of charge clusters ("cluster charge glass") located in CuO_2 planes, which seem to coexist with charge-poor antiferromagnetic domains that are frozen at such low T. The charge glass behavior is accompanied by the emergence of a hysteretic positive magnetoresistance (MR) and the difference between zero-field cooled and field-cooled $R(B = 0)$ [4]. The hysteresis and memory exhibited by the MR are further used as a practical tool to detect the underlying charge glassiness in $La_{2-x}Sr_xCuO_4$ (LSCO) as a function of doping x. For that purpose, the in-plane MR was measured in a series of molecular-beam-epitaxy grown LSCO thin films with $0.03 \leq x \leq 0.08$ [5] that extends from the insulating into the superconducting region. Signatures of charge glassiness were observed at low T over a wide range of x, and they were used to map out a (T,B) phase diagram of the charge glass state in LSCO. The charge glass behavior is clearly suppressed with doping. Furthemore, a large and abrupt change in the MR curves and in the phase boundary are observed for a small change in x from 0.05 to 0.055. A detailed analysis strongly suggests the presence of superconducting fluctuations for $x \geq 0.055$ and a coexistence of the charge glass state with superconductivity.

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The electronic properties of $Sr_{1-x}La_xCuO_2$: an electron-doped cuprate.

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Abstract. Most of the studies on e-doped cuprates have been conducted on one cuprate family[1] : $Ln_{2-x}Ce_xCuO_4$ (Ln= Pr, Nd, La…) while a number of hole-doped cuprates have been investigated. The compound $Sr_{1-x}La_xCuO_2$ is another e-doped cuprate with a very simple structure called the "infinite layer" structure only composed of CuO_2 planes separated by (Sr, La) layers. However it is very difficult to synthesize it: ceramic samples are made under high pressure and no single crystals have been obtained so far. The studies on this compound have been first conducted on ceramic or oriented powder samples[2] and more recently on epitaxial thin films which allowed to perform studies of the transport properties on single crystal-like samples[3-7]. I will review the electronic properties of this compound in the superconducting and in the normal state by contrasting them with the properties of hole-doped cuprates.

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Multiple Andreev Reflection Spectroscopy of FeAs-based High Tc Superconductors

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Abstract. Novel superconducting compounds based on rare earth oxypnictides REO(F)FeAs (RE = La, Sm, Gd, etc.) [1] are currently in the focus of research interest. The Fermi surface for 1111 system consists of quasi-2D hole sheets centered at the Γ point and two electron sheets at the M points of the first Brillouin zone. Correspondingly, many of the available theoretical and experimental data indicate that the FeAs based materials are multiband superconductors [2]. Several data were reported in favor of s± or s++ order parameter symmetry, making the experimental situation regarding the 1111 compounds uncertain. The magnitude and structure of the superconducting gap Δ is intimately related to the pairing mechanism. ARPES measurements are not sensitive enough to resolve fine details of Δ on the sub-meV scale. That makes this parameter accessible nearly exclusively from point contact spectroscopy. However, for 1111 compounds which have the highest T_c, the available experimental data on Δ are rather inconsistent [2], even for the most intensively studied SmO(F)FeAs. Various types of conclusions have been obtained including d-wave like, single gap s-like, and multi-gap behavior. We performed recently the superconducting gap measurements in nearly optimally doped GdO(F)FeAs, and CeO(F)FeAs samples by SNS Andreev spectroscopy using the break junction technique [3]. Until now gap measurements have not been done for Gd-1111, an analogue to Sm-1111 superconductor with similar $T_c \sim 53$K. We have unambiguously detected the presence of two superconducting gaps, whose values averaged over large number of spectra are $\Delta_L = 10.5 \pm 2$ meV, $\Delta_S = 2.3$ meV for GdO(F)FeAs, and $\Delta_L = 8$, $\Delta_S = 1.7$ meV for CeO(F)FeAs. It is also found that the gap values for various RE-1111 compounds scale linearly with Tc.

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- 100 Years of Superconductivity - Experimental Facts and Theoretical Ingredients for The Pairing Mechanism in HTS Cuprates

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Abstract. Accumulating experimental data for the the structure and origin of the *bosonic spectral function* in high-temperature superconducting (HTS) cuprates at and near optimal doping are discussed. Some global properties of the bosonic spectral function, such as its shape and number and positions of peaks, are extracted from *optics, neutron scattering, ARPES and tunnelling measurements*. These analysis gives convincing evidence for strong electron-phonon interaction (EPI) in HTS cuprates (at and near the optimal doping) with large EPI coupling constant is approximately 1-3. This implies some important ingredients for the microscopic theory of d-wave pairing in HTS cuprates at and near the optimal doping. These are: strong EPI, strong correlations - both incorporated in an extended Migdal-Eliashberg theory for EPI in strongly correlated systems. The latter give rise to the forward scattering peak (FSP) which in conjunction with the weakly screened Madelung EPI in the ionic-metallic structure of layered HTS cuprates makes EPI responsible for the strength of Cooper pairing, while the residual Coulomb interaction (by including spin fluctuations) triggers d-wave pairing [1].

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Microwave Cooling of Josephson Plasma Oscillations

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Abstract. The radiation pressure is used for cooling atoms, ions and optomechanical devices. In a Fabry-Pérot interferometer in which one of the two mirrors vibrates, the Brownian motion of the vibrating mirror and hence its effective temperature can surprisingly be lowered by increasing the power of light. There is a straightforward analogy with a Josephson junction irradiated with microwave photons, where the phase difference between the wavefunctions of two superconductors, the Josephson phase, takes the role of the mirror position. I'll show that the microwave field acts on the Josephson phase as the radiation pressure does on a vibrating mirror. Specifically, when coupled with a high quality microwave cavity, the Josephson junction generates sideband resonances for each cavity mode. Out-of-equilibrium phase heating or cooling is achieved by microwave radiation at these sidebands, corresponding to the Stokes and anti-Stokes scattering, respectively. Cooling and heating increase with microwave power.

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Manipulation of individual microscopic two-level systems in amorphous oxide

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Abstract. Experiments with quantized Josephson plasma oscillations in tunnel junctions display signatures of coherent coupling to individual microscopic defects acting as two-level systems (TLSs). These defects manifest themselves by avoided level crossings in microwave spectroscopy data reflecting the dependence of the Josephson plasma frequency on the current flowing through the junction. They are currently understood as nanoscale dipole states emerging from metastable lattice configurations in amorphous dielectrics forming the oxide layer forming the tunnel barrier of Josephson junction. Such dipolar TLSs couple to the electrical field inside the junction which oscillates at the Josephson plasma frequency. I will present our recent experiments in which we use a Josephson junction for manipulating the quantum state of a single TLS. These experiments allow to directly measuring of the energy relaxation T_1 and dephasing T_2 times of an individual microscopic dipole-like TLS. Driving Rabi oscillations of the junction tuned close to a resonance with TLS leads to the observation of true 4-level dynamics [1]. The multi-photon spectroscopy allows for direct probing of hybridized states in the combined junction-defect coupled quantum system [2]. New method of direct microwave driving made it possible to study the temperature dependence of coherence times of individual TLSs [3]. Moreover, the observation of TLSs which have much longer coherence times than the macroscopic qubit renders them interesting for quantum information processing purposes, which we experimentally explored by generating entanglement between two TLSs mediated by the qubit [4].

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Lattice Anomalies In Iron Pnictides

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Abstract. The discovery of a new family of superconductors, the Fe pnictides,[1] has attracted the interest of scientific community since they have a high transition temperature and many similarities with the cuprates. As in cuprates, the undoped compound is an antiferromagnet (AF) that becomes metallic upon doping and at certain levels superconducting. It appears that lattice effects and the geometry of the $FeAs_4$ tetrahedra are important to the properties of the Fe-based pnictides, including superconductivity.[2] In a high quality oxygen deficient $NdFeAsO_{0.85}$ sample with T_c=53.5K [3] high resolution synchrotron diffraction data[4,5] and Fourier Transform Infrared (FTIR) measurements[6] have shown lattice anomalies at ~180K. In more detail, the low temperature FTIR studies indicated a slight softening of an As phonon mode at this temperature.[6] On the same compound the high resolution synchrotron diffraction data collected with a dense sampling in the temperature range 10-295K revealed that the structural modifications start around ~180K as in the IR data and disappear at T_c.[4,5] Evidence of a similar softening at the spin density wave transition temperature ~178K and an anomaly across T_c has been observed in a Raman study of superconducting $S_{1-x}K_xFe_2As_2$.[7] In a femtosecond spectroscopic study of a $SmFeAsO_{0.8}F_{0.2}$ superconductor the presence of a pseudogaplike feature with an onset above 180K was induced.[8] Besides, in the non-superconducting $LaFeAsO_{1-x}F_x$ a lattice anomaly has been detected also at ~180K that disappears upon AF ordering.[9] Similar effects that have been detected in other pnictides indicate that these characteristics might be a general feature in these compounds. The lattice anomalies apparently are not connected with a structural phase transition. The disappearance of the anomaly crossing T_c and its association with the superconducting Fe-As planes point to a connection with the superconducting carriers.

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Long-range Spin-triplet Proximity Effect in Josephson Junctions with Multilayered Ferromagnets

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Abstract. Long-range spin-triplet superconducting correlations that are induced in heterostructures made of superconductors with the usual singlet pairing and inhomogeneous ferromagnets have attracted considerable attention recently [1]. This exotic state, even in momentum (s-wave) and with odd in frequency spin-triplet pairing, has significantly larger penetration length. As a result, the Josephson supercurrent through very thick/strong ferromagnets was observed [2-4]. Dominant spin-triplet effect on the supercurrent can be realized after inserting a singlet-to-triplet "converter", two thin layers of weak ferromagnet (F') placed between superconductors (S) and a thick/strong ferromagnet (F), acting as a "filter" which suppresses the short-range correlations in SF'(F)F'S heterostructures [5, 6]. However, in the simplest heterostructures with ferromagnetic bilayer, SF_1F_2S, the influence of misalignment of magnetizations on the Josephson current cannot be attributed to the emergence of long-ranged spin-triplet correlations [7].

We present theoretical study of the Josephson effect and pairing correlations in planar SF_1F_2S junctions that consist of conventional superconductors connected through two metallic monodomain ferromagnets with transparent interfaces. Both singlet and triplet pair amplitudes, the Josephson current-phase relations, and density of states for arbitrary orientation of magnetizations are calculated from the self-consistent solutions of Eilenberger equations in the clean limit and for moderate disorder in ferromagnets. We have found that the long-range spin-triplet correlations give dominant second harmonic in the Josephson current-phase relation of highly asymmetric SF_1F_2S junctions [8]. The resulting ground state degeneracy of the Josephson junction (like at 0-pi transtions) is now experimentally accessible and has important potential applications in the field of quantum computing: Quantum superposition of macroscopically distinct states in the absence of an external magnetic field, and quantum interferometers (SQUIDs) which operate with two times smaller flux quantum [9].

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Infrared study of correlated systems

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Abstract. Infrared spectroscopy is a powerful technique in the study of condensed matter since the energy of electronic excitations and lattice vibrations fall in its range. It is very useful in the study of electronic correlations, electron-phonon interactions or some structural correlations. Very often these measurements need a broad spectral range and a high brilliance available at synchrotron light sources. In view of the creation of an infrared beamline at the Swiss Light Source, few research topics and experiments will be highlighted.

Graphene Nanopores: Structure, Properties and Function

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Abstract. Graphene is an exceptional material for high-speed electronics, as well as a revolutionary membrane material due to its strength and atomic thickness. Nanopores in membranes of graphene are currently regarded as candidates for ultrafast DNA sequencing. The unique band structure of graphene dictates phenomena that affect its surface properties, electronic properties, and interactions with ions and molecules in a way that is to date poorly understood.

In this talk, we present results1 on the translocation of individual DNA molecules through nanopores created in graphene membranes2. Unlike traditional solid-state nanopore materials that are insulating, graphene is an excellent electrical conductor, and its use opens the door to a new future class of nanopore devices in which electronic sensing and control is performed directly at the pore. Due to the thin nature of the graphene membranes, and the reduced electrical resistance3, we observe larger blocked currents than for traditional solid-state nanopores. We also show how ionic current noise levels can be reduced with the atomic-layer deposition of a few nanometers of oxide over the graphene surface.

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Zero-modes and The Structure Of Dirac's Vortex Core in Graphene

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Abstract. The vortex in any $O(2)$ order parameter on graphene's honeycomb lattice is known to produce zero-energy states. I will discus how these rather special states in the middle of the spectrum induce local competing order in the core of the vortex. The local order parameters in general close the algebra $Cl(3) \times U(1)$, where $Cl(3)$ is the three dimensional Clifford algebra, with the members of this algebra depending on the type of order supporting the vortex. The superconducting order will be discussed in some detail, and the curious duality between the topological insulation and the superconductivity in graphene will be pointed out.

Spin pumping in magnetic tunnel junctions and topological insulators: Theory and experiment

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Abstract. The pursuit of the "second-generation" spintronics has been focused on harnessing *coherent spin states*. The salient examples of phenomena involving both coherent spins and their time evolution is the *spin-transfer torque* (STT) and its Onsager reciprocal effect,[1] termed *spin pumping* because it occurs in setups without any applied bias voltage, where microwave driven precessing magnetization of a single ferromagnetic (F) layer emits *pure* spin current into adjacent normal metal (N) layers. While pumped spin current has been detected by converting it into ~10 nV voltage signal in $N_1|F|N_2$ junctions, a puzzling and much larger signal ~1 μV was measured in our recent experiments[2] on F|I|N tunnel junctions with AlO_x insulating barrier I. This observation is unexpected in both standard scattering theory and nonequilibrium Green function (NEGF) in the rotating frame[3] approaches to pumping which predict no signal at adiabatic level ~ω and only a small correction ~ω^2. However, neither of these two approaches is capable of taking into account *strong spin-orbit coupling* (SOC) directly at the F|N pumping interface, such as the Rashba one demonstrated to exist in recent experiments on STT in F|I|N junctions.[4] Unlike the recent theoretical efforts[1] on STT in the presence of SOC, very little is known about such effects on spin pumping. Here we discuss novel solution to time-dependent NEGFs, which describes pumping in the presence of SOC exactly at the level of one microwave photon absorption or emission processes, to explain ~ω voltage signal observed experimentally.[2] A similar device, with strong interfacial SOC, can be created by the fabrication of F|TI heterojunctions where TI is a newly discovered three-dimensional (3D) topological insulator whose SOC generates band gap in the bulk and metallic states on the surface with quasparticles behaving as massless Dirac fermions (akin to graphene but with spin splitting of states due to SOC). Microwave driven magnetization of F|TI junction will lead to voltage signal of spin pumping whose unique features can be employed to detect quantum Hall liquid on the surface of TI in proximity to F. Finally, we discuss pumping into a 2D topological insulators (TI) whose helical edge states lead to quantized pumped spin current even at very small input microwave power thereby offering a prospect for *giant spin battery effect*.[5]

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Numerical Study Of Critical Behavior Of Two-dimensional Nonequilibrium Zero-temperature Random Field Ising Model

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Abstract. We present a numerical study of nonequilibrium zero-temperature random field Ising model in two dimensions. We have found that the model displays a critical behavior for disorder $R_c = 0.54 \pm 0.02$ and external magnetic field $H_c = 1.275 \pm 0.020$, when magnetization is $M_c = 0.00 \pm 0.01$. The pertaining critical exponents are: exponent $\beta = 0.15 \pm 0.04$ (giving scaling of magnetization with disorder at the critical field), size exponent $\tau = 1.54 \pm 0.05$, cutoff exponent $\sigma = 0.10 \pm 0.01$ and correlation length exponent $\nu = 5.15 \pm 0.20$. Our findings are based on scaling analysis and collapsing of data, obtained in extensive simulations of systems with linear sizes up to $L = 131072$, which were sufficiently large to clearly display the critical behavior.

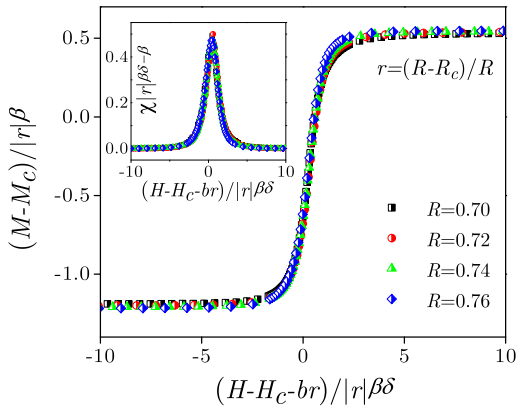

FIGURE 1. Scaling collapse of magnetization M (main panel) and susceptibility χ curves (inset) for disorders $R = 0.70 - 0.76$ and system size $L = 131072$. The curves are averages of 30 random field configurations for each R.

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Helically Coiled Carbon Nanotubes: Symmetry Based Study

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Abstract. The first report of experimental evidence of regularly coiled carbon nanotubes [1] appeared in 1994. They were predicted to have excellent electro-magnetic properties. However, geometrical structure, formation mechanism and theoretical aspects of these nanotubes still remain unresolved [2]. In this work a simple model of hexagonal, helically coiled single wall carbon nanotubes is proposed and their line group symmetry [3] is determined. Further, electronic band structure and optical absorption of the coiled nanotubes in relaxed configurations is calculated by means of fully symmetry adopted density functional tight binding method implemented into the POLSym code [4]. Electrical and optical properties of the straight and coiled carbon nanotubes of different chiralities are compared and analyzed.

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Testing the models of quasicrystals using their images in direct space

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Abstract.

We tested the broadly used model of icosahedral Al-Pd-Mn to the STM (scanning tunnelling microscopy) images of its clean surfaces perpendicular to the symmetry axes. We placed the surfaces in the model over the most dense layers of atoms (see, for example [1]), inspired by the Bravais' rule for ordinary crystals. Latter we compared the appearance of the surfaces to their simulations [2]. We concluded that the model, produced out of the diffraction data and put on an ideal icosahedral tiling in the direct space needs some corrections, either in the position of Al atoms, or in the distribution of the atomic positions.

Now we study the old HREM (high-resolution electron microscopy) [3] and the recent STEM (scanning transmission electron microscopy) [4] images of the decagonal/pentagonal Al-Cu-Co and relate the atomic positions to an ideal pentagonal tiling [5]. Already in the direct space, without using the coding of the model, we are able to show that the old model [6], based only on the diffraction data and put on the same tiling [5] overestimates the density of certain 5f symmetric atomic local configurations in the quasicrystal [7].

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$Al_3(LiSc)$ Core/shell Ordered Nanostructures Embedded in Solids

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Abstract. This study will illustrate the importance of understanding the fundamental features that underlie the behavior of nanoscale phases with coherent interfaces embedded in a solid matrix and their role in the evolution of microstructure in materials. The fundamental principles established using model alloy systems are employed in the design and testing of new materials such as systems for energy-related technologies. The effect of Li addition on core/shell precipitate formation in the ternary AlLiSc alloys has been studied by a range of advanced microscopy and spectroscopy techniques, such as high resolution TEM with exit wave reconstruction, atomic resolution HAADF imaging, and energy filtered electron energy loss spectroscopy (EELS), combined with the first principle calculation and continuum thermodynamic modeling to uncover the role of Li. For the ternary AlLiSc alloy we show a way of producing a uniform distribution of coarsening resistant monodispersed $Al_3(LiSc)$ core/shell particles (see Figure 1) in an Al matrix with unusually narrow size distribution. This approach uses differential diffusivities and solubilities of Li and Sc in an Al matrix. Our model shows that the complex precipitation pathway can be fully understood within the framework of classical theories of nucleation and growth.

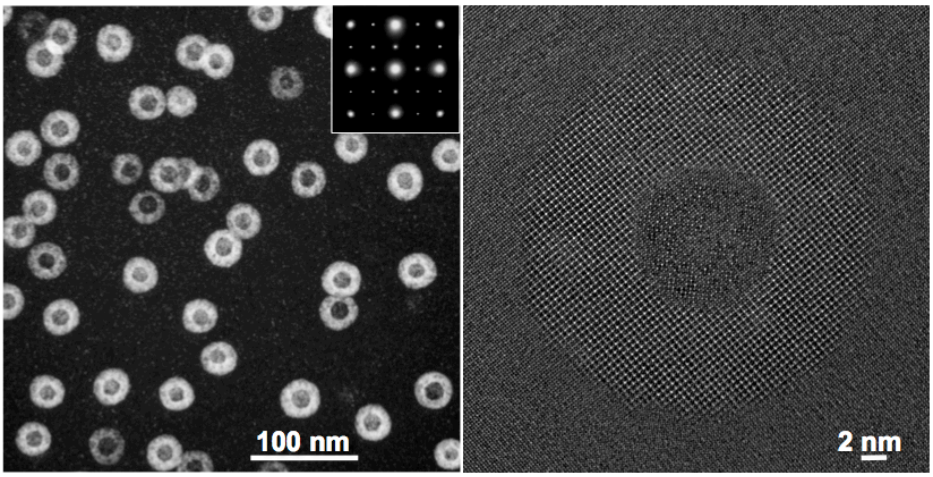

Figure 1. Dark field TEM micrograph of an AlLiSc alloy imaged with the (110) superlattice reflection, showing uniform distribution of core-shell nanoparticles with $L1_2$ structure; inset shows <001> zone axis diffraction pattern (left) and high resolution TEM micrograph of a single $Al_3(LiSc)$ core-shell nanoparticle (right).

Acknowledgements. Electron microscopy was performed at the National Center for Electron Microscopy, which is supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. VR acknowledges support of Nanotechnology and Functional Materials Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, funded by the European FP7 project No. 245916.

Bandgap Narrowing in Titanium Oxide Semiconductors by Non-Compensated Anion-Cation Codoping for Enhanced Visible Light Photoactivity

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Abstract. With the seminal discovery of water splitting by Fujishima and Honda in the early 1970s, titanium dioxide (TiO_2) emerged as the premier photocatalysts for solar energy utilization.[1] However, TiO_2 has a wide intrinsic band gap and absorbs light only in the ultraviolet region resulting in less than 3% solar energy conversion efficiency. Reducing the band gap of TiO_2 is the main avenue for increasing the conversion efficiency. In this talk I discuss a conceptually new approach for bandgap narrowing of TiO_2 and other wide bandgap photocatalysts using non-compensated codoping.[2] Non-compensated codoping consists of simultaneous doping using two dopants with opposite but unequal oxidation states. The electrostatic attraction within the anion-cation dopant pair enhances both the thermodynamic and kinetic solubility, and the non-compensated nature ensures the creation of tunable intermediate bands that effectively narrow the bandgap. The key features of the concept are demonstrated using first-principles calculations. The codoping of TiO_2 with the non-compensated Cr-N pair was studied in a form of nanoclusters synthesized by sol-gel methods and thin films grown by pulsed laser deposition. The compositional, structural, electrical, and photocatalytic properties of TiO_2 codoped with the non-compensated Cr-N pair were characterized using, XRD, XPS, STS, and EPR. The location of the electronic states introduced by Cr-N codoping of TiO_2 thin films were studied by x-ray absorption, x-ray emission and resonant photoemission spectroscopy. The x-ray spectroscopic data show that Cr-N codoping effectively reduces the bandgap of TiO_2 from 3.2 to 1.8eV with new delocalized states associated with Cr-N codoping appearing at the top of the valence band.

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Tuning Electronic Properties of Graphene-based Nanostructures by the Hydrogenation

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Abstract. We applied Density Functional Theory (DFT) to investigated the role of adsorbed hydrogen on electronic properties of graphene as well as metallic single-wall carbon nanotubes (CNTs). The favorable H adsorption structures at free-standing graphene and at the graphene layer deposited on Ir(111) surface are identified from the computational simulations supported with the state-of-the-art experiments [1–3]. We show that patterned H adsorption on graphene supported by Ir(111) induces a band-gap of at least 0.4 eV.
The DFT calculations demonstrate that upon H adsorption, initially metallic CNTs transform to magnetic semiconductors with electronic properties remarkably similar to those of graphene nanoribbons with zig-zag edges.

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Ion Beam Induced Modifications of Metal (Fe or Co) Thin Films/Si bilayers

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Abstract. The aim of this talk is to briefly review our experimental findings and our attempt in modeling the atomic transport processes and reactions across the metal/semiconductor interface, at the energies where nuclear stopping prevails. For the particular case of noble-gas ion induced reactions in metal (Fe or Co) thin films/Si we have studied in detail the formation and growth of silicides as a function of the ion-beam mass, energy, fluence, charge state and substrate structure and sample temperature, using a combination of analyzing methods such as Rutherford backscattering, X-ray diffraction, transmission electron microscopy and conversion electron Mössbauer spectroscopy. Ion beam mixing of thin films/Si bilayers due to Ar and Xe ion irradiations were investigated. The effect of a 1.0 keV Ar^+ ion pre-amorphization of the Si substrate on interface mixing in thin films/a-Si bilayers was analyzed. In order to interpret the mixing rates in this most general case, we considered mixing through thermal local or global spikes and compound phase formation.

Multi-scale Molecular Designing of Nanoparticles and Advanced Materials

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Abstract. The science and technology of nanostructured materials have gained worldwide prominence in recent years as areas with great potential for new technological and cultural progress. Nano-structured particles and compact materials with particle sizes smaller than 100 nm can be synthesized by various bottom-up and top-down methods. A variety of innovative methods for obtaining nanoparticles with highly controlled properties at molecular and nano levels, developed in our laboratory, will be reviewed in this presentation. They include aerosol, mechanochemical and sonochemical synthesis, various methods involving centrifugal dispersion of melted and dissolved products, sol-gel and chemical precipitation, as well as various polymerization procedures and methods for the fabrication of inorganic/organic nanocomposites and polymers. We will present numerous examples that illustrate the preparation of oxide, non-oxide, metallic, polymer and composite nanoparticles and experimental data related to size-dependent properties of nanomaterials. Attention will also be drawn to the designing of full-density nano-structured materials by powder processing without the influence of additional field during sintering, using only the sintering of nano-powders – a method recently developed in our laboratory. In brief, the presentation will cover a broad range of advanced materials, including engineering, optical, electronic, energy and catalytic materials, as well as biomaterials and pharmaceutical materials.

Rainbows with crystals and nanotubes

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Abstract. This talk is devoted to the crystal rainbow effect, which occurs in ion channeling in crystals and nanotubes. The effect is a consequence of the interference of the contributions of the atomic strings of the crystal to the channeling process. We shall begin with a detailed description of crystal rainbows. Then, it will be demonstrated that the crystal rainbow effect can be modeled simply and accurately by catastrophe theory. After that, we shall analyze the evolution of the angular distribution of channeled ions with the crystal thickness. The analysis will include the rainbow cycles, and the effects of spatial focusing and angular focusing of channeled ions. This will lead us to the theory of crystal rainbows. It will be demonstrated that it is the proper theory of ion channeling. Further, we shall describe how the effect of spatial focusing of channeled ions can be used for a subatomic microscopy. The talk will be continued with the rainbow effect occurring with carbon nanotubes. That will be followed by a consideration of the channeling star effect appearing with bundles of carbon nanotubes. Finally, it will be shown how an ion beam can be guided by a bent carbon nanotube.

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Localization-Delocalization Transitions of Semi-Flexible Bio-polymers

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Abstract. In the first part of this talk, we discuss the conformational behavior of DNA molecules adsorbed on cationic lipid membranes that are supported on grooved, one-dimensionally periodic micro-structured surfaces. We elucidate a striking ability of these periodically structured membranes to stretch DNA coils, in terms of surface curvature dependent potential energy attained by the adsorbed DNA molecules. Due to it, DNA molecules undergo a localization transition causing them to stretch by binding to highly curved sections of the supported membranes. In the second part of this talk, we discuss the unbinding of long semi-flexible bio-polymers from long line-like attractive potential wells (columnar traps). We reveal that this phase transition is an exactly solvable problem of statistical mechanics.

Theoretical Concepts for Dynamic Force Spectroscopy of Molecular Complexes

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Abstract. Reserach of the kinetics of molecular binding and the strength of forces that bind living molecules has been made possible by the dynamic force spectroscopy measurements [1–3]. Complexity of the problem steams from the size and geometry of molecules with number of binding sites, as well as the experimental setup itself—the measurements are done at finite, dynamically varying forces. Therefore suitable theoretical concepts are needed to interpret the experimental data in order to extract the quantitative measures of the binding forces, form of the potential and the lifetime of bond at *natural conditions* in the absence of external forces. Here we briefly outline how the reaction-rate theory [4] can be adapted for the situations where the focre-loading rate depends on the force itself. Based on the theory of complex systems, a methodology for the selection of force–distance curves is introduced [5] to cope with the enhanced fluctuations at the nanoscale objects. We demonstrate these theoretical concepts at work by nalaysing the sets of experimental data on peptide–RNA complex from HIV1 virus [3].

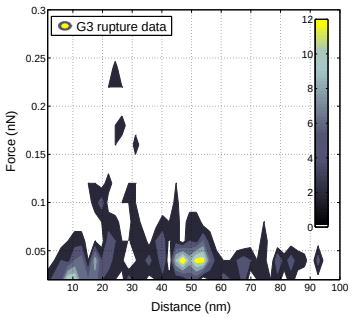

FIGURE 1. Rupture pattern for a set of similarity-related Force–Distance curves [5].

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Numerical Simulations of Complex Systems in Quantum and Classical Physics

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Abstract. In this talk we review our recent research on numerical simulations of various complex may-body systems. First, we will give an overview of the effective action approach [1–7] for numerical calculation of path integrals for non-relativistic many-body quantum system using a hierarchy of recursive relations derived from the underlying Schrödinger equation for general transition amplitudes. The use of the effective propagator expanded to high orders in the short time of propagation substantially speeds up the convergence of Path Integral Monte Carlo algorithm for calculation of general transition amplitudes, partition functions and expectation values. We will also present time-dependent formalism that allow numerical study of dynamics of quantum systems in time-dependent potentials.

In the second part of the talk, we will present molecular dynamics numerical simulations of granular materials [8–10]. In particular, we will present study of compaction of dense granular materials under the influence of vertical tapping. We analyze the compaction process for various values of friction coefficient and coefficient of normal restitution, and find that the time evolution of the density is described by the Mittag-Leffler function of order $0 < \alpha < 1$. We characterize the local organization of granular material in terms of contact connectivity and distribution of the Delaunay free volumes. Our analysis at microscopic scale provides evidence that compaction is mainly due to a decrease of the number of the largest pores. An interpretation of the memory effects observed for a discontinuous shift in tapping intensity is provided by the analysis of the time evolution of connectivity numbers and volume distribution of pores.

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Raman scattering on nanomaterials

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Abstract. The conventional Raman scattering spectroscopy is one of the most used and powerful techniques for characterization of nano-sized materials and structures. By proper analysis of optical mode shift and broadening in nanomaterials based on phonon confinement model, it is possible to deduce about the influence of various effects like particle size and size distribution, strain, change of phonon dispersion, substitutional effects, defect states and nonstoichiometry, electron-molecular vibration coupling. We have demonstrated potentials of this technique in CeO_2 and TiO_2 nanocrystalline systems analyzing their optical phonon properties.

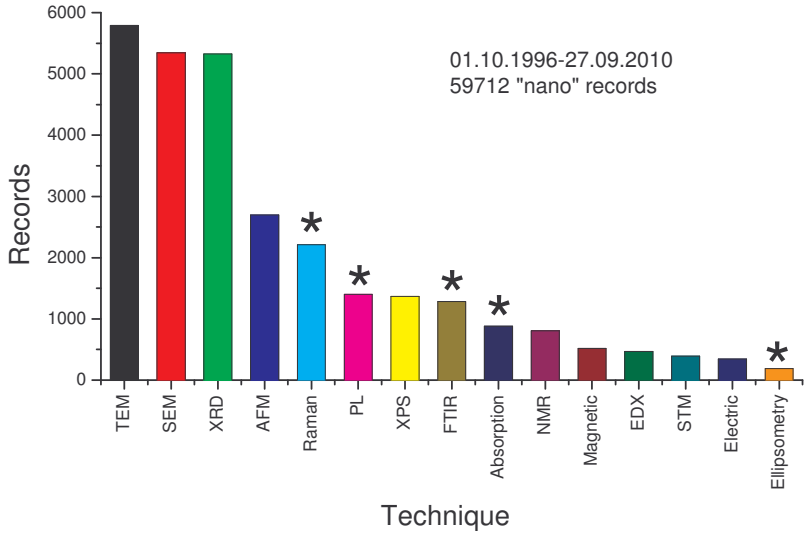

FIGURE 1. The most used techiques for nanomaterial characterization. Number of records in the period January 1996- July 2010, for the listed characterization techniques under the 58021 "nano" records (Source: ISI Web of Science).

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Mechanical and electrostatic molecular orbital gating in a single Zn-porphyrin molecule

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Abstract. Our ability to control charge transport in single-molecule devices depends heavily on our understanding of the conformation of a metal-molecule-metal junction. The electronic interaction of the molecule with the metallic electrodes determines both the alignment and the spacing of the energy levels that participate in charge transport. While previous reports have indicated a large influence of the junction configuration on the low-bias conductance of single-molecule junctions, spectroscopic information is scarce. In the few studies of current-voltage characteristics that exist, level positions were generally reported to be dependent on contact chemistry rather than configuration. Here, we demonstrate giant mechanical tunability in molecular junctions. The ability to adjust the distance between the electrodes in the nanometer range and to change the electrostatic potential in the junction with a gate electrode allows us to monitor the current-voltage characteristics of a thiol-anchored Zn-porphyrin molecule over several junction configurations and across different transport regimes. Depending on the particular geometry transport through both the HOMO and the LUMO molecular orbital can be observed. Our findings demonstrate that the electronic transport in a molecular junction can be modulated substantially by changing its conformation and offers prospects for mechanically driven molecular devices.

p-wave Superconductivity on Honeycomb Lattice

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Abstract. A topological (time-reversal invariant p-wave) superconductor in two dimensions was proposed in, X.-L. Qi, T.L. Hughes, S. Raghu, and S.-C. Zhang, Phys. Rev. Lett. 102, 187001 (2009), with two counterpropagating Majorana edge modes of opposite spin. We discuss p-wave order parameter instabilities of interacting fermions on honeycomb and bilayer honeycomb lattice to find if these systems may support the topological superconducting phase. We find that indeed most natural spin-independent nearest neighbor attractive interactions on bilayer honeycomb lattice (in an effective description) lead to two kinds of Cooper pairs with $p_x + i\, p_y$and $p_x - ip_y$ pairing, but due to fermion (spin and valley) doubling problem we do not find Majorana modes. If we suppress the spin (consider triplet pairing) the system becomes gapless in its bulk and lose its topological features.

Optical Spectroscopy of Single and Few-Layer Graphene

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Abstract. Here we present our research on optical properties of single and few-layer graphene obtained by mechanical exfoliation of the natural NGS graphite. The optical characterization involves micro Raman spectroscopy, UV/VIS spectroscopic ellipsometry and NIR FT reflectometry of graphene flakes on oxidized n-doped silicon wafers with a nominal oxide thicknesses of 100 and 300 nm. All instruments are equipped with a microscopic optics enabling a micrometer-size spot on the sample. The sample quality and determination of the flake thickness (number of graphene layers) is based on combined AFM and Raman measurements. As a result the optical parameters (*n*, *k*) and the optical conductivity (in units of the universal optical conductivity, $\sigma_o=e^2/4\hbar$) of graphene are determined.

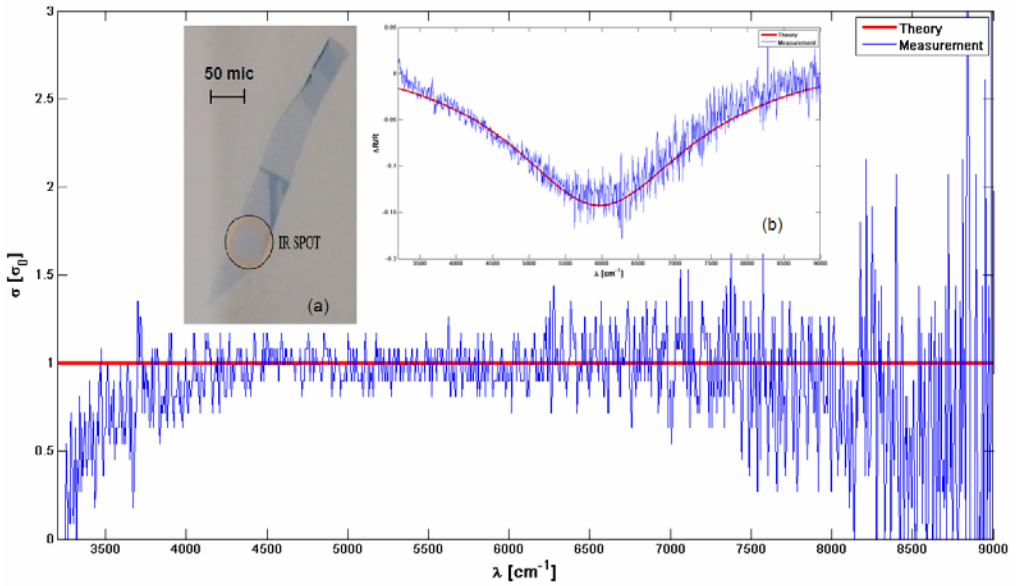

FIGURE 1. Retrieved conductivity of a large graphene flake (a) from the IR $(R_{gs}-R_s)/R_s$ spectrum (b) in units of the universal optical conductivity σ_o.

Contributed Speakers:

1	Stevan Nađ Perge	Delft University of Technology
2	Tatjana Vuković	University of Belgrade
3	Zorica Konstantinović	Institut de Ciencia de Materials de Barcelona
4	Mihajlo Vanević	Delft University of Technology
5	Vladimir Juričić	Universiteit Leiden
6	Ivana Petković	Centre CEA de Saclay
7	Patric May	Technische Universität Berlin
8	Radmila Panajotović	Open University
9	Ivan Belča	University of Belgrade
10	Ivica Bradarić	Institute of Nuclear Sciences Vinča, Belgrade
11	Ivana Vidanović	Institute of Physics Belgrade
12	Darko Tanasković	Institute of Physics Belgrade
13	Jaćim Jaćimović	EPFL, Lausanne
14	Viktor Cerovski	Institute of Physics Belgrade
15	Mihailo Čubrović	Lorentz Institute, Leiden University
16	Nenad Lazarević	Institute of Physics Belgrade
17	Nenad Vukmirović	Institute of Physics Belgrade
18	Igor Stanković	Institute of Physics Belgrade
19	Alberto Pomar	Institut de Ciencia de Materials de Barcelona
20	Milorad Milošević	Universiteit Antwerpen
21	Milan Radović	EPFL, Lausanne
22	Vladimir Jovanović	Institute of Physics Belgrade

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Single spins in InAs nanowires

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Abstract. We demonstrate coherent control of single spins in InAs nanowires. InAs is a promising material for spin qubits due to the strong spin-orbit interaction. Single electron spins are isolated in quantum dots that are defined in nanowires by local gate electrodes. In order to initialize and readout qubit states, we use double quantum dot configuration tuned to the spin blockade regime [1, 2]. Pauli spin blockade between triplet and singlet states is used to prepare the two spins in the triplet configuration and to distinguish between singlet and triplet states during the readout stage. We observe Rabi oscillations driven by electric dipole spin resonance (EDSR) and mediated by spin-orbit interaction. The highest Rabi frequency achieved is $\sim$ 57MHz, an order of magnitude faster compared to EDSR in GaAs/AlGaAs 2d electron gas [3, 4]. Due to a difference of 0.25 in Lande g-factors for the two dots we can selectively address the two spins with gigahertz electric fields. Ramsey decay time of $T_2^* = 8 \pm 1$ns suggests that nuclei spin bath is the main source of decoherence for this system [5]. Coherence time can be extended using spin-echo and dynamical decoupling techniques.

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Diffraction Intensities From Nanotubes: Fingerprints Of Symmetry

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Abstract. Many physical properties of various organic and inorganic nanotubes are directly influenced by tubes' geometry, while available techniques of sample growth give mixtures of nanotubes with diverse chiralities. Commonly, tube's characterization is based on theoretical calculations of diffraction intensity developed for carbon nanotubes [1, 2]. Still, tubes are often multi-wall and heterogeneous structures, so information obtained by such methods are not always reliable and sufficient. Therefore, fast simulation and analysis of diffraction patterns is of great importance.
Here we use symmetry of nanotubes to achieve this goal. As every tube is a monoperiodic system, i.e. its symmetry is described by one of the line groups [3], we utilize recently developed symmetry based calculations of diffraction intensities [4, 5] for the line group orbits. First, the method is applied on a single-wall carbon nanotube, as this is a single-orbit system with biunique relation between the symmetry group parameters and the tube's structure. The effect of tube's symmetry on the intensity distribution is discussed and particular features of the diffraction patterns are linked to group parameters. Next, diffraction intensities of double-wall nanotubes are analyzed. Derived expressions for total scattering amplitude in terms of group parameters of the individual walls enable us to elucidate all symmetry aspects of intensity distribution. Also, effects of mutual position of the walls can be analyzed. Finally, characterization of multi-wall carbon and molybdenum disulfide nanotubes is discussed. Presented results give better insight into intensities distribution along layer lines and provide important information needed for structural studies of nanotubes.

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Directed Self-Assembly in Manganite Thin Films

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Abstract. Oxide thin films often exhibit a tendency toward self-organized growth forming regular arrays of three dimensional nanostructures. This behavior offers enormous potential for the implementation of new nanodevices, while at the same time attracts great attention due to their rich physics. Among them, manganese perovskites showing colossal magnetoresistance and half metallic characteristics have emerged as promising candidates for miniature spintronic devices. Complex oxide thin films are often elastically strained, due to film-substrate lattice mismatch, and this lattice strain can, in some cases, select preferential growth modes leading to the appearance of different self-organized morphologies. In this work we report on the controlled fabrication of self-organized nanostructures in highly epitaxial $La_{2/3}Sr_{1/3}MnO_3$ thin films [1]. By carefully controlling growth rate dramatic changes of the surface morphology can be induced: from very flat surface, through nanometric mounds and nanoholes [2]. Best-defined nanoholes form in coherently grown films at low misfit irrespective to its sign [3]. These self-assembled features appear to be useful nanotemplate as demonstrated in the case of assisted self-assembly of Au nanoparticles (Figure 1).

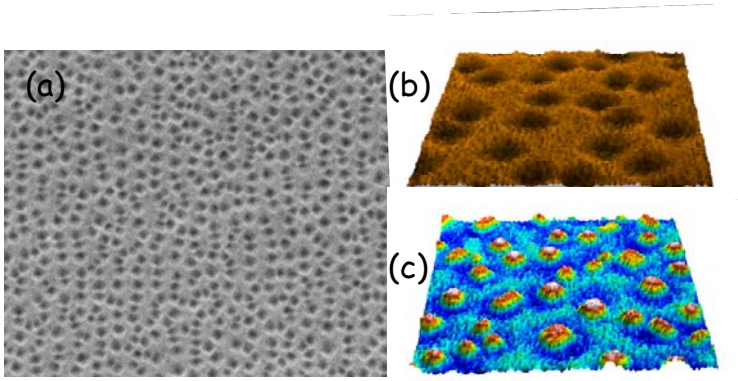

FIGURE 1. (a) Nanohole pattern of $La_{2/3}Sr_{1/3}MnO_3$ (SEM 3000x2500 nm^2 image). Small area 3D SEM image 500x500 nm^2 of bare film (b) and film with Au particles (c)

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Effects of Metallic Contacts on Electron Transport in Graphene

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Abstract. At a metal-graphene interface, the difference in work functions determines the direction of charge transfer and doping of the graphene layer. We report on a first-principles study of the conductance through graphene suspended between Al contacts as a function of junction length, width, and orientation. The charge transfer at the leads and into the freestanding section gives rise to an electron-hole asymmetry in the conductance and in sufficiently long junctions induces two conductance minima at the energies of the Dirac points for suspended and clamped regions, respectively. We obtain the potential profile along a junction caused by doping and provide parameters for effective model calculations of the junction conductance with weakly interacting metallic leads. Our first-principles results justify the widely used effective models of metal-graphene junctions.

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Quantum Criticality in Graphene

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Abstract. Half-filled graphene in its ground-state is a semimetal, which is a consequence of peculiar Dirac-like nature of its low-energy quasiparticles. Weak short-range interactions, such as nearest-neighbor Coulomb and on-site repulsion, for instance, are irrelevant near the semimetallic ground-state. However, when sufficiently strong they may lead to various quantum semimetal-insulator transitions that may be viewed as condensed-matter analogues of the chiral symmetry breaking in particle physics.

In this talk, I will address some of the general questions that arise in this context, namely, what interactions are allowed by the symmetries of the honeycomb lattice, as well as what symmetries are broken at the transition, which is intimately related to the question of the nature of the order parameter describing the transition [1]. I will also argue that a quantum field theory of the Gross-Neveu-Yukawa-type describes quantum-critical behavior of the interacting graphene system, and discuss some consequences of this scenario, in particular, emergent Lorentz symmetry at the critical point and universal amplitudes at the transition [2]. Finally, I will address the role of the weak long-range Coulomb interaction at the metal-insulator critical point [3].

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High Frequency High Magnetic Field Response of Graphene Monolayers

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Abstract. We study the electronic magnetotransport in graphene at rf frequencies in the few GHz to $\sim$ 50GHz range. Our aim is to investigate the dynamics of charge carriers in the quantum Hall regime. The graphene sample is placed in a break made in a coplanar waveguide and the transmitted power is measured. In order to isolate the response of the sample from the direct transmission between the input and output waveguides, the graphene electron density distribution is modulated with a side gate and the resulting modulation in the transmitted power detected via a standard lock-in technique.

The fixed frequency graphene response as a function of magnetic field reveals two different components. One is symmetric in B and dominates under large side gate voltage, and the other shows reproducible fluctuations revealed only at low gate voltage modulation amplitude. The first part is thought to be related to the bulk conductivity and the fluctuations to the carrier dynamics close to the edge. Interestingly, the amplitude of the fluctuations depends on the trajectory of the carriers, since the parity with respect to magnetic field reversal is not conserved. We thus demonstrate the chiral nature of the transport. We assume that the fluctuations of impedance originate in the scattering from localized states close to the edge of the sample.

Double-resonant Raman scattering in graphene

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Abstract. Since its discovery, graphene attracted much attention due to its unique material properties [1]. The linear band dispersion leads to its exceptionally good transport properties, which paves the way for graphene applications such as integrated circuits, field-effect transistors (FETs) and chemical sensors. Graphene without perturbations, i.e., no substrate interaction, gives insight into the intrinsic bandstructure and phonon dispersion. Interactions with a substrate might have impact on bandstructure and phonon dispersion. In addition, the electron mobility is even enhanced for free-standing graphene [2-4].
In bilayer graphene the transport properties are different from single layer graphene due to the tunneling of charge carriers between the two layers: With increasing charge carrier density, the mobility decreases for single-layer graphene but increases for bilayer graphene [5].
Here, we present an analysis of the different scattering processes in the double resonance Raman process of graphene and bilayer graphene. There is an ongoing debate about the so-called inner and outer processes [6], where inner (outer) refers to scattering by phonons with wave vector between Γ-K (K-M). We discuss different scattering combinations and show that only the combination of inner and outer processes can explain the Raman intensities. A one-dimensional calculation of the Raman intensity reproduces the experimentally measured spectra very well and further supports a contribution of both inner and outer processes. Furthermore, we show that in uniaxially strained graphene a clear assignment of double-resonant Raman peaks to different scattering processes can be given. Here, we present an analysis of the different scattering processes in the double resonance Raman process of graphene and bilayer graphene. There is an ongoing debate about the so-called inner and outer processes, where inner (outer) refers to scattering by phonons with wave vector between Γ-K (K-M). We discuss different scattering combinations and show that only the combination of inner and outer processes can explain the Raman intensities. A one-dimensional calculation of the Raman intensity reproduces the experimentally measured spectra very well and further supports a contribution of both inner and outer processes. Furthermore, we show that in uniaxially strained graphene a clear assignment of double-resonant Raman peaks to different scattering processes can be given.

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XPS Study on Effects of Electron-beam Irradiation of Thin Condensed DPPC Films

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and Gölzhäuser A[2]

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Abstract. Phospholipids, as relatively short amphiphilic polymers, and among them the DPPC (1, 2-dipalmitoyl-sn-glycero-3-phosphocholine), are suitable for production of artificial biomaterials and in combination with cholesterol and proteins present a practical model for the study of transport and signalling in the model cell membrane. On the other hand, low-energy electrons are proved to be the most abundant secondary species created in the irradiation of the living tissue by high-energy ionizing radiation (X- and γ- rays, ions, etc), creating dangerous molecular fragments from nucleic bases [1] and breaking the strands of the DNA [2], but also proved to be an efficient tool in production of bio-chips on the self-assembling molecular (SAM) structure [3].

In our present study, DPPC molecules were deposited as a thin film (mono- and multilayer) on a gold-coated silicon substrate or on a silicon wafer and irradiated by electrons of energy between 5 and 200 eV and the shifts and intensity of the binding energies of C 1s, O 1s, P 2p, and N 1s atoms are observed through analysis of the photo-electrons emitted from the target before and after electron irradiation. Overall, most damage to the monolayer film is caused by cutting the methyl groups from nitrogen and phosphate group from the rest of the molecule. The least effect of electron irradiation is shown on the P 2p band, regardless of the incident energy. The effects are significantly smaller for 5 and 200 eV electrons than for energies in between, which is encouraging for the idea of using these phospholipids as a substrate for amino-acid, protein and DNA irradiation with electrons below 5 eV, where the dissociative electron attachment to these molecules have been previously observed [1, 2] to produce highly reactive chemical species. Main questions for further study are concerning the presence of water clusters trapped around polar head and the dynamic of its release due to the interaction with the electron beam. Equally important is the knowledge of bond orientation, homogeneity of the monolayer and the difference in the electron beam interaction with a monolayer and a bilayer.

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AFM Indentation And Electrolytical Oxidation For Production Of Nanopyramids

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Abstract. Atomic Force Microscope (AFM) nanoindentation is used for pretexturing Al samples in order to prepare them for electrolytic process in barrier film forming electrolyte. Similar technique was used to obtain the matrix of nanoindents with rectangular symmetry as a precursor for pore initiation in electrolytic process in porous film forming electrolytes[1,2]. Barrier film forming electrolytes produce non-porous oxide films parallel to sample's surface and according to that nanoindents become molds for nanoobjects grown during electrolytic process. Complete experiment encompasses: Al surface pretreatment, indentation, electrolytic oxidation and removal of Al. Shape and dimension of grown alumina nanoobjects depend on AFM tip shape as well as on indentation force. As the shape of diamond AFM tip used in the experiment was pyramidal, resulting nanoobjects were pyramids with dimensions ranged from 50 nm to 1200 nm. The AFM tapping mode scan of nanopyramids is shown on FIGURE 1.

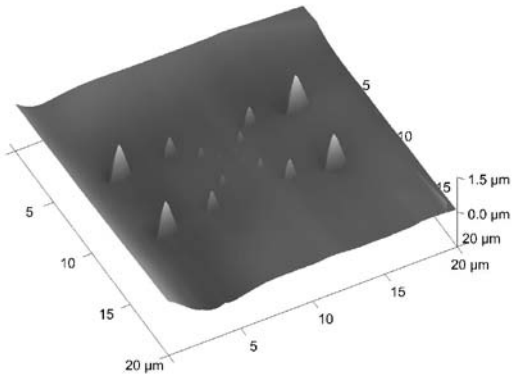

FIGURE 1. Alumina nanopyramids-result of AFM indentation and electrolytic oxidation

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The Experimental Signatures of Orbital Liquid Ground State in Ferromagnetic Metal $SrRuO_3$

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Abstract. $SrRuO_3$ is the end member of the Ruddlesden-Popper series of ruthenates $Sr_{n+1}Ru_nO_{3n+1}$ (n=∞), where n denotes the number of Ru-O layers separated by Sr-O layers, and crystallizes in orthorhombically distorted (Pbnm) perovskite structure. Besides conventional ferromagnetism below 163 K, this compound shows strong non Fermi liquid behaviour in electrical resistivity above 11 K with $\rho \sim \sqrt{T}$ dependence above T_c, and violation of the Mott-Ioffe-Regel limit[1,2,3,4]. We present experimental evidence of related anomalies in electrical resistivity, dc and ac magnetic susceptibility, and specific heat, appearing deeply within ferromagnetically ordered state in $SrRuO_3$. The absence of Jahn-Teller distortion in this regime[5] rules out conventional orbital order, forcing one to describe these in terms of an orbital liquid ground state coexisting with ferromagnetic spin order[6]. We show how the interplay between spin and orbital degrees of freedom interacting via weak spin-orbit coupling gives rise to the observed anomalies, emphasizing the important role of t_{2g} orbital degeneracy in bad metallic 4d-shell based transition metal oxides with an almost ideal perovskite based structure.

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Nonlinear BEC Dynamics Induced By Harmonic Modulation Of Atomic *s*-wave Scattering Length

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Abstract. In the recent experiment [1], a Bose-Einstein condensate of ^{7}Li has been excited by a harmonic modulation of the atomic *s*-wave scattering length via Feshbach resonance. Combining an analytical perturbative approach with numerical simulations we analyze the resulting nonlinear dynamics of the system on the mean-field Gross-Pitaevskii level. Related excitation spectra are presented and prominent nonlinear features are found: mode coupling, higher harmonics generation and significant shifts in the frequencies of collective modes. We indicate how nonlinear dynamical features could be clearly observed in a future experiment and compared to our theoretical results.

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Phase Diagram and Energy Scales in the Anderson Lattice Model

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Abstract.
Transport and thermodynamic properties of heavy fermion materials are dominated by the electrons from partially field f-shells. At high temperatures f-electrons act as local moments while at low temperatures they are hybridized with the conduction electrons and form heavy quasiparticles. The crossover temperature T^* can be tuned by changing the hybridization V which in experiments can be easily achieved by changing the pressure. The functional dependence $T^*(V)$ is, however, still a subject of controversy. In this work we address this question by solving the the Anderson lattice model with one f-orbital per lattice site, the simplest model which describes generic features of heavy fermions. The resistivity and magnetic susceptibility results obtained within dynamical mean field theory (DMFT) give the exponential dependence of T^* on hybridization V with only slightly renormalized effective Kondo coupling $J_K \propto V^2$ as compared to the case of dilute impurities. While our solution of DMFT equations using continuous time quantum Monte Carlo impurity solver is numerically exact, it neglects intersite correlations. To determine their importance, we have also solved the model and obtained the phase diagram within cluster extension of DMFT. We used real-space cellular DMFT (CDMFT) implementation with two sites in a unit cell. The antifferomagnitic region is in this case much narrower having smaller critical hybridization V_c and Néel temperature. T_N is of the order of 1/1000 of half-bandwidth which is several times smaller than in DMFT solution and is of the same order of magnitude as in the experiments on various heavy fermion systems. For $V > V_c$ we find that the nonlocal correlations are negligible at temperature $T^*(V)$ and that T^* is the same as given by local DMFT solution. For $V < V_c$, however, CDMFT solution indicates that crossover energy scale $T^*(V)$ is determined by intersite RKKY interactions.

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Pressure dependence of the Kondo regime in $Co_{1/3}NbS_2$

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Abstract. NbS_2 is a layered 2D conductor which shows superconductivity at ambient pressure at 7.1 K. Upon intercalation of Co in the van der Waals gap between the layers, the magnetic moments of the Cobalt atoms suppress superconductivity in $Co_{1/3}NbS_2$. Their strong interaction with the conduction electrons in the plane shows up in the marked decrease of the resistivity when the triangular lattice of Co atoms orders antiferromagnetically at T_N = 26 K. We have investigated the pressure (p) dependence of the resistivity up to 4.3 GPa in a broad temperature range (40 mK – 300 K). In the p-T phase diagram we observe the suppression of T_N and the appearance of a Kondo regime. The crossover is interpreted within the Doniach phase diagram. Surprisingly, this Kondo regime shows a non-monotonic pressure dependence. At low pressures it steeply decreases with increasing p, fully disappears at 2.2 GPa and reappears above 3.2 GPa. Above this pressure it increases with p. For the interpretation of these unconventional results, the break-up of the fragile triangular order with pressure, the creation of a Kondo spin-liquid and the presence of residual spin impurities are considered.

Dependence of the mobility edge on the boundary hopping of the infinite-size Anderson model

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Abstract. Dependence of the mobility edge W_c of the $3d$ Anderson model on the boundary hopping term t is studied using the high-precision numerical calculation of the smallest Lyapunov exponent and its finite-size scaling properties for box and Lorenzian distribution of on-site energies, and demonstated that $W_c(t)$ reaches its maximum for $t \approx 0.25$, while the critical exponent ν is independent of t within 95% confidence intervals, for both distribution. Results imply that the Anderson transition cannot be described in terms of the local order parameter.

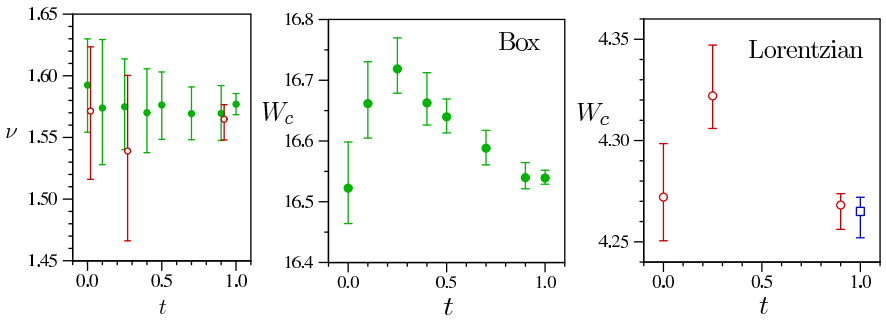

FIGURE 1. Obtained values of $\nu(t)$ for the both studied distributions of disorder (left panel, open symbols for Box, filled for Lorentzian distribution), as well as $W_c(t)$ (the middle and right panels). The value $W_c(t=1)$ is from Ref. [1], while the remaning results are from Ref. [2].

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Fermionic Quantum Criticality From AdS/CFT Correspondence

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Abstract. We study ordering phenomena and quantum phase transitions in strongly correlated electron systems from the viewpoint of AdS/CFT correspondence [1]. The correspondence is a dual classical description of strongly coupled quantum systems coming from string theory, and provides a controlled framework that is free of the fermion sign problem. We first show how the basic workings of the Fermi statistics (Pauli principle, Fermi surfaces, Fermi momentum) are encoded in AdS/CFT [2, 3]. A number of distinct states are found to exist, characterized by either Landau Fermi liquid scaling or by non-Fermi liquid exponents, and separated by critical points similar to those found in heavy fermion systems. We further study some ordering phenomena: quantum Hall effect [4], electron-hole (exciton) pairing and Cooper pairing. The last shows a remarkable dichotomy between the systems with Fermi liquid ground states, where the BCS mechanism gives rise to the conventional textbook superconductivity, and the systems with quantum critical ground states where the same BCS pairing mechanism leads to power-law scaling of the gap equation and an increase in critical temperature, characteristic of unconventional superconducting materials.

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Raman Scattering Study Of $FeSb_2$ Single Crystals

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Abstract. The lattice dynamics of $FeSb_2$ has been investigated by using Raman spectroscopy method as well as first-principles calculations based on ultra-soft pseudopotential method. Polarized Raman scattering spectra of the $Fe_{1-x}Co_xSb_2$ and $Fe_{1-x}Cr_xSb_2$ ($0 \leq x \leq 1$) single crystals are measured at different temperatures in the 80–200 cm^{-1} wavenumber range. All six Raman-active modes, predicted by factor-group analysis, are experimentally observed and assigned. Calculated phonon energies in Γ point showed good agreement with the experimental data for all modes except B_{3g} mode. The highest energy B_{1g} symmetry mode shows significant line asymmetry due to phonon-mode coupling-width electronic background. The coupling constant reaches the highest value at about 40 K and after that it remains temperature independent. Additional broadening comes from the temperature-induced anharmonicity. Below 40 K the coupling is drastically reduced, in agreement with transport properties measurements. Alloying of $FeSb_2$ with Co and Cr produces the B_{1g} mode narrowing, i.e., weakening of the electron-phonon interaction. In the case of A_g symmetry modes we have found a significant mode mixing.

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Charge Transport in Organic Electronic Materials

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Abstract. Semiconducting conjugated polymers have become the materials of great interest for the use in electronic and optical devices, such as field-effect transistors, light-emitting diodes and solar cells. It is therefore of paramount importance to understand the carrier transport in these materials. Transport in disordered organic materials was until recently modelled only using phenomenological approaches that assume certain spatial and energetic distribution of electronic states and certain form of transition probabilities between them. As such, they lack the predictive power. We have developed an approach that links the atomic structure of the material to its electrical properties without the introduction of any fitting parameters [1]. The approach is based on a multiscale methodology that links the relevant quantities at four length scales. The simulations yield the temperature dependence of hole mobility in amorphous P3HT polymer consistent with experimental results from the literature [1]. Furthermore, using this approach it was possible to test the adequacy of previous simplified models. It was found that the Miller-Abrahams model is not sufficient for describing the hopping probabilities between the states [2] and that the concept of electronic temperature cannot be used to describe carrier heating in electric field [3].

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Aggregation Kinetics of Short Range Attractive Particle Suspensions: Brownian Dynamics Simulations vs. Fractional Smoluchowski Equation

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Abstract.

We revisit the aggregation dynamics of particles interacting with short-range attractive interaction. Using Brownian Dynamics simulations we follow the relaxation of a homogeneous, thermodynamically unstable system towards equilibrium by agglomeration. The dynamics of this transition is found to be subdiffusive and characterized by the creation of clusters exhibiting an exponential size distribution. If particle density is sufficiently high, formed clusters will further agglomerate into a single cluster spanning the system. We introduce a phenomenological time scaling law in order to collapse data for a range of diffusion rates and densities onto a single universal curve. Furthermore we demonstrate, that this class of systems and their dynamical features can be modelled by a fractional Smoluchowski coagulation equation. The underlying coagulation rates are seen to exhibit a simple dependency on cluster size. Agglomeration of particles in suspensions is common in many technological and biological processes and their unusual properties are intensively exploited in industrial applications, from environment protection to nano-particle production. Approximate description of structural parameters evolution introduced here should be applicable to the family of systems where agglomeration and diffusion rates are comparable.

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Introduction Of Magnetic Nanoparticles In $YBa_2Cu_3O_7$ Films Grown By Chemical Methods

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Abstract. The controlled introduction of secondary phase nanoparticles in the YBCO matrix has been proved as an efficient way to enhance vortex pinning [1]. Recent works have proposed that the ferromagnetic character of theses secondary phases could lead to a novel and greatly improved pinning mechanism. After a brief review of our precedent results on nanostructured superconductinf films [1], we will show our recent results in the compatibilization of colloidal suspensions of spinel nanoparticles with trifluoroacetate-based precursor solutions of YBCO to obtain epitaxial YBCO/magnetic nanocomposites. In particular we will analyze the coexistence of magnetism and superconductivity in these nanocomposites. We will discuss the enhanced pinning properties of these YBCO nanocomposites and we will explore further capabilities of the above chemical approach.

This work is supported by MEC (MAT2008-01022), Generalitat de Catalunya, Consolider Nanoselect and EU(HIPERCHEM and NESPA)

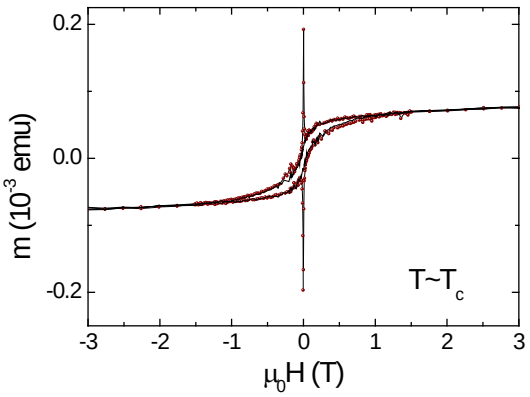

FIGURE 1. Magnetic hysteresis loop close to the superconducting transition temperature of an $YBa_2Cu_3O_7/CoFe_2O_4$ nanocomposite thin film. Both superconducting and ferromagnetic loops are clearly observed.

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Vortex Interactions in Two-Band Ginzburg-Landau Theory

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Abstract. Several years ago [1], Babaev and Speight predicted existence of the semi-Meissner state in two-band superconductors, the superconducting state with intercalating regions of high and low vortex density. The naive explanation for such a state was found in the possibility that two coupled Cooper-pair condensates in two-band superconductors may be of type-II and type-I respectively, and could therefore cause short-range repulsive and long-range attractive vortex-vortex interactions. This was claimed to be verified experimentally by Moshchalkov *et al.* in 2009 [2], and was coined as "type-1.5 superconductivity" in single-crystal MgB_2. To date, the theoretical Ginzburg-Landau (GL) approach of Babaev has been heavily criticized (e.g. by Kogan and Schmalian [3]) for its general noncompliance with the strict conditions of the GL derivation, while the experiments of Moshchalkov experienced reservations of the MgB_2 community (where MgB_2 is widely recognized as a purely type-II superconductor). Moreover, Brandt and Das [4] pointed out that inhomogeneous vortex distributions do not necessarily signify type-1.5 behavior, and were observed earlier even in single-band superconductors.

In this talk, I present the analytic and numeric results revealing the true nature of the "type-1.5" vortex behavior and conditions for its appearance, based on the microscopic parameters of superconductivity, and the two-band Ginzburg-Landau theory derived to higher order terms [5]. I further discuss the unique vortex states predicted by our formalism, and their behavior as a function of field, temperature, and applied dc current.

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When Superconductivity Meets Magnetism: Electronic, Magnetic and Structural Properties of $YBa_2Cu_3O_{7-x}$ /$La_{1-x}Sr_xMnO_3$ Heterostructures

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Abstract. The relationship between superconductivity and magnetic order in high-temperature superconducting (HTSC) copper oxides is an important issue for both fundamental and applicative research (spintronics). The recent progress in manufacturing heterostructures enables us to engineer atomic-scale materials, and provides an opportunity to study the interplay between superconductivity and magnetism. Knowing that the valence electrons in cuprates as well as in manganites are subject to strong magnetic interactions, the magnetization at the interface accompanied with the charge transfer are expected to have a crucial influence in these systems.
To study the interplay between superconductivity and magnetism (i.e. influence of magnetic field on electron paring, the proximity effect, the change of charge carrier concentration, etc), we are investigating a series of n(**YBCO**)/m(**LSMO**) bilayers and multilayers (n and m are numbers of YBCO and LSMO unit cells respectively grown on STO (001)). We are using Angle Resolved Photoemission Spectroscopy (ARPES) (study of electronic structure), Polarized Neutron Reflectometry (PNR) (to reveal the depth profile of the magnetic induction) and Resonant Inelastic X-ray scattering (RIXS) measurements (for resolving the low energy magnetic excitations in with orbital sensitivity).

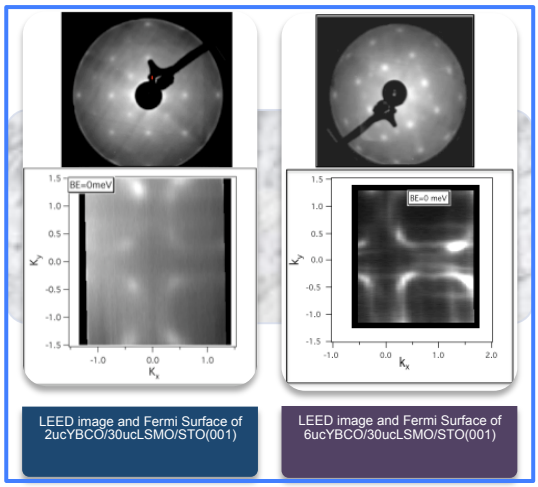

FIGURE 1. Fermi surfaces and corresponding LEED patterns of two YBCO/LSMO bilayers.

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Magnetic Field Dependence Of Anisotropy Of In-plane Angular Magnetoresistance Of Electron-doped $Sr_{1-x}La_xCuO_2$ Thin Films

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Abstract. We studied the normal state magnetoresistance of underdoped superconducting epitaxial $Sr_{1-x}La_xCuO_2$ thin films by applying a high magnetic field up to 22 T parallel to the CuO_2 planes and by varying the orientation of a field of given intensity in order to probe the underlying spin system. This infinite layer compound which has the simplest structure of all the cuprates presents a monotonic negative in-plane magnetoresistance with an anisotropic angular dependence which depends on the doping level [1] and on the field intensity [2]. Angular dependence of the in-plane magnetoresistance at highest magnetic fields is the same for films with different doping levels [2]. We compare our observations with the corresponding ones for the other electron-doped family $Ln_{2-x}Ce_xCuO_4$ (Ln=Nd, Pr, La) and we attribute them to a manifestation of antiferromagnetism which appears to be only due to spins in the CuO_2 planes.

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Effective Carrier Interaction in Semiconductor Thin Films and Quantum Dots

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Abstract. It is shown that within the two-dimensional (2D) approximation the effective carrier interaction [1, 2] (electron-electron/electron-hole) in semiconductor thin films $V_{\rm int}^{\rm eff}(\rho_{ij}) \equiv \langle k/r_{ij}\rangle_{\perp} = kf(\rho_{ij})/\rho_{ij}$, where $k = e^2/(4\pi\varepsilon_0\varepsilon_r)$, depends on the layer thickness d but it is not sensitive to the form of quantum well $V_{\perp}(z_i)$ [2] (see Fig. 1). Here $r_{ij} = (\rho_{ij}^2 + z_{ij}^2)^{1/2}$ is the full (three-dimensional, 3D) distance between two charged quasiparticles (carriers), whereas $\rho_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2]^{1/2}$ and $z_{ij} = z_i - z_j$ are the corresponding lateral and vertical components, respectively, and ε_r is the relative dielectric constant of the semiconductor. The so-called screening function $f(\rho_{ij})$ is determined for two simplest quantum well models: (i) the one-dimensional infinite square well and (ii) the parabolic well (linear harmonic oscillator). These two potentials can be understood as the hard/soft wall limiting cases keeping in mind that a more realistic model may have a form between (i) and (ii). The screening function $f(\rho_{ij})$ in the case (ii) can be expressed in an analytical form which, consequently, can be used as a general (model-independent) formula [2]. As an example, we have considered the electrons localized in a quantum dot created in a semiconductor thin layer (see Fig. 1). It is demonstrated that, when the quantum well confinement is much stronger than the lateral one, the results obtained using the 2D approach with the effective potential are in a good agreement with the full 3D calculations [2].

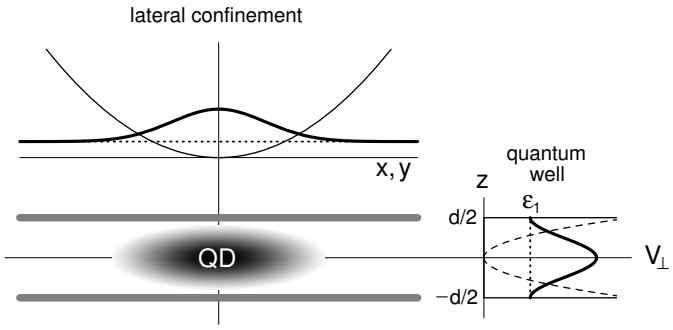

FIGURE 1. The localization of a QD in the semiconductor layer of the thickness d (bottom left) and schematic plots showing the corresponding lateral (top) and perpendicular (right) confinements, as well as the lowest levels (dotted lines) and the probability distributions (thick lines).

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High Energy Nitrogen Ions Channeling Implantation in <110> and Randomly Oriented Silicon Crystals

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Abstract. The accurate description of the depth profile of ions implanted in crystals is important in the scientific as well as in the technological context[1]. Nitrogen is an interesting alternative to oxygen in the production of SOI substrates due to its high stability and electrical resistivity, extreme radiation hardness and excellence as diffusion barrier for mobile ions[2]. This work reports on the experimentally obtained depth profiles of 4 MeV $^{14}N^{2+}$ ions implanted in the <110> and randomly oriented silicon crystals. The ion fluence is 10^{17} particles/cm^2. The nitrogen depth profiling is obtained using Nuclear Reaction Analysis (NRA) method, via the study of $^{14}N(d,\alpha_0)^{12}C$ and $^{14}N(d,\alpha_1)^{12}C$ nuclear reactions, and using the SIMNRA and SRIM 2008 computer simulation codes. During the implantation, the RBS/C spectra were measured on the nitrogen implanted and on the crystal virgin spots. They provide information on the amorphization of the silicon crystals induced by the ion implantation.

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Determination of Iron Charge State in Quaternary Diluted Magnetic Semiconductors

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Abstract. X-ray Absorption Near Edge Structure (XANES) measurements carried out at Deutsches Elektronen-Synchrotron DESY were employed to investigate the local electronic structure of Fe ion in quaternary diluted magnetic semiconductors $Cd(Zn)_{1-x}Fe_xTe_{1-y}(Se,S)_y$. Closer inspection of the pre-edge structure appearing in the Fe K edge XANES spectra (see Figure 1.) revealed the existence of Fe ion in the mixed valence 2+/3+ configuration in all investigated compounds. When going from $Cd_{0.97}Fe_{0.03}Te$ through $Zn_{0.98}Fe_{0.02}Te_{0.91}Se_{0.9}$ to $Cd_{0.98}Fe_{0.02}Te_{0.97}Se_{0.03}$, where Fe shares the same local environment composed of Te atoms only [1], the intensity of the pre-edge peak increases and so does the amount of Fe^{2+} component. The shape of the pre-edge structure completely differs in $Cd_{0.99}Fe_{0.01}Te_{0.97}S_{0.03}$, where the presence of two types of anions in the immediate surrounding of Fe [1] favours its higher oxidation state.

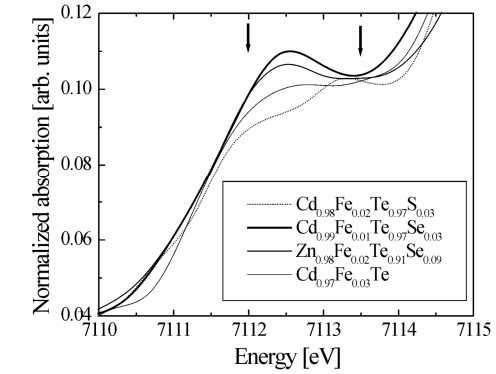

FIGURE 1. Pre-edge structure of the investigated compounds Fe K-absorption edge XANES spectra. Arrows indicate the energy position of Fe^{2+} and Fe^{3+} components.

ACKNOWLEDGEMENT. The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under the Grant agreement N° 226716.

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M-point Phonon Eigenvectors Of The Honeycomb Lattice Obtained By Group Projectors

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Abstract. In the case of materials (for example monolayer graphene) belonging to the honeycomb lattice, symmetry alone is sufficient to determine phonon eigenvectors at Γ-, M- and K-points of the Brillouin zone. We have extended earlier calculation [1] for K-point phonons to the M-point phonons (both in-plane and out-of-plane). Eigenvectors obtained by us using Wigner's method of group projectors are identical with those obtained by molecular method [2] and force constants calculations [3] done for graphene. This confirms once more the power of group theoretical applications in physics.

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Plasma Electrolytic Oxidation of Aluminum in Heteropolyacids

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Abstract. Morphology, composition and microhardness of oxide coatings formed during DC plasma electrolytic oxidation (PEO) of aluminium in heteropolyacids (12-tungstosilicic acid and 12-tungstosilicic acid) were investigated. Oxide coatings were characterized by optical emission spectroscopy, AFM, SEM-EDS, XRD and Raman spectroscopy. Oxide coatings morphology is strongly dependent on process duration, while microhardness decreases with extended PEO time. The microdischarges characteristics were studied as well and it is shown that size of microdischarges becomes larger, while the surface density of microdischarge sites becomes lower, with increasing PEO time. Optical emission spectrum of microdischarges has several intensive band peaks caused by electronic transition in Al, W, O, H atoms. On the base of experimental results it has been concluded that compositions of oxide coatings formed during the PEO are tungsten bronzes.

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Scanning Probe Microscopy of Graphene

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Abstract. Application of graphene for a field effect transistor requires understanding of the graphene electrical properties and finding appropriate methods for its structuring. We employ scanning probe microscopy for studying charging/discharging processes and for lithography of graphene and few-layer graphene flakes on SiO_2/Si substrate. Prior to any manipulation of the flakes, their topography and height were measured using the tapping mode atomic force microscopy. Kelvin probe microscopy and electric force microscopy were done in order to measure initial distribution of surface potential and surface charges. Charging of the graphene flakes was done with a biased tip in the contact mode. Evolution of the injected charge carriers within the graphene flakes was recorded using Kelvin probe microscopy revealing rate of discharging process. Using the electric force microscopy and the simple capacitor model for the graphene/SiO_2/Si, the amount of injected charges is determined. Structuring of graphene flakes was done using dynamic plowing lithography, that is, scratching lithography with a vibrating tip in order to avoid tearing and displacing of the flakes. This technique enables writing of trenches within graphene flakes in a controlled manner.

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Simulation Study of Anisotropic Random Sequential Adsorption on a Triangular Lattice

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Abstract. Random sequential adsorption of extended objects on a two-dimensional triangular lattice is studied under anisotropic conditions by means of Monte Carlo simulations. Depositing objects are *k*-mers of various lengths. In addition to the anisotropic RSA of pure shapes, we also performed some simulations for a ten-component mixture of k-mers covering 2,3,...,11 lattice sites, and we investigate the effects of the anisotropy on the adsorption of the mixture components. Approach to the jamming limit is found to be exponential, of the form $\theta(t) \sim \theta_{jam} - \Delta\theta \exp(-t/\sigma)$ for all the objects, for the ten-component mixture of *k*-mers, and for each of the components. We concetrate here on the influence of the degree of anisotropy on the kinetics of deposition processes.

Quantum Channeling of 1 MeV Positrons in a Very Short (11, 9) Single-Wall Carbon Nanotube

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Abstract. In this work, the quantum channeling effect in transmission of 1 MeV positrons through very short single-wall carbon nanotubes has been investigated. The nanotube length is varied from 10 to 200 nm. The initial positron quantum state is represented by the Gaussian function, with the dispersion equal to the critical quantum transverse de Broglie wave length for the channeling and the center corresponding to the impact parameter of the positron. The evolution of the quantum state on the nanotube length is obtained using the numerical solution of time-dependent Schrödinger equation and the Moliére's expression for the positron-carbon interaction potential. For the numerical integration of time-dependent Schrödinger equation method based on Chebyshev propagation sheme is used. The positron spatial and angular distributions for different nanotube length has been analyzed and compared with the corresponding classical 1.84 GeV proton spatial and angular distributions[1,2].

Keywords: Time dependent Schrödinger equation, Channeling, Positron

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Off-Center Hydrogen Impurity In Spherical Quantum Dot In Electric Field

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Abstract. The effect of the parallel electric field on the energy levels, with given values of the magnetic quantum number, of the off-center hydrogen impurity in GaAs/AlAs spherical quantum dot with finite barrier potential confinement is investigated. Energies are calculated using method of the matrix diagonalization with eigenfunctions of the Hamiltonian of the on-center hydrogen impurity as a basis functions, which are expressed in terms of Kummer's function. The variations of the energies and probability densities, for given electron state, as a function of the position of impurity *D*, radius of the quantum dot R_0, potential barrier height V_0 and strength of electric field *K* were discussed. We found that the strong electric field changes the character of some impurity electron states in the sense that the electron is not strongly localized around the position of the hydrogenic impurity.

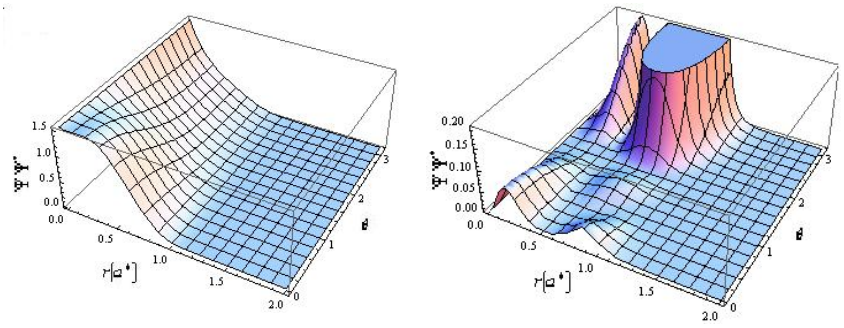

FIGURE 1. Probability density in the ground state (m=0) of off-center hydrogen impurity without (left panel) and with applied electric field (right panel). (D=0.5, R_0 =1 and K=400 in effective atomic mass units)

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Quantum Channeling of 1 MeV Positrons in a Very Short (11, 9) Single-Wall Carbon Nanotube

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Abstract. In this work, the quantum channeling effect in transmission of 1 MeV positrons through very short single-wall carbon nanotubes has been investigated. The nanotube length is varied from 10 to 200 nm. The initial positron quantum state is represented by the Gaussian function, with the dispersion equal to the critical quantum transverse de Broglie wave length for the channeling and the center corresponding to the impact parameter of the positron. The evolution of the quantum state on the nanotube length is obtained using the numerical solution of time-dependent Schrödinger equation and the Moliére's expression for the positron-carbon interaction potential. For the numerical integration of time-dependent Schrödinger equation method based on Chebyshev propagation sheme is used. The positron spatial and angular distributions for different nanotube length has been analyzed and compared with the corresponding classical 1.84 GeV proton spatial and angular distributions[1,2].

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Exfoliated MoS_2 Nanotubes

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Abstract. Preparation of single molecular layer of inorganic solid molybdenum disulfide (MoS_2), out of the crystalline 2H -MoS_2 has been reported in 1984. [1] but, there have been no reports on attempt to exfoliate transition-metal disulphide nanotubes.
The MoS_2 co-axial nanotubes (nanotube supplier: Nanotul Ltd.) were lithium intercalated in a solution of butyl lithium in hexane at room temperature [1]. The exfoliation occurs by immersing intercalated sample into water, with extensive centrifuging and washing with distilled water. Very anisotropic molecular-layer flakes reveal unique phenomena, when nanoparticles behave as "quasi"-molecules and can self-assemble into single crystal dendritic structures. TEM micrograph (Fig. 1) clearly shows presence of monolayers. The structural transformation from *2H*- to *1T*- crystalline polytype of MoS_2 has been observed. The shift towards higher energies (smaller wavelengths) in the optical absorption spectrum, compared to the bulk material and nanotubes, is observed, revealing quantum confinement effect. Results of scanning electron microscopy, transmission electron microscopy, scanning tunneling microscopy, uv-vis spectroscopy, X-ray diffraction as well as X-ray photoelectron spectroscopy of this unique graphene analogy will be presented.

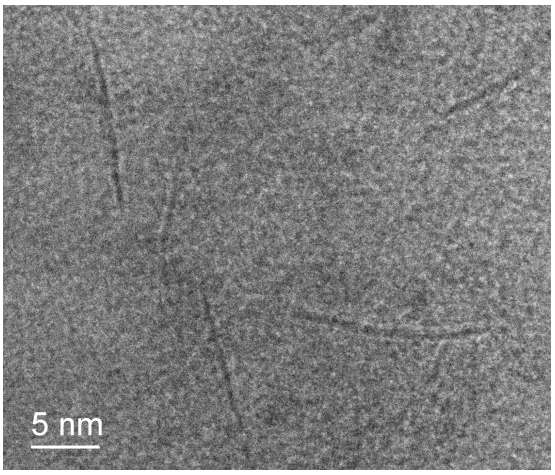

FIGURE 1. TEM micrograph of exfoliated MoS_2 nanotubes, with clearly visible monolayers .

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Optical Characterization of Single Layer and Few Layer Graphene

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Abstract. Graphene, a single layer of carbon atoms packed tightly into a honeycomb lattice, has been attracting wide attention due to its unique electrical, optical and mechanical characteristics. In order to fully understand this system and put in practical use remarkable effects that are manifested within, detailed characterization of its optical and electrical parameters is required. Here, we report on optical characterization of single layer and few layer graphene via infrared spectroscopy and spectroscopic ellipsometry. Micromechanically exfoliated graphene samples are prepared on SiO_2/Si substrate. Samples are then used for the characterization in NIR range by FT IR spectroscopy. Obtained reflectance is used for retrieving complex refraction index and conductivity of the sample in measured range. In the visible and UV range characterization is done by spectroscopic ellipsometry. Results are again used for retrieving complex refraction index and conductivity of the sample. In the measured ranges conductivity saturates to universal optical conductivity due to dominance of its interband component. Obtained results are in agreement with both theoretical and experimental data reported by other groups.

Influence Of Iron Doping On Band Gap Of $Ce_{1-x}Fe_xO_{2-y}$ Nanocrystals

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Abstract. We have investigated optical properties of $Ce_{1-x}Fe_xO_{2-y}$ (x=0.01,0.03,0.05) nanocrystals using spectroscopic ellipsometry. Several analytical models were applied in the analysis of optical dispersion of complex dielectric function and band gap variation. Samples were synthesized using hydrothermal method at relatively low (200 ^oC) calcination temperature. Average particle size was evaluated from the x-ray diffraction data. Using Raman spectroscopy we have observed increase in oxygen vacancy concentration with Fe doping. Optical absorption edge shifts more towards visible spectral range as the dopant content increases (up to 5%) as a consequence of increased oxygen vacancy concentration which induce additional levels within the gap. Shifting of the optical band gap makes these materials potential candidates for application in the field of photocatalysis.

Microstructural And Vibrational Properties Of Nanocrystalline CeO_2 Modified By Oxygen Point Defects

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Abstract. Oxygen vacancies cause several important changes in nanostructured CeO_2 oxygen storage and ionic conduction properties. Microstructural changes of nanocrystalline CeO_{2-x} annealed at different temperatures ranging from 200 ºC to 500 ºC were investigated by X-ray diffraction and Raman spectroscopy methods. It was demonstrated that the oxygen vacancies content changed significantly with increasing of annealing temperature playing an important role in the observed microstructural changes of the annealed samples. The observed microstrain changes dominate over the crystallite size effect. A new mode, classified as a probable surface mode, was observed in the Raman spectra at ~480 cm^{-1}, appearance of which can be explained by defective structure and disorder in ceria lattice.

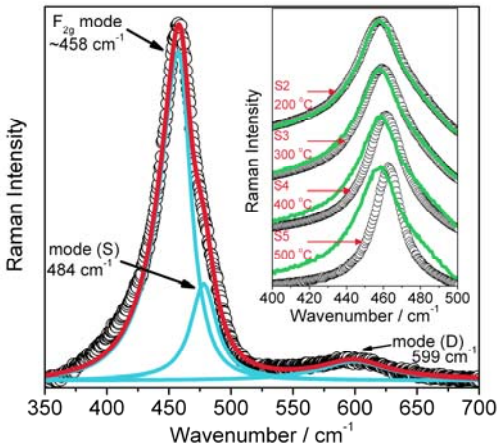

FIGURE 1. Raman spectrum of CeO_{2-x} annealed at 200 °C (circles) fitted with phonon confinement model and Lorentzian function (lines). Inset: Raman spectra before and after annealing at 200-500 °C.

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Phase diagram of the frustrated J_1-J_2 Heisenberg spin-1/2 model on the body-centered cubic lattice

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Abstract. Using spin Green's function method we study the influence of the frustration and quantum fluctuations on the magnetic ordering of the spin-1/2 Heisenberg antiferromagnet on the body-centered cubic lattice (bcc) (J_1-J_2 model) in the ground state (T=0 K). We analyze previously demonstrated two magnetic phases: Neel-phase (AF_1) with two sublattices for small J_2 and collinear antiferromagnetic phase (AF_2) with four sublattices for high values of J_2. Within the Tyablikov's approximation (RPA) we obtain the analytical expressions for the internal energy, sublattice magnetic moment and corresponding Neel temperature in the absence of magnetic fields. Using numerical simulations the phase transition from AF_1 to AF_2 is found for $p=J_2/J_1\cong0.76$ at absolute zero and $p=J_2/J_1\cong0.71$ in the vicinity of the Neel temperature. We also study the Neel temperature dependence on the parameter ratio J_2/J_1. Our conclusions are compared to the other methods' results.

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Electron Spin Resonance Study of $SeCuO_3$

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Abstract. We have carried out 9.4 GHz ESR temperature dependent ($5-300$ K) measurements on a single crystalline sample of $SeCuO_3$ for three different crystal orientations. The ESR spectra originating from $S=1/2$ of Cu^{2+} consist of a single broad exchange narrowed Lorentzian absorption profile. The extracted temperature dependence of absolute spin susceptibility was found to be in good agreement with SQUID data. The compound undergoes the antiferromagnetic (AF) phase transition at $T_N=8$ K as was evidenced through the disappearance of the ESR spectra below T_N as well as seen from the distilled AF correlations inferred from the Curie-Weiss behaviour of the susceptibility. The line-width behaviour obeys the Kubo-Tomita temperature law of spin relaxation from room temperature down nearly to 50 K below which it starts to diverge and finally vanishes at T_N. Based on the behaviour of the g-factor, line-width, and susceptibility, magnetic fluctuations have been conjectured to lower the mean-field transition temperature drastically. The system belongs to the Cu-O based family possessing magneto-electric coupling induced by the magnetic fluctuations and promises to be exploited for multiferroic applications.

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Magnetic Properties of Fe^{2+}/Fe^{3+} Doped CeO_2 Nanocrystals

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Abstract. We have measured magnetic properties of pure and Fe-doped ($Ce_{0.88}Fe^{2^+/3^+}_{0612}O_{2-}$) ceria nanocrystals in two different valence states. Fe-doped samples show strong magnetic properties at room temperature. Saturation magnetization in doped samples increases with valence state change, showing that not only the oxygen vacancies but also valence state of iron plays significant role in magnetic properties. Raman spectra of these samples suggest that electrons in highly oxygen deficient $Ce_{0.88}Fe^{2^+/3^+}_{0.12}O_{2-\delta}$ samples are delocalized onto Ce(Fe)-O(VO)-Ce(Fe) orbitals.

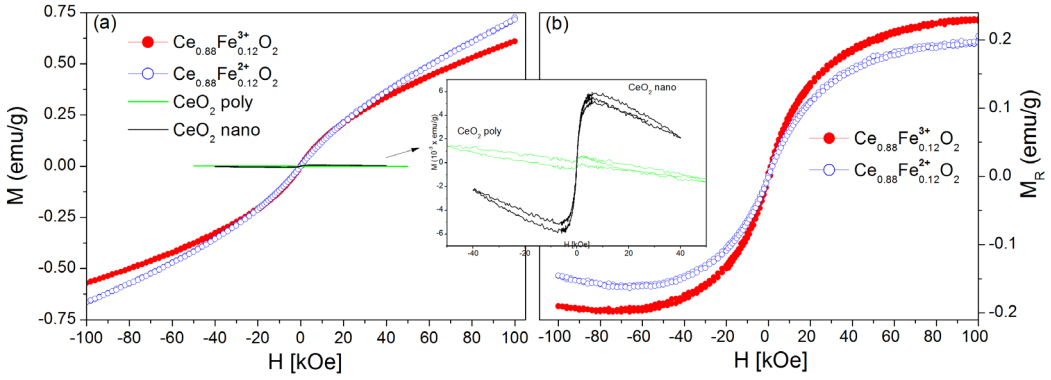

FIGURE 1. Magnetic properties of pure and iron doped $CeO_{2-\delta}$ nanocrystals. (a) Room temperature magnetization curves of pure and 12% Fe-doped samples. (b) The same data after subtracting the paramagnetic contribution.

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Critical Chain Length And Charge Transfer In $YBa_2Cu_3O_{6+x}$

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Abstract. Doping, p, of the superconducting CuO_2 planes in $YBa_2Cu_3O_{6+x}$ material crucially depends on the length of CuO chains formed in the oxygen deficient CuO_x planes, since only chains longer or equal to some critical chain length, l_{cr}, can provide holes for charge transfer to the CuO_2 planes. Recently, it was shown that the 60K plateau in $T_c(x)$ dependence could be explained as a consequence of the corresponding plateau existence in the $p(x)$ dependence. This constant value of doping p is achieved if the critical chain length is equal to some optimal critical chain length, $l_{cr,opt}$, which can be determined for every temperature T which enables stabilization of the Ortho II structural phase. In the present study we have determined $l_{cr,opt}$ for the set of different temperatures by calculating p as a function of l_{cr} in the range of oxygen concentrations which span the region of Ortho II phase (x>0.5). It was found that $l_{cr,opt}(T)$ dependence follows an exponential law: $l_{cr,opt}(T)=A\exp(B/T)$. Additionally, the $T_c(x)$ dependence was calculated and compared with the existing experimental results. Implications of the choice of l_{cr} for the shape of the calculated $T_c(x)$ curve are shortly discussed.

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Study on the Origin Of 60K Plateau in $T_c(x)$ Dependence in $YBa_2Cu_3O_{6+x}$

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Abstract. Two possible causes for the 60K plateau existence in the $T_c(x)$ dependence in $YBa_2Cu_3O_{6+x}$ superconductor were studied here in detail: the stripe formation followed by T_c suppression around p=1/8 doping, and development of the Ortho II structural order resulting in constant value of doping p in the range $0.50<x<0.65$. We have analyzed available experimental results for the $T_c(p)$ dependence and its discrepancy from the universal $T_{c,univ}(p)$ relation. It was clearly shown that stripe formation reduces T_c only beyond x=0.60, where 60K plateau already fades out. Thus, the conclusion was made that stripes cannot be considered of great importance for the 60K plateau development. On the other hand, it was shown that for every temperature T=const, which stabilizes Ortho II structural phase, there can be found such a value of critical chain length, l_{cr}, (defined in a way so that only CuO chains of length $l \geq l_{cr}$ can supply holes to superconducting layers) which provides nearly constant doping $p(x)=const$ between x=0.50 and $x \approx 0.65$. Since this range of oxygen concentrations is exactly the range of 60K plateau extension, the conclusion was drawn that Ortho II ordering can be considered as a main cause for the 60K plateau formation.

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Influence of Ortho–II Structural Phase on the 60K Plateau Formation in $YBa_2Cu_3O_{6+x}$

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Abstract. In the present study, we have employed the two dimensional ASYNNNI model to study how the Ortho–II structure formation influences doping, p, of the superconducting CuO_2 planes in $YBa_2Cu_3O_{6+x}$ high-T_c superconductor. It was shown that if the direct repulsive interaction between next nearest oxygen atoms (V_3), present in the Hamiltonina of the ASYNNNI model, is neglected the Ortho–II ordering is destroyed and doping p becomes a linearly increasing function of oxygen concentration x in the range $0.50 \leq x \leq 0.65$, for any choice of critical chain length l_{cr} (defined so that CuO chains of length $l<l_{cr}$ cannot transfer holes to the CuO_2 planes). Consequently, the $T_c(x)$ dependence, obtained by the employment of universal T_c versus p relation, does not exhibit experimentally observed 60K plateau. The results presented here indicate that formation of Ortho–II structural phase is a key factor for the 60K plateau emergence in $T_c(x)$ dependence.

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Pressure effects on the transport coefficients of $Ba(Fe_{1-x}Co_x)_2As_2$

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Abstract. We report on the temperature dependence of the resistivity and thermoelectric power under hydrostatic pressure up to 2.5 GPa of the itinerant antiferromagnet $BaFe_2As_2$ and the electron-doped superconductor $Ba(Fe_{0.9}Co_{0.1})_2As_2$. We observe a hole-like contribution to the thermopower below the structural-magnetic transition in the parent compound that is suppressed in magnitude and temperature with pressure. Pressure increases the contribution of electrons to transport in both the doped and undoped compound. In the 10 % Co-doped sample, we used a two-band model for thermopower to estimate the carrier concentrations and determine the effect of pressure on the band structure. We found that pressure increases the band overlap and the number of charge carriers, similar to the effect of doping with charge carriers.

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Large Polaron in Transverse Magnetic Field

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Abstract. It has been argued for a long time that large polaron states may have crucial role in the charge and energy transport in some very important quasi 1D substances such as biological macromolecules, α–helix and DNA [1–3], and quasi 1D conductors–highly conducting organic salts and polymers from the polyacetylene family [4]. Theoretical investigations of transport processes in these media has been commonly carried on within the pure 1D models neglecting the possibility of transverse motion. However, realistic quasi 1D substances are not purely one dimensional but highly anisotropic systems which may have significant consequences on polaron properties. This especially concerns the adiabatic limit where even tiny transverse coupling may destroy 1D polaron [5, 6]. That is, the one–dimensionality of system is the prerequisite of the polaron formation and stability. In this paper we examine the possibility of the existence of large 1D polaron confined to a single chain in a substances built up of a collection of the parallel molecular chains embedded in realistic 3D lattice. Such system may be described by the 3d Holstein's molecular crystal Hamiltonian with anisotropic electron hopping. As a mechanism of confinement we have considered the external magnetic field directed across the molecular chain. It was shown that the stable large polaron states extended over the finite region within the crystal may exist in these media for a certain values of system parameters and strength of magnetic field. Polaron parameters such as effective mass, transverse and longitudinal radii are calculated explicitly in terms of these parameters. On the basis of these results possible role of polaron mechanism in the long haul charge and energy transfer is critically examined.

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Quantum Critical Transport Near the Mott Transition

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Abstract. We perform a systematic study of incoherent transport in the high temperature crossover region of the half-filled one-band Hubbard model. We demonstrate that the family of resistivity curves displays characteristic quantum critical scaling of the form $\rho(T,\delta U) = \rho_c(T) f(T/T_o(\delta U))$, with $T_o(\delta U) \sim |\delta U|^{z\nu}$, and $\rho_c(T) \sim T$. The corresponding β-function displays a "strong coupling" form $\beta \sim \ln(\rho_c/\rho)$, reflecting the peculiar mirror symmetry of the scaling curves. This behavior, which is surprisingly similar to some experimental findings, indicates that Mott quantum criticality may be acting as the fundamental mechanism behind the unusual transport phenomena in many systems near the metal-insulator transition.

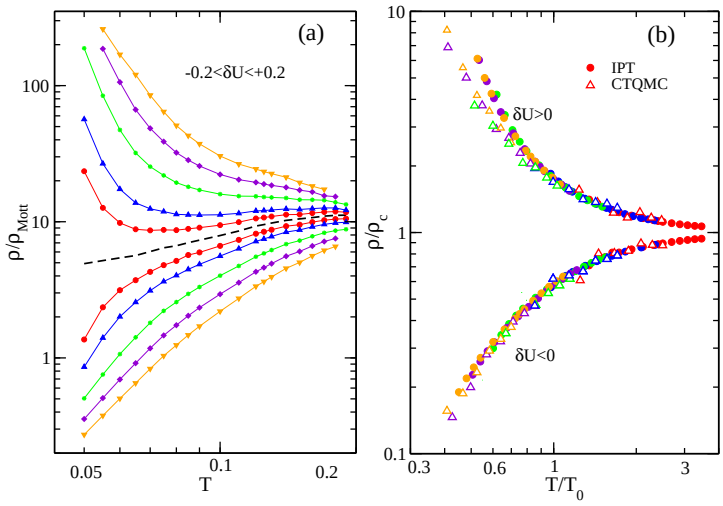

FIGURE 1. (a) DMFT resistivity curves as function of temperature along different trajectories $-0.2 \leq \delta U \leq +0.2$ with respect to the instability line $\delta U = 0$ (black dashed line). Data are obtained using IPT impurity solver. (b) Resistivity scaling; essentially identical scaling functions are found from CTQMC (open symbols) and from IPT (closed symbols).

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Wigner-Mott Scaling of Transport Near the Two-Dimensional Metal-Insulator Transition

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Abstract. Thermal destruction of heavy quasiparticles often dominates the transport behavior of many strongly correlated materials. It typically leads to pronounced resistivity maxima in the incoherent regime around the coherence temperature T^*, reflecting the tendency of carriers to undergo Mott localization following the demise of the Fermi liquid. This behavior is best pronounced in the vicinity of interaction-driven (Mott-like) metal-insulator transitions, where the T^* decreases, while the resistivity maximum ρ_{max} increases. Here we show that, in this regime, the entire family of resistivity curves display a characteristic scaling behavior $\rho(T)/\rho_{max} \approx F(T/T_{max})$, while the ρ_{max} and $T_{max} \sim T^*$ assume a power law dependence on the quasi-particle effective mass m^*. Remarkably, precisely such trends are found from an appropriate scaling analysis of experimental data obtained from diluted two-dimensional electron gases in zero magnetic fields. Our analysis provides strong evidence that inelastic electron-electron scattering – and not disorder effects – dominates finite temperature transport in these systems, validating the Wigner-Mott picture of the two-dimensional metal-insulator transition.

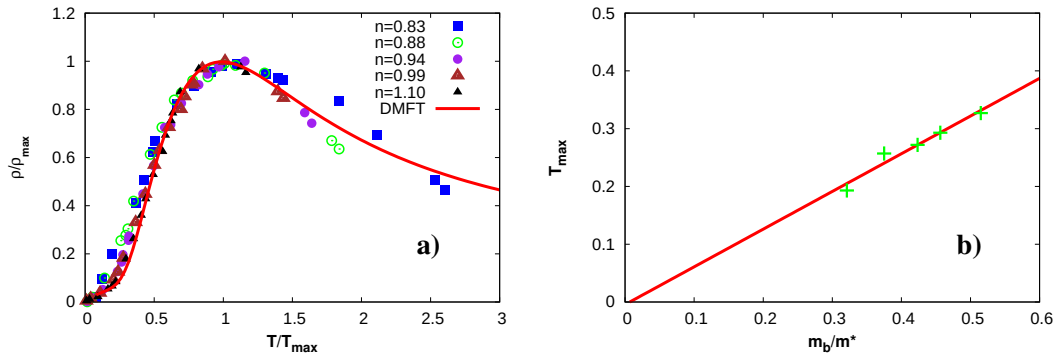

FIGURE 1. Scaling analysis applied on Si-MOSFETs. Experimental data are taken from V. M. Pudalov et al., Physica (Amsterdam) **3E**, 79 (1998). Panel a) shows scaled experimental resistivity data (dots) and scaling curve (red line) obtained with DMFT. Panel b) shows temperature dependence of effective mass of the same experimental data.

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Scaling Properties of the Hand Tremor Movements in Essential Tremor

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Abstract. We have used the Wavelet Transform (WT) and the Detrended Fluctuation Analysis (DFA) methods to analyze hand tremor movements in essential tremor (ET). We have analyzed the time series comprised of peak-to-peak (PtP) intervals, extracted from regions around the first three main frequency components of the power spectra (PwS) of the recorded tremors, in two different recording conditions (before and after the addition of wrist-cuff load). Our goal was to distinguish between multiple sources of ET, and to separate the influence of peripheral factors on ET.
Our results show that, in ET, the values of relevant scaling exponents of the main frequency component of recorded tremors change after the addition of load, and that the two main components of ET tremor frequency spectra, otherwise indistinguishable without load, become significantly different after inertial loading. Finally, our results also show that the scaling behavior of the calculated functions changes as well—the calculated WT scalegrams and DFA functions display a shift in the position of the crossover when the load is added. We conclude that the difference in behavior of the WT and DFA functions between different conditions in ET could be associated with the expected pathology in ET, or with some additional mechanism that controls movements in ET patients.

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Crossover phenomena in Critical Ising Strips with Arbitrary Surface Fields: Exact Variational Results

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Abstract. Critical $(T = T_c)$ Ising strip characterized by *arbitrary* surface magnetic fields h_1 and h_2 $(h_1 \neq h_2, h_1 h_2 \geq 0)$ is considered by exact variational formulation of a two-dimensional Ising model of Mikheev and Fisher. *Exact* local energy density profiles in various regimes of the fields variables y_i $(i = 1,2)$, $y_i = D^2 h_i^2 L$ (L is a width of the strip and D is a metrical factor) show strong *nonmonotonous* behavior near the confining boundaries. Quite general *exact* results on the Casimir amplitudes demonstrate that they are strikingly influenced by variable boundary conditions in that they may change their nature from attractive to repulsive one,with significant accompanying variation of its intensity.

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Fractal properties of percolation clusters in mesoscopic neural networks with small-world topology

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Abstract. We present a study on spike packet propagation in a mesoscopic-scale network of neuronal pools exhibiting small-world properties, consistent with the recent findings [1]. The coarse-graining of neural dynamics is carried out along the lines of the modified Gerstner-Kistler assembly model [2], appropriate to describe the phenomenon of transient synchronization. To a certain extent, spike packet propagation is not unlike the spreading of soliton-like excitations, giving rise to spatiotemporal patterns that represent the generalization of the long-standing notion of synfire chains [3]. One may follow up the emergence of the largest synchronized connected component within the formalism of a percolation transition [4]. Applying the finite-size scaling method, we obtain the dependence of critical probability on the synaptic strength and refractoriness, allowing one to discuss the interplay between the network topology and the dynamical features of its constituents, with potential implications to in vitro cultures [5, 6].

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Formation of Phase Transitions in Ultrathin Dielectric Films

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Abstract. This paper presents the results of research conducted in the field of QSE of ultrathin dielectric films. Method of choice is the method of Green's functions which proved to be a very powerful tool for theoretical research in solid state physics. Among many other properties of materials, such as optical, conductive, etc, through this method it is possible to find critical values of parameters corresponding to the phase transitions from bulk to localized states of excitons. This analysis is valid for four layered film, e.g. for film with five crystallographic planes, since that type of ultra thin film was the object of research. Conditions for occurrence of one, two, three, or even four localized states have been found and analyzed.
Keywords: ultrathin films, excitons, Green's functions, localized states

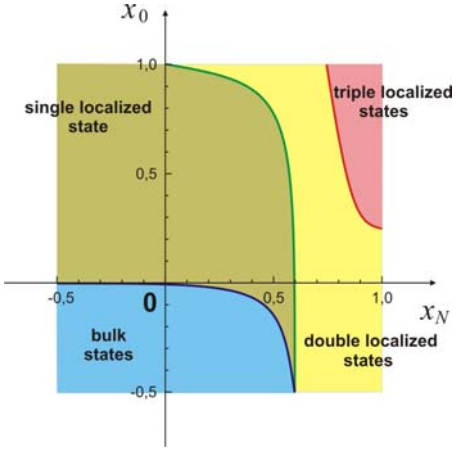

FIGURE 1. Phase transitions from bulk to single, double, triple and quadruple localized exciton states

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Effects of Different Treatments on the Structural and Spectral Properties of $SrTiO_3$ Single Crystal

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Abstract. We studied the effects of different treatments on the structural and spectral properties of $SrTiO_3$. These treatments include doping by Re and Me ions and modification of surface of single crystals using plasma treatment. Quasistationary compression plasma flow was produced by magnetoplasma compressor. Dielectric spectroscopy measurements were performed in the frequency range from 70kHz to 10MHz and in the temperature range from 30K to room temperature. The microstructure and morphology of modified sample surface were investigated by scanning electron microscopy, standard XRD and low-angle grazing incidence diffraction method. Due to possibility of setting up an incident X-ray beam to the low angle the grazing incidence method allows investigations of the crystal structure of the surface layers in material. Dielectric measurements showed that doping by rare-earth ions (Sm, Nd) significantly influences the dielectric properties especially at temperature around antiferodistorzion phase transition at 105K, unlike doping by iron-ions (Mn, V, Fe). Differences in dielectric properties are discussed on the basis of degree of packing of ions. XRD analyze showed that recrystallization occurred under conditions of high dynamic pressure and high thermodynamic parameters gradients. It was seen that the surface treatment by hydrogen plasma caused recrystallization of surface layer of treated sample, i.e. creating a polycrystalline layer. Analysis of the SEM data shows that quasi-ordered structures of order of 10^{-6}-10^{-9} m in size were formed on the surface.

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Semi-flexible Hamiltonian Walks on 3- and 4-simplex Fractal Lattices

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Abstract. Semi-flexible Hamiltonian walks (SHWs) are self-avoiding random walks that visit every site of the lattice, and which are weighted according to the number of bends in the walk. SHWs were introduced in 1956 by Flory [1] in order to model the compact phase of semi-flexible polymers and the globule-crystal transition. In spite of its ostensible simplicity, there are not many results for this model, and some of them contradict each other [2–8]. Therefore, it is instructive to study this problem on fractals, whose self-similar structure enables an exact recursive method for obtaining various thermodynamic quantities. In addition, results of such analysis might give some insight into the behavior of real bio-polymers, which are semi-flexible and fulfil their biological function while they are in compact conformations, resided in nonhomogeneous crowded environment inside the living cell. Here we present the main results of our recent study of SHWs on 3- and 4-simplex fractal lattices [9]. In particular, we have established the asymptotic form of the partition function, with temperature dependent scaling parameters, as well as the corresponding critical exponents, and investigated the possibility of the phase transition between a compact molten globule and ordered 'crystal' state.

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Semiflexible Polymer Chains on Plane-filling Fractals

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Abstract. The lattice semiflexible self-avoiding walk model is used in polymer physics in order to describe relevant aspects of different phenomena, such as protein folding, adsorption of semiflexible homopolymers, transition between the disordered globule and the crystalline polymer phase, behavior of semiflexible polymers in confined spaces, or influence of an external force on polymer systems [1–5]. In spite of numerous studies, a scanty collection of exact results has been achieved so far, even for the simplest lattice models. Here we present the results of our recent exact renormalization group (RG) study [6] of semiflexible polymer chains on an infinite family of the plane-filling (PF) fractals. The fractals are compact, that is, their fractal dimension d_f is equal to 2 for all members of the fractal family enumerated by the odd integer b ($3 \leq b < \infty$). For various values of stiffness parameter s of the chain, on the PF fractals (for $3 \leq b \leq 9$) we calculate exactly the critical exponents ν (associated with the mean squared end-to-end distances of polymer chain) and γ (associated with the total number of different polymer chains). In addition, we calculate ν and γ through the Monte Carlo RG approach for b up to 201. Our results show that, for each particular b, critical exponents are stiffness dependent functions, in such a way that the stiffer polymer chains display enlarged values of ν, and diminished values of γ. On the other hand, for any specific s, the critical exponent ν monotonically decreases, whereas the critical exponent γ monotonically increases, with the scaling parameter b.

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Hamiltonian Walks on Modified Rectangular Lattice

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Abstract. Hamiltonian walks (HWs) are self-avoiding random walks that visit each site of the lattice exactly once. Apart from being interesting in their own right, in polymer physics they are used as models of collapsed polymers and also as lattice toy-models of proteins. It is expected that the number of Hamiltonian walks Z_N scales as $\omega^N \mu^{N^\sigma} N^a$, with the number of lattice sites $N \gg 1$. Values of the constants ω, μ and σ depend on the properties of the underlying lattice, but whereas connectivity constant ω and critical exponent σ are the same for open and closed HWs, value of μ depends on the HW type also. For all regular lattices the exponent σ depends on the lattice dimensionality only as $\sigma = (d-1)/d$. Since exact determination of the number of HWs on a lattice is hard combinatorial problem, confirmation of the expected asymptotic relation for Z_N by direct enumeration or other methods barely exists [1–3]. Recently, it was found for HWs on some fractal lattices that not both correction factors (μ^{N^σ} and N^a) to the leading exponential factor ω^N are always simultaneously present [4–6]. In these papers it was also argued that the origin of the correction μ^{N^σ} for HWs on fractal lattices is not the same as for regular lattices, but lies in the subtle topological properties of fractals. Here we study HWs on modified rectangular lattice [7, 8] by applying an exact recursive scheme for enumeration of different types of HWs. By analyzing the series of numbers obtained in such a way, we show that $Z_N \sim \omega^N \mu^{N^\sigma}$, where $\sigma = 1/2 = (d_f - 1)/d_f$, with $d_f = 2$ being the fractal dimension of the lattice, and $\omega = 1.169$. In contrast to all previously studied hierarchical lattices, not only that the value of μ differs for open and close HWs, but it also depends on the parity of the lattice order.

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Relaxation properties in diffusive model of dimers with constrained movements on a triangular lattice

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Abstract. We study the relaxation process in a two-dimensional lattice gas model, based on the concept of geometrical frustration. In this model the particles are dimers which can both randomly translate and rotate on the planar triangular lattice. We monitor, for different densities, several quantities: mean square displacement, the self-part of the van Hove correlation function, and the self intermediate scattering function. We observe a considerable slowing down of diffusion on a long-time scale when suppressing the rotational motion of dimers; our system is subdiffusive at intermediate times between the initial transient and the long-time diffusive regime. We show that the self-part of the van Hove correlation function exhibits, as a function of dimer displacement, a stretched exponential decay at intermediate times. The self intermediate scattering function (SISF), displaying slower than exponential relaxation, suggests the existence of a heterogeneous dynamics. For each value of density, the SISF is well described by the Kohlrausch-Williams-Wats law. The characteristic timescale $\tau(q_n)$ is found to decrease with the wave vector q_n according to a simple power-law, $\tau(q_n;\rho_0) \propto q_n^{-\delta}$, with the same exponent $\delta = 2.70 \pm 0.07$ for all densities ρ_0. Furthermore, the slowing down of the dynamics with density ρ_0 is consistent with the scaling law $1/\tau(q_n;\rho_0) \propto (\rho_c - \rho_0)^{\varkappa}$, with the same exponent $\varkappa = 3.34 \pm 0.12$ for all wave vectors q_n. The density ρ_c is approximately equal to the closest packing limit, $\theta_{CPL} \lessapprox 1$, for dimers on the two-dimensional triangular lattice.

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Effect of Low Energy N^{4+} Irradiation on Structural Characteristics of Ethylene-Norbornene Copolymer Films

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Abstract. The effect of ion irradiation on structural characteristics of ethylene-norbornene copolymer was studied using Raman and Fourier transform infra-red (FT-IR) spectroscopy. Polymer samples were irradiated with 60 keV N^{4+} ions to various fluences ranging from 10^{13} to 10^{16} cm^{-2}. The FT-IR spectra showed that the absorption peaks of ketone and aldehyde groups increase with the increase of fluence, confirming the processes of surface oxidation and C=C bonds formation. Raman scattering analysis shows that carbon enriched zones formed in irradiated ethylene-norbornene exhibit a noticeable degree of tetragonal hybridization.

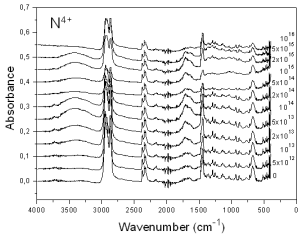

FIGURE 1. FT-IR spectra of ethylene-norbornene samples irradiated with N^{4+} ion beams.

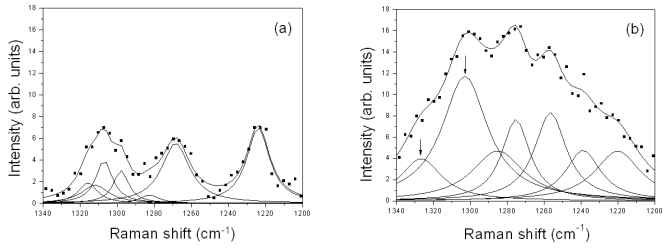

FIGURE 2. Lorentzian deconvolution of Raman spectra of ethylene-norbornene samples unirradiated (a) and irradiated (b) with N^{4+} ions for the fluence of 10^{16} cm^{-2}.

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Investigation of influence of finite-size scaling and aspect ratio on stick percolation

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Abstract.
On the basis of high-efficiency algorithm for Monte Carlo simulation, we investigate finite scaling and aspect ratio influence on percolation of stick networks. We find that aspect ratio of the system strongly influences moments of percolation probability distribution function. Based on our simulation results, we introduce correction of finite size scaling law for variable aspect ratio. In this way, system of percolating stick is completely described. With given dimensionality, percolating rule, boundary conditions, and aspect ratio, all percolating systems of stick fall on the same scaling function. For infinite cluster, we show that percolating probability at percolation threshold shows excellent agreement with Cardy's prediction for lattice percolation[1].

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Network-Based Methodology for Analysis of Complex Systems: Theory & Applications

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Abstract. Complex systems across different scales can be represented by networks, whose structural properties are closely related with dynamical features of the system [1]. Mesoscopic inhomogeneities, which can be detected as topological subgraphs (communities), often indicate existence of *functional units*, as for instance in protein interactions, gene-expression correlations [2], or Web-based social networks [3]. We present a systematic methodology for detecting the functional units or communities from the empirical data in complex systems. It is based on mapping the data onto suitable type of networks and the eigenvalue spectral analysis of the Laplacian operator on these networks. We demonstrate the methodology on complex modular graphs grown by computer codes, as benchmark structures [4], and apply it to find Web-based communities from the data of Blog users [3]. The methodology is suitable for finding the dynamic substructures in the assemblies of nano-systems, which can be mapped onto complex networks [5].

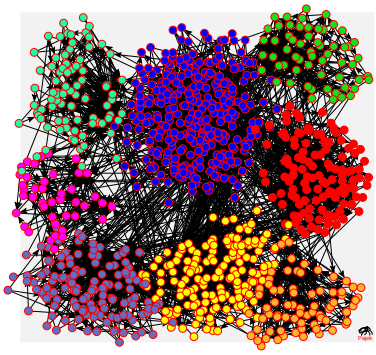

FIGURE 1. An example of complex network with marked topological modules [4].

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Altering Glass Transition of TPD thin Films with UV Light

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N,N´-Bis(3-methylphenyl)-N,N'dyphenilbenzidine (TPD) is a hole-transport material used in electroluminescent devices whose glass transition temperature, Tg, depends on the film thickness.[1] For sufficiently thin films (d<30 nm), dewetting of amorphous TPD films deposited on a on fused-silica or an ITO substrate occurs even at room temperature.[2] Following a brief report on increased thermal stability of UV irradiated TPD films,[3] we investigated the underlying mechanism responsible for it. From proton NMR and mass spectrometry measurements, coupled with morphology (AFM) and spectroscopy (UV-VIS) studies, we find that photo-excited TPD species react with oxygen in air. This leads to partially oxidized TPD films whose increased thermal stability we ascribe to stronger hydrogen bonding of photo-oxidized TPD species with hydrophilic substrates.

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