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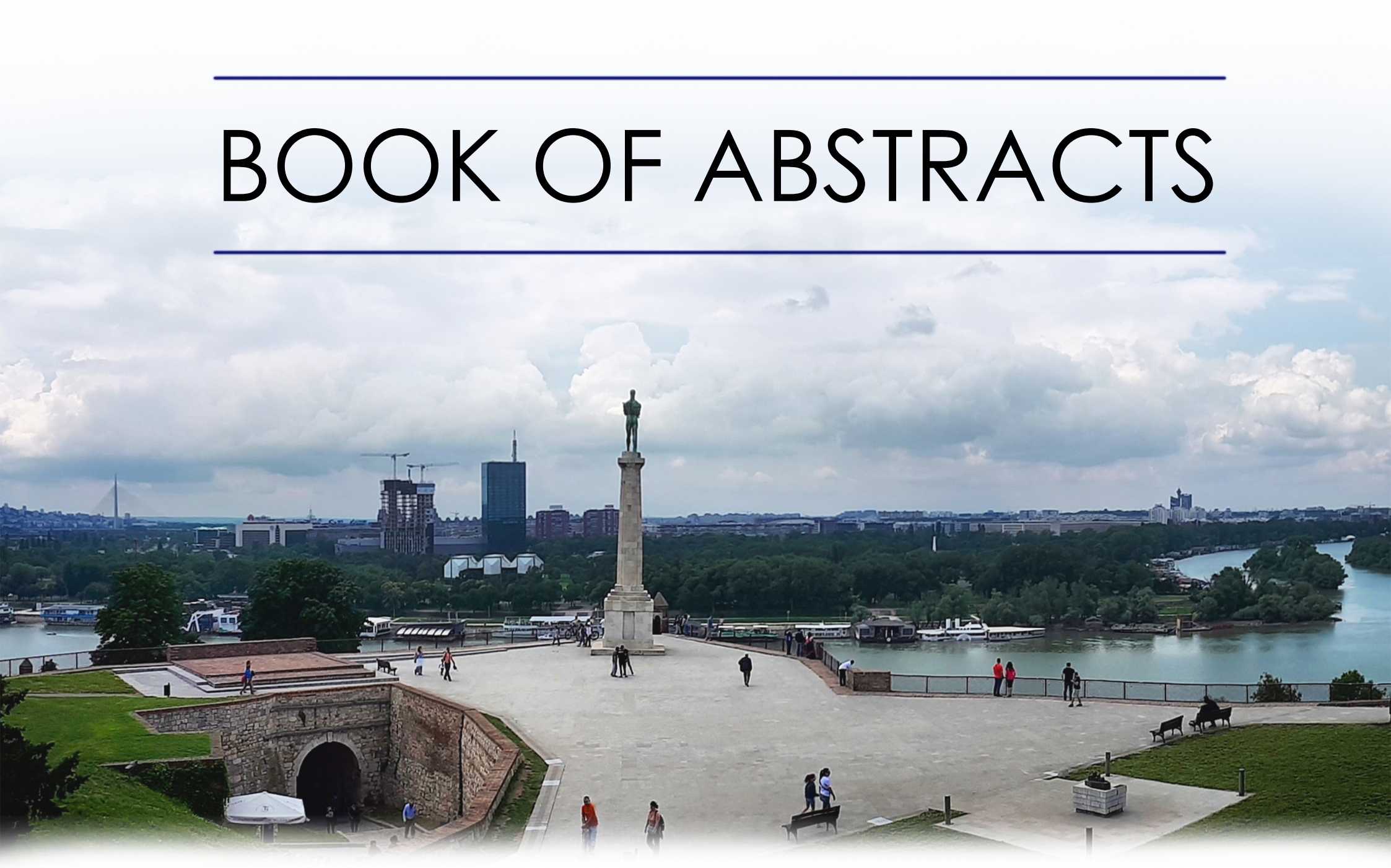
The 20th Symposium on Condensed Matter Physics

BOOK OF ABSTRACTS



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XX SYMPOSIUM ON CONDENSED MATTER PHYSICS SFKM 2019

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- Qingming Zhang, Lanzhou University and Institute of Physics, Chinese Academy of Sciences

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DNA-Based Dendrimers: Novel Macromolecules With Peculiar Characteristics

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Abstract. We present a joint theoretical-experimental study of a novel class of macromolecules, the so-called dendrimer-like DNAs (DL-DNAs). They have recently been synthesized from the enzymatic ligation of Y-shaped DNA unit, a three-armed structure consisting of double-stranded DNA (ds- DNA), formed via hybridization of three single-stranded DNA chains (ss-DNA), each of which has partially complementary sequences to the other two [1]. To describe such dendrimers of various generations we have employed a bead-spring model, in which base-pairs of a single DL-DNA molecule are modeled by charged monomers, whose interactions are chosen to mimic the equilibrium properties of DNA correctly. We have performed Molecular Dynamics Simulations and we have also employed dynamic/static light scattering in order to determine equillibrium properties and conformational characteristics of all-DNA dendrimers as well as the behavior of their solutions. We have investigated their behavior in ionic solution, paying particular attention on their salt-responsiveness. Our computational and experimental results reveal that the DL-DNAs are rigid objects with low internal monomer concentration, regular voids in their interior, with high persentage of absorbed counterions, and that show high resistance to stimuli-responsiveness [2]. These properties shape the behaviour of their solutions. Namely, both experimental as well as computational results show anomalous structure factor of dense DL-DNA solutions, as it had been predicted theoreticaly in Ref [3]. In this way we have found the object which was a missing puzzle in understanding the full phase diagram of star polymer solutions.

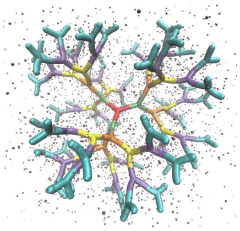

FIGURE 1. 6th generation of the dendrimer composed of Y-shaped DNA building blocks.

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Spectroscopy of few-layer superconducting $NbSe_2$

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Abstract. Tunnel junctions, an established platform for high resolution spectroscopy of super- conductors, require defect-free insulating barriers; however, oxides, the most common bar- rier, can only grow on a limited selection of materials. We show that van der Waals tunnel barriers, fabricated by exfoliation and transfer of layered semiconductors, sustain stable currents with strong suppression of sub-gap tunneling [1], [3]. This allows us to measure the spectra of bulk (20 nm) and ultrathin (3- and 4-layer) $NbSe_2$ devices at 70 mK. These exhibit two distinct superconducting gaps, the larger of which decreases monotonically with thickness and critical temperature. The spectra are analyzed using a two-band model incorporating depairing. In the bulk, the smaller gap exhibits strong depairing in in-plane magnetic fields (see Figure1), consistent with high out-of-plane Fermi velocity to be related to 3D character of electron band associated to this gap [2]. In the few-layer devices, the large gap exhibits negligible depairing, consistent with out-of-plane spin locking due to Ising spin– orbit coupling. In the 3-layer device, the large gap persists beyond the Pauli limit as also expected for Ising superconductors. Recent experiment in high magnetic field give a critical field of about 30 T.

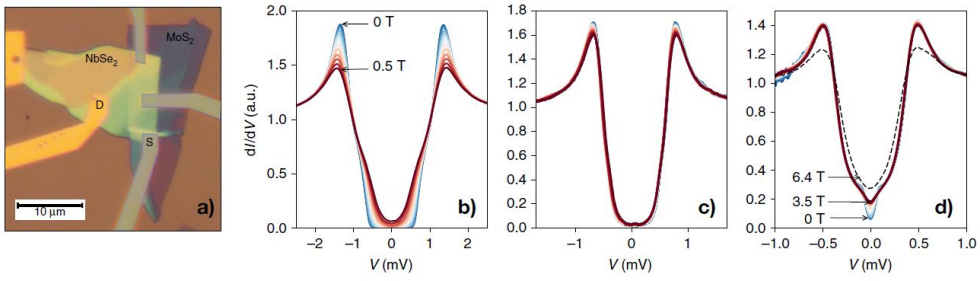

Figure 1: Tunneling conductance to parallel magne2c fields. **a)** Op2cal image of the tunnel junc2on device. The yellow-green flake is a 50–20 nm thick $NbSe_2$ (20 nm at the source electrode) and the purple-blue flake is a 4–5 layer MoS_2. Au electrodes are deposited on the leL to serve as ohmic contacts (yellow) and on the right to serve as tunnel electrodes (purple). **b)** dI/dV curves at increasing magne2c field parallel to the $NbSe_2$ layers of the bulk sample. **c)** and **d)** Same for the 4- layer and 3-layer device at $0 < H_{||} < 3.5$ T. Dashed line in d): dI/dV curve taken with the 3-layer device at uncompensated parallel field of 6.4 T.

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Polar Micro Bricks in an Active Bath

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Abstract. Artifical or biological microswimmers perform active motion by some internal propulsion mechanism enabling them to swim forward. A collection of these microswimmers constitutes an active bath that has exceptional properties. For example, when passive particles, which do not self-propel, are suspended in such a bath, they are stochastically pushed around and, more importantly, their motion can be rectified if they have a polar shape. We design specially shaped passive particles, which we term *micro bricks*, so that they exhibit large directed drift motion, when immersed in the active bath. We perform Brownian dynamics simulations of the active bath in two dimensions, and explore different shapes of immersed micro bricks with the goal to make their effective velocity as large as possible so that they manuver quickly. Essential are grooves, where active particles from the bath accumulate and push the brick forward. On the opposite edge active particles are guided to the side so that they do not push against the brick so efficiently.

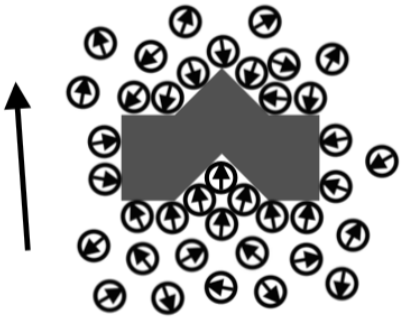

FIGURE 1. Active particles push the brick in the direction of the arrow.

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Disordered Configurations of the Glauber Model on Two-Dimensional Networks

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Abstract. We analyze the ordering efficiency and the structure of disordered configurations for the zero-temperature Glauber model on Watts-Strogatz networks obtained by rewiring 2D regular square lattices. In the small-world regime, the dynamics fails to reach the ordered state in the thermodynamic limit. Due to the interplay of the perturbed regular topology and energy neutral stochastic state transitions, the stationary state consists of two intertwined domains, manifested as multi-cluster states on the original lattice. Moreover, for intermediate rewiring probabilities, one finds an additional source of disorder due to the low connectivity degree, which gives rise to small isolated droplets of spins. We also examine the ordering process in paradigmatic two-layer networks with heterogeneous rewiring probabilities. Comparing the cases of a multiplex network and the corresponding network with random inter-layer connectivity, we demonstrate that the character of the final state qualitatively depends on the type of inter-layer connections.

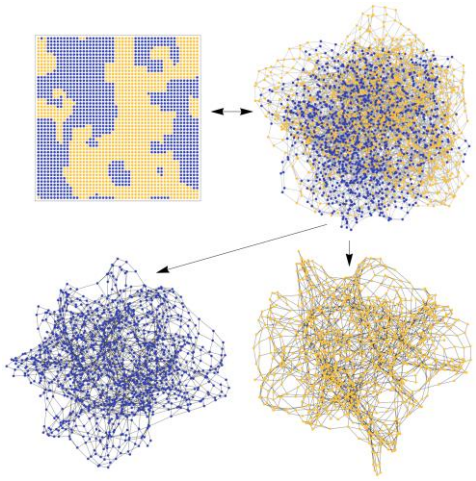

FIGURE 1. A disordered configuration with two domains comprises a multi-cluster state on the lattice.

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Topological quantization and gauge invariance of charge transport in liquid insulators

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Scuola Internazionale Superiore di Studi Avanzati, Trieste

Abstract. According to the Green–Kubo theory of linear response, the conductivity of an electronically gapped liquid can be expressed in terms of the time correlations of the adiabatic charge flux, which is determined by the atomic velocities and Born effective charges. We show that topological quantization of adiabatic charge transport and gauge invariance of transport coefficients allow one to rigorously express the electrical conductivity of an insulating fluid in terms of integer-valued, scalar, and time-independent atomic oxidation numbers, instead of real-valued, tensor, and time-dependent Born charges.

Nematic Fluctuations In Iron Based Systems

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Abstract. The origin and interplay of nematicity, magnetism, and superconductivity in iron based materials are still a subject of current research. The fluctuations which precede the ordered phases provide an additional probe for these phenomena. Using Raman spectroscopy we study fluctuations in $Ba(Fe_{1-x}Co_x)_2As_2$ (x = 0-0.051) as a function of temperature, symmetry, and doping. Our results provide evidence for critical spin fluctuations, suggesting a spin driven mechanism of the nematic and magnetic order. We discuss similarities with related systems such as $EuFe_2As_2$ and FeSe.

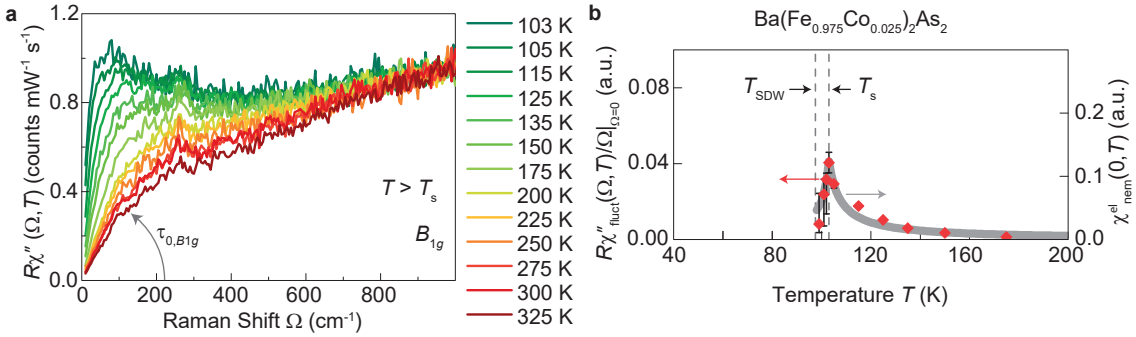

FIGURE 1. Fluctuations in $Ba(Fe_{0.975}Co_{0.025})_2As_2$. **a** Due to the response from fluctuations above the structural phase transition at $T_s \approx 103$ K the spectral weight at low energies and the initial slope $\tau_{0,B1g}$ increase upon cooling. **b** The initial slope (red diamonds) exhibits a maximum at T_s, but the fluctuations only vanish at the magnetic ordering temperature T_{SDW}. The maximum is reflected in the temperature dependence of the electronic nematic susceptibility χ^{el}_{nem} (grey) when the fluctuations couple to the lattice.

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Hydrogen-induced high-temperature superconductivity in two-dimensional materials: The case of hydrogenated monolayer MgB2

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Abstract. In seminal work of 1968 Ashcroft showed that dense metallic hydrogen, if ever produced, could be a high-temperature superconductor, owing to its very high Debye temperature, as a result of its minimal mass, enabling very strong phonon-mediated superconducting pairing according to the Bardeen-Cooper-Schrieffer (BCS) theory [1]. Currently, it has been well established that hydrogen-based compounds under ultra-high pressure, such as the polyhydrides H3S [2] and LaH10 [3,4], superconduct through the conventional electron-phonon coupling mechanism to attain the record critical temperatures (*T*c) known to date.

We will demonstrate that the intrinsic advantages of hydrogen for phonon-mediated superconductivity can be exploited in a completely different system, namely two-dimensional (2D) materials [5]. Namely, we found that hydrogen adatoms can strongly enhance superconductivity in 2D materials. Firstly, Van Hove singularities in the electronic structure, originating from atomic-like hydrogen orbitals, lead to a strong increase of the electronic density of states, thus enhancing the electron-phonon coupling. Furthermore, the emergence of high-frequency hydrogen-related phonon modes in this system boosts the electron-phonon coupling further.

As a concrete example, we will focus on the effect of hydrogen adatoms on the superconducting properties of monolayer MgB2 [6,7], which we investigated by solving the fully anisotropic Eliashberg equations, in conjunction with a first-principles description of the electronic and vibrational states, and the coupling between them. We will show that hydrogenation leads to a high *T*c of 67 K, which can be boosted to over 100 K by biaxial tensile strain. This proves that hydrogenation of a 2D material can indeed induce strong electron-phonon coupling and high-*T*c superconductivity, as exploited in the bulk hydride compounds with record *T*c's to date [3,4], yet without the need to apply excessively high pressures that hamper practical applications.

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Quantum Geometry Of Topological Josephson Matter

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Abstract. Quantization effects due to topological invariants such as Chern numbers have become very relevant in many systems, yet, key quantities as the quantum geometric tensor providing local information about quantum states remain experimentally difficult to access. Recently, it has been shown that multiterminal Josephson junctions constitute an ideal platform to synthesize topological systems in a controlled manner [1, 2]. We theoretically study properties of Andreev states in topological Josephson matter and demonstrate that the quantum geometric tensor of Andreev states can be extracted by synthetically polarized microwaves [3]. The integrated absorption provides direct evidence of topological quantum properties of the Andreev states.

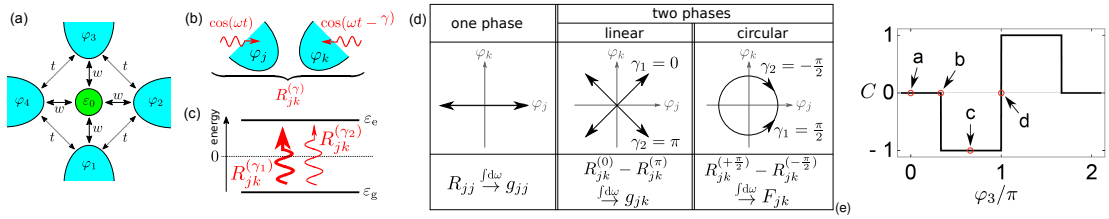

FIGURE 1. Application of polarized microwave spectroscopy in multiterminal junctions. (a) Microscopic model of the 4-terminal Josephson junction. Four superconducting leads, each with a phase φ_j ($j = 1,2,3,4$), are connected to a normal level ε_0 via the couplings w and nearest leads are connected by $t \ll w$. (b) A periodic modulation of two phases φ_j and φ_k at frequency ω leads to transitions with rates of absorption $R_{jk}^{(\gamma)}$, where γ is the relative phase between the modulations. (c) The absorption rates R_{jk} between the ground and the excited state depends on γ. (d) Schema of how to extract the elements of the quantum geometric tensor $\chi_{jk} = g_{jk} - iF_{jk}/2$ (metric tensor g and Berry curvature F). Driving of a single phase φ_j extracts the diagonal elements g_{jj}, while linear (circular) driving of two phases φ_j and φ_k, $j \neq k$, extracts the off-diagonal elements g_{jk} (F_{jk}). (e) The Chern number is obtained by integration $C(\varphi_3) = \int d\varphi_1 d\varphi_2 F_{12}/2\pi$ and is non-trivially quantized for certain values of the control phase φ_3.

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Local Orbital Degeneracy Lifting as a Precursor to an Orbital-Selective Peierls Transition

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Abstract. Fundamental electronic principles underlying all transition metal compounds are the symmetry and filling of the d-electron orbitals and the influence of this filling on structural configurations and responses. Curiously, some of the transition metal systems feature a large discrepancy between the long-range ordering temperatures (tens to hundreds of Kelvin) and the energy scales of the underlying electronic phenomena involved (hundreds to thousands of meV). I will address this often ignored and largely unexplained disparity through a study of one such compound, $CuIr_2S_4$ (CIS) spinel, where the orbital degrees of freedom play crucial role. $CuIr_2S_4$ displays temperature driven metal to insulator transition (MIT), where the low temperature insulating state consists of long range ordered Ir^{3+} ($5d^6$) and Ir^{4+} ($5d^5$) ions, with a four-fold periodicity, an example of tetrameric charge ordering [1]. Concurrently, spin dimerization of Ir^{4+} pairs occurs within the tetramer, with large associated structural distortions (0.5 Å) as they move towards each other, making this charge-order particularly amenable to detection using structural probes [2]. Notwithstanding the complexities of the insulating state, including formation of remarkable three-dimensional $Ir^{3+}{}_8S_{24}$ and $Ir^{4+}{}_8S_{24}$ molecule-like assemblies embedded in the lattice, its quasi-one-dimensional character was unmasked, and MIT attributed to an orbital-selective Peierls mechanism, postulated from topological considerations [3]. By utilizing a sensitive local structural technique, x-ray atomic pair distribution function analysis, we reveal the presence of fluctuating local-structural distortions deep in the high temperature metallic regime of $CuIr_2S_4$ [4]. The distortions are the fingerprints of a precursor high temperature state that enables the rich phenomenology observed at low temperature. Through judicious chemical substitutions, we show that this hitherto overlooked fluctuating symmetry lowering has electronic origin that can be understood as a local, fluctuating, orbital-degeneracy-lifted (ODL) state. Observation of the ODL state provides a natural way to understand the observed energy-scale discrepancy in a rage of transition metal systems. Our study also presents a very new view on MIT and related phenomena in the material studied - CIS, and CIS-derived spinel systems and experimentally verifies that the orbital sector indeed drives the physics in this material class. Our study exemplifies that such states exist but are difficult to detect and should be studied in a more systematic manner. The ODL state, characteristic of the high temperature regime, could be a critical ingredient and a missing link enabling more comprehensive understanding of phenomena as widespread as nematicity, pseudogaps, metal insulator transitions, spin glass behavior etc. The presentation will also spotlight a few other important ODL systems, such as FeSe and $NaTiSi_2O_6$.

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Anomalous Magnetism in $CaRuO_3$

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Abstract. Perovskites represent the wide class of materials exhibiting many different physical properties ranging from superconductivity, colossal magnetoresistance to ferroelectricity. Calcium ruthenate crystallizes in the orthorhombic modification of the ideal cubic perovskite structure, within which rotation and tilting of the oxygen octahedra play an important role in defining the properties of this material. It is widely believed that $CaRuO_3$ is located close to a quantum critical point due to the strong non-Fermi-liquid behavior expressed in the temperature dependence of electronic transport, optical conductivity, and specific heat [1-6]. We show here through detailed magnetic measurements that temperature dependence of the magnetic response of the system corresponds to the critical slowing of spin fluctuations towards T = 0 K [7]. We confirm these observations by magnetic measurements of $CaRu_{0.97}Ti_{0.03}O_3$, which show a pronounced magnetic response corresponding to the anomalies observed in the pure compound.

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Quantum State Manipulation and Relaxation Mechanisms in Single Atom Magnets

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Abstract. In the gas phase, single atoms have magnetic spin and orbital moments given by Hund's rules. Once these atoms are surface adsorbed, the symmetry is broken by the crystal or ligand field created by the chemical bonds. This creates magneto-crystalline anisotropy in the orbital moment, and through spin-orbit coupling, also in the spin moment. Through the low coordination, the orbital moment can largely be preserved resulting in magneto-crystalline anisotropies that can be up to three orders of magnitude larger than in bulk of the respective element [1]. This has created the hope to realize magnetic bi-stability in individual surface adsorbed atoms. We have indeed discovered two atom substrate combinations where single atoms exhibit stable magnetization at zero magnetic field. One is Ho/MgO(100) grown on Ag(100) [2] and the second Dy/graphene grown on Ir(111) [3]. Both systems continue to reveal surprises that we will talk about.

Single Ho atoms on MgO(100)/Ag(100) are the smallest and most stable magnets known today [2,4]. At 8 T external field, their onset temperature for switching from the metastable to the stable state is 45 K, and up to 35 K their coercitive field is far above 8 T [4]. Their magnetic state can be read and written with tunnel electrons [4,5]. However, their ground state and zero-field stability remained open issues. Using antiferromagnetic tips with robust zero-field spin-contrast [6], we determine the ground state and find that the nuclear spin states convert avoided level crossings to real ones at zero field, while at small fields they create a series of avoided level crossings. Landau-Zener tunneling at these crossings can be used to prepare the magnetic states without implying electrons [7].

Dy atoms on graphene on Ir(111) exhibit giant spin-contrast in STM images of up to 60 pm apparent height difference between up and down magnetization. We interpret this exceptionally large tunnel magneto resistance as 5d and 6s states being strongly polarized, due to Dy transferring almost an entire electron to graphene [8]. Together with Dy, many other rare-earth atoms adsorbed on graphene exhibit intense high energy inelastic conductance steps. Their origin is an intra-atomic spin-excitation between the 4f and 5d/6s spin-moments. For a given valence, the exchange energy between these moments is largely independent of the 4f element. Consequently, we observe a linear behavior of excitation energy with filling of 4f levels [9].

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Fröhlich allowed GaN Silent Modes in Raman Spectroscopy

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Abstract. Silent modes are those which are Raman and infrared forbidden. However, under resonant conditions (laser energy close to the band gap) we were able to observe the B_{1l} silent mode of GaN, while the B_{1h} could not be observed. The observation only in resonant conditions points out to a Fröhlich electron-phonon coupling. But, since the silent modes do not have a dipole moment, Fröhlich coupling cannot take place. The double Dutch have actually sense by realizing the isotopic compositions of both Ga and N. The isotopic composition also explains why the low energy mode is observed while the high energy silent modes is still silent.

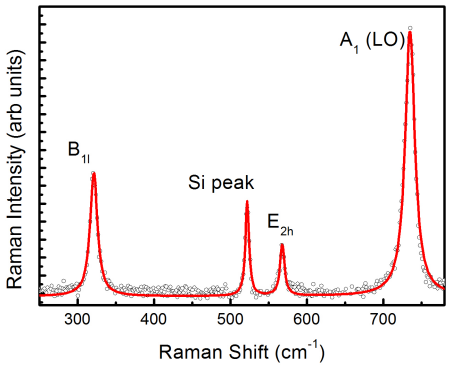

FIGURE 1. Resonant Raman spectrum of extremely narrow GaN nanowires.

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Theoretical Electron and Electron-Positron Momentum Densities of Transition Metals and their Compounds in the presence of Many-body Correlation Effects.

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Abstract. Valuable information about the nature of many-electron interactions in transition metals and their compounds is obtained from experiments based on Com pton and positron annihilation spectroscopy the later especially in the form of angular correlation of annihilation radiation measurements. These experiments access the electron momentum density and the momentum density of annihilating electron-positron pairs. Here we review theoretical state of the art techniques that combine Density Functional and Dynamical Mean Field Theory which allows to calculate the electron momentum densities. We survey recent experiments and calculations for paramagnetic and ferromagnetic transition metals and half-metallic ferromagnets.

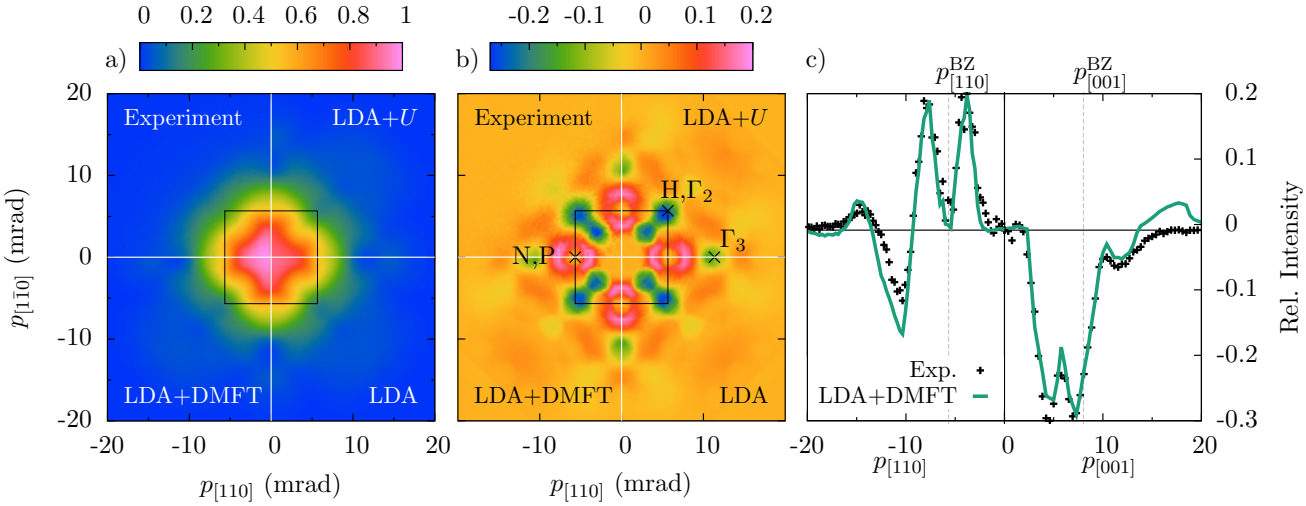

FIGURE 1. Experimental and theoretical results for Vanadium: (a) 2D-ACAR $\tilde{N}(p_x, p_y)$ spectra; (b) anisotropy $A(p_x, p_y)$ spectra. The color scale indicates the signal intensity relative to $\tilde{N}(0,0)$. The points Γ_2 and Γ_3 correspond to the $(1,1,0)$ and $(1,0,0)$ reciprocal lattice vector, respectively. With respect to the **k**-basis the N-point of the Brillouin zone has the coordinates $\mathrm{N}(0,\pi/a,\pi/a)$; (c) the cross sections of 2D-ACAR anisotropies ([001] projection) along the [110] and [100] directions illustrate the difference between experimental and DMFT anisotropies. Black crosses: experiment; green curve: LDA+DMFT calculations. The dashed lines indicate the Brillouin zone boundaries $p^{BZ}_{[110]/[100]}$ along the [110] and [100] directions, respectively.

Peculiar Electronic Dispersions in Two-Dimensional Materials Caused by Symmetry

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Abstract. Two-dimensional materials are spatial atomic arrangements that are periodic in two directions, but are finite in the third, orthogonal direction. Most of their physical properties are determined by the functional dependence of the electronic energy near the Fermi level on the electron wave vector i.e. by the electronic dispersion. Until recently only three types of electronic dispersions were known in two-dimensional materials: Dirac (as in graphene), semi-Dirac (as in black Phosphorus) and quadratic (as in MoS_2). In this talk we show that certain symmetries of non magnetic, time-reversal symmetric, two-dimensional materials with no spin-orbit coupling (SOC) leads unavoidably to new, forth type of electronic dispersion we called the Fortune teller (FT) dispersion [1]. Even more, inclusion of SOC leads to another type of peculiar electronic dispersion, which is generalization of both Dirac and FT dispersions. The physical properties of materials which these new dispersions induce are still to be investigated theoretically.

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Metal surface induces strong acoustic plasmons in chemically doped graphene

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Abstract. Recent theoretical considerations[1,2] have demonstrated that freestanding graphene doped with alkali metals (AC_x) supports strong Dirac and weak acoustic plasmons. Here we show that when AC_x is deposited on a metallic surface, the intense Coulomb screening completely washes out these collective modes. However, even small increase of separation between AC_x and metallic surface (Δ) causes recovery of AC_x plasmonic properties and especially the enhancement of acoustic plasmons intensities not present in the freestanding case. We shall explain the physical background of these intriguing phenomena. The studied systems consist of lithium- and cesium-doped graphene deposited on Ir(111) surface.

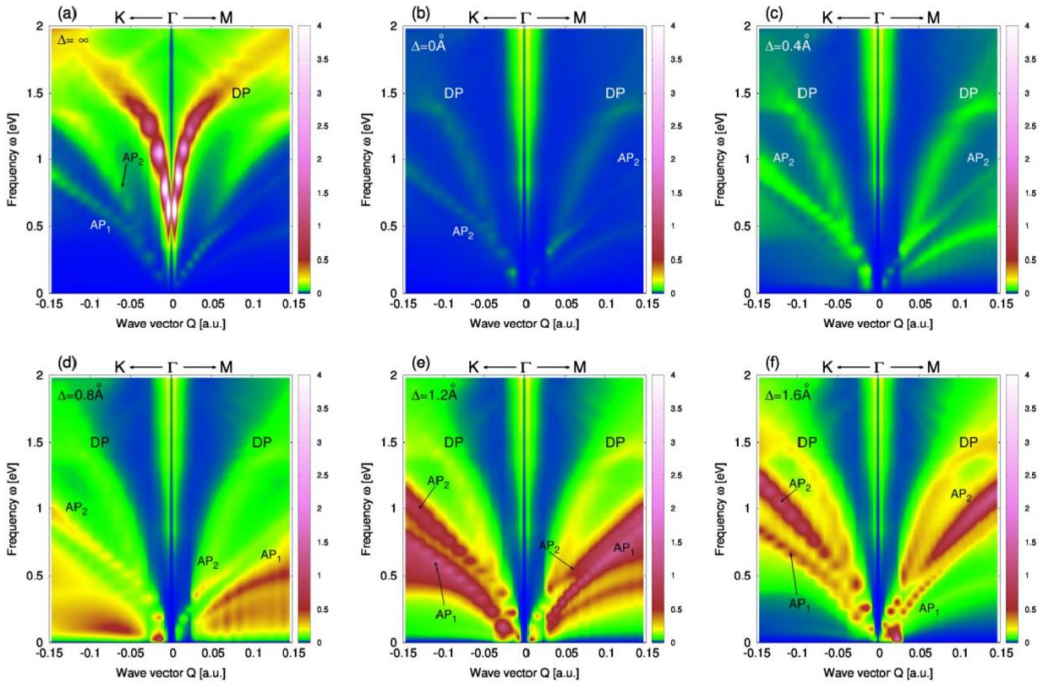

Figure 1: The EELS intensity in CsC8/Ir(111) composite for (a) $\Delta=\infty$, (b) $\Delta=0$, (c) $\Delta=0.4$Å, (d) $\Delta = 0.8$Å , (e) $\Delta = 1.2$Å and (f) $\Delta = 1.6$Å.

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Fluorescent nanostructured materials for cell bioimaging applications – fabrication and physical properties

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Abstract. Fluorescent imaging nanoprobes belong to a group of nano-sized materials devised to improve the spatial resolution of the images and enable the monitoring of biological events at the cellular and molecular levels. The optical properties of nanoprobes can be adjusted for specific applications by controlling their size, morphology, composition and surface chemistry. In addition, since they display favourable pharmacokinetic features, the nanoprobes can be designed for targeting drug delivery. Here, we will present the physical and structural properties of two types of fluorescent nanostructures developed recently in our group: partially reduced graphene oxide (prGO) and tryptophan-riboflavin bifunctionalized gold nanoparticles.

Partially reduced graphene oxide (prGO) was studied as a potential nanoprobe for the fluorescent microscopy of cancer cells. prGO, an intermediate form between graphene oxide (GO) and graphene, was prepared by the partial reduction of the previously prepared graphene oxide nanosheets with hydrazine. The reduction results with an increase in fluorescence of the GO sheets due to a change in ratio of the sp2 and sp3 carbon sites. The fluorescence intensity is dependent on the reduction time and it was found that it reaches maximum 6 min after introduction of hydrazine. The sample used in bioimaging studies was extracted from the dispersion at this particular time and then the reduction process was left to proceed to saturation until highly reduced graphene oxide (rGO) was obtained. The morphology and composition of the GO, prGO and rGO samples was studied by scanning transmission electron microscopy coupled with energy dispersive spectrometry (STEM-EDS). UV-vis and photoluminescence (PL) spectroscopies were used to investigate their optical properties. Deep-UV fluorescent bioimaging studies of the human Huh7.5.1 cancer liver cells incubated with fluorescent GO, prGO and rGO nanosheets were performed on DISCO beamline of synchrotron SOLEIL (France). After internalization of prGO sheets by the cells, a strong increase in the intensity of fluorescence signal was observed. In the spectral window from 420 to 480 nm, the fluorescence intensity off the prGO incubated sample was 2.5 times higher than the intensity of the autofluorescence of the control sample.

The other nanoprobe is the hybrid nanostructure obtained by functionalization of gold nanoparticles with amino acid tryptophan and vitamin riboflavin. Deep-UV fluorescence microscopy was used to study the interaction of functionalized nanoparticles and Huh7.5.1 cells. Since the wavelength of tryptophan fluorescence corresponds to the wavelength at which riboflavin absorbs, the resonance energy transfer (RET) process may occur between these two biomolecules. The fluorescence spectroscopy was used to study RET between the fluorophores when they are free in solution and when they are attached to surface of gold nanoparticles. The results showed that the energy transfer will be improved in the presence of the nanoparticles. It was also observed that the photobleaching dynamics of fluorescent centres in Huh7.5.1 cells upon 280 nm excitation would be different when the cells were treated by functionalized nanoparticles. By monitoring the changes in the photobleaching dynamics of the fluorophores, it was possible to

identify the areas in which accumulation of the nanoparticles takes place, although the particles were smaller than the spatial resolution of the images.

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Neural network based reverse-back procedure for photoacoustic electronic characterization of semiconductors

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Abstract. In this paper, a procedure for determining the coefficient of ambipolar diffusion of semiconductors based on their photoacoustic response is developed. The procedure is based on the processing of the experimental response using previously designed neural network which accurately performs thermal characterization and determines the thickness of the semiconductor sample combined with a reverse-back procedure in which the theoretical model of the photoacoustic response is used, which depends on the coefficient of diffusion of charge carriers in nonlinear mode. With the parameters obtained this way, theoretical photoacoustic response is repeatedly generated and compared to the experimental signal until a satisfactory match is achieved. Experimental measurements were previously performed on Si n-type circular plates with thicknesses levels of 830 μm, 417 μm and 128 μm using a transmission minimum volume open-cell experimental set-up. The accuracy of the procedure is discussed. The coefficients obtained by this procedure show good agreement with letarture predictions.

Keywords: photoacoustic, semiconductors, artificial neural networks, thermal diffusion, thermal expansion, photothermal, inverse problem, n-type silicon, reverse-back procedure

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The vibrational properties of CrI_3 single crystals

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Abstract. CrI_3 is a two-dimensional layered material and a ferromagnetic [1] with Curie temperature of 61K [1,2] and first order phase transition that occurs at 220K [3,4]. This class of materials has recently gained a lot of intention due to numerous potential applications. Here we represent our work consisting of both experimental and theoretical Raman scattering study of CrI_3 lattice dynamics. Based on our results we can distinguish two different phases for CrI_3 with monoclinic ($C2/m$) being the high-temperature and rhombohedral ($R\bar{3}$) phase being the low-temperature phase. Abrupt changes to the spectra were found at the first order phase transition which was located at $T_S \approx$ 180 K, lower than in previous studies. In contrast to the prior reports we found no sign of phase coexistence over temperature range exceeding 5 K [5].

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Classification of Quasi-One-Dimensional Topological Crystalline Phases: Topological Quantum Chemistry Approach

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Abstract. The problem of topological crystalline phases classification has so far been approached from various aspects. Recently, a new description, topological quantum chemistry (TQC) has been introduced [1]. Namely, it is well known that for particular system, its symmetry group and symmetry types of atomic orbitals located on the Wyckoff positions (occupied by atoms) determine the induced *band representation*. It is shown that all the band representations are sum of the finite number of *elementary band representations*. Then the topological properties of these prototypic band structures (as well as of and their combinations) can be read out from the properties of the associated graphs.

This technique, with few amends, is applied to quasi-one-dimensional systems. All possible elementary band representations (EBRs) are classified for all 13 families of line groups in both cases when the spin-orbit interaction is omitted or included. Symmetry-protected topological semimetal band structures [2] are singled out with the underlined mechanism. Topological phases with obstructed atomic limit are also selected.

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Why are hybrid halide perovskites exciting materials?

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Abstract. Recently, it has been shown that $CH_3NH_3PbI_3$ is very promising material in photovoltaic devices [1] reaching light conversion efficiency (η) up to 22% [2]. A strong research activity has been focused on the chemistry of the material to establish the most important parameters which could further improve η and to collect photons from a broad energy window. The major trend in this field is in photovoltaic device engineering although the fundamental aspects of the material are not yet understood.

In my laboratory we have devoted considerable effort to the growth of high quality single crystals at different length scales, ranging from large bulk crystals (up to 100 mm3) through nanowires [3,4] down to quantum dots of tens of nanometers of linear dimensions. The structural tunability of the material allows to study a broad range of physical phenomena including electrical and thermal transport, magnetism, optical properties, band structure by photoemission etc. With a selected set of measurements, I will demonstrate our enthusiasm for this material both in basic science and in device applications [5,6].

Acknowledgement: The work has been performed in collaboration with Endre Horvath, Massimo Spina, Balint Nafradi, Peter Szirmai, Alla Araktcheva, Pavao Andricevic, Andrzej Sienkiewicz, Claudio Grimaldi, Hugo Dil, and many others.

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Macroscopic Variability in Modular Neural Networks

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Abstract. Macroscopic variability is an emergent feature of neural networks, typically manifested as slow rate oscillations, which consist in spontaneous switching between the episodes of elevated neuronal activity and the quiescent episodes. The switching dynamics between the collective states is especially relevant for the activity of neocortical pyramidal neurons, and is believed to facilitate or mediate different types of learning and memory. We demonstrate the conditions that facilitate switching dynamics, focusing on the interplay between the different sources of noise and the heterogeneity in network topology. We consider modular (clustered) networks of rate-based neurons subjected to external and intrinsic noise, and derive a reduced model which describes the collective network dynamics in terms of a set of coupled second-order stochastic mean-field systems associated to each of the clusters. The model allows one to estimate the different contributions to effective macroscopic noise and qualitatively indicates the parameter domains where switching dynamics may occur. By analyzing the corresponding mean-field models in the thermodynamic limit, we highlight the differences in the mechanisms behind the switching phenomenon in non-clustered and clustered networks. In case of a non-clustered random network, switching is confined to a small parameter region, whereby the underlying mechanism resembles the motion of a noise-driven particle in a double-well potential. The switching mechanism qualitatively changes due to clustering, which is shown to promote multistability. Due to faciltatory role of clustering, the switching phenomenon gains robustness, occurring in a considerably broader parameter region compared to the case of a non-clustered network.

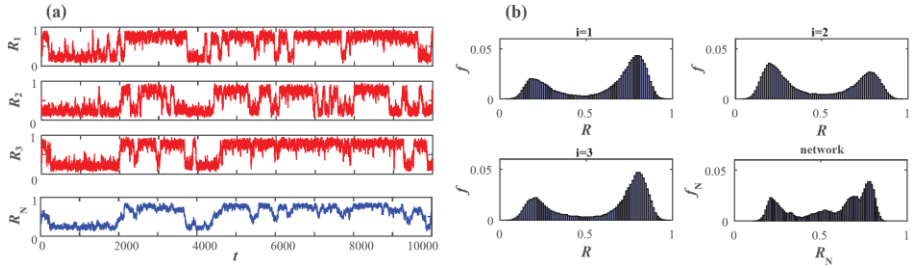

FIGURE 1. Example of switching dynamics in a clustered neural network. In panel (a) are shown the time traces of mean rates of individual clusters $R_i(t)$ and the network activity $R_N(t)$, whereas in (b) are illustrated the corresponding probability distributions.

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Analysis of the Frenkel excitons dynamics in pentacene

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Abstract. In the last few decades organic molecular solids have been matter of both theoretical and experimental studies, due to their potential applications in various organic devices. The dispersion relation for noninteracting excitons and the influence of perturbative correction is examined in the case of pentacene structure [1] and compared with the results given in [2], obtained by inelastic electron scattering at room temperature. Although [2] showed that noninteracting bosonic Hamiltonian can not be used to obtain the same behaviour as the one acquired by experimental data, in [1] one can see that this conclusion may be rather too strong. In [1] theoretical dispersion curves along four different directions in the Brillouin zone, were obtained using noninteracting bosonic Hamiltonian. These curves follow the periodicity of the experimental data. It was also shown in [1] that perturbative corrections are negligible since the exciton gap in dispersion relation is huge in comparison to exchange integrals. For these calculations perturbation theory developed in [3, 4] was used.

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Engineering Quantum States with Superconducting Quantum Circuits

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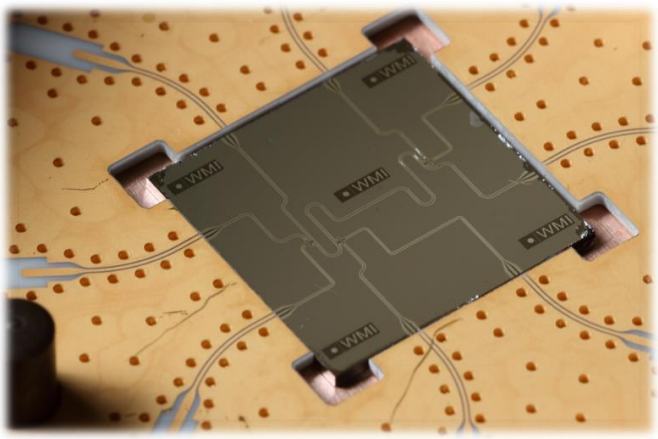
Abstract. Superconducting quantum circuits represent a highly successful solid-state platform, allowing us to engineer quantum states and thereby to study fundamental quantum effects and develop key components of future quantum technology. Examples are the tailoring of light-matter interac-tion, the development of sources and detectors for quantum light, or the implementation of quantum information processing, quantum metrology and quantum simulation systems. Meanwhile, several companies such as Google, IBM, Intel or Rigetti have started the race towards a universal quantum computer based on a superconducting hardware platform.

I will summarize the recent progress in the design, fabrication and performance of superconducting quantum bits [1-4] and address some key problems related to scaling-up superconducting quantum circuits to complex systems required to make solid-state based quantum information processing a reality. Superconducting circuits also have triggered the prospering subfield of quantum microwave communication & sensing [5-8], which aims at developing novel components, experimental techniques, and theory models building on the quantum properties of continuous-variable propagating microwaves. It provides the foundations for distributed quantum computing & communication via microwave quantum local area networks or sensing applications based on the illumination of an object with quantum microwaves (quantum radar).



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Real-Time Study of the Dynamics of Oxygen Vacancy Ordering at Heterostructure Complex Oxide Interfaces

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Abstract. The defect chemistry driven by oxygen vacancy formation provides an astonishing range of mechanisms for creating and compositional tuning of functionality in transition metal oxides. The cooperative interactions between vacancies can produce subtle differences in the structural arrangement of defects. Such oxygen vacancy ordering was found instrumental in a wide range of exotic behavior including high-temperature superconductivity and multiferroicity. The transformation between different structures is governed by vacancy dynamics, the transport of oxygen vacancies in and out of the sample and their migration across interfaces. The effects of vacancy dynamics are particularly important at surfaces and interfaces making the growth of thin films and heterostructures the premier method for developing greater control of oxygen vacancy profiles. In this talk I present a new approach for controlling oxygen vacancy dynamics illustrated by growing an oxygen deficient $SrTiO_3$ cap layer on a thin film of $La_{2/3}Sr_{1/3}MnO_3$ by pulsed laser deposition (PLD). The $SrTiO_{3-\delta}$ capping layer "extracts" oxygen from the $La_{2/3}Sr_{1/3}MnO_3$ film resulting in oxygen vacancy ordering leading to a phase transition from a perovskite (PV) to a brownmillerite (BM) phase in the buried layer. We use a new system that combines real-time X-ray diffraction (SXRD) with *in situ* hard X-ray photoemission spectroscopy (HAXPES) to characterize the spectroscopic signature and electronic structure associated with structural transformations identified by SXRD during PLD film growth. The $SrTiO_{3-\delta}$ film growth is monitored by time-resolved measurements of the SXRD intensity at the $(0\ 0\ 0.5)$ anti-Bragg position where a dramatic increase in intensity reveals the doubling of the PV unit cell in the buried layer indicating formation of the BM phase. This feature creates an extremely powerful combination of diffraction and spectroscopy enabled by the ability of HAXPES to penetrate the $SrTiO_{3-\delta}$ cap layer and characterize the electronic structure of the buried $La_{2/3}Sr_{1/3}MnO_{3-\delta}$ layer. Better understanding of oxygen vacancy ordering can provide new insight into the role of the coupling between structural and electronic degrees of freedom underlying the multiple instabilities in strongly correlated oxides responsible for a wide range of intriguing phenomena such as metal insulator transitions and a variety of orbital and magnetic ordering.

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Electronic Collective Modes as a Diagnostic Tool for Pairing in Superconductors

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Abstract. The superconducting energy gap $\Delta_{\mathbf{k}}$ is intimately related to the interaction potential $V_{\mathbf{k},\mathbf{k}'}$ that is at the origin of Cooper pairing. Usually only the dependence of the gap on momentum $\mathbf{k}$ is analyzed, for instance by angle resolved photoemission spectroscopy (ARPES), for obtaining information on the type of pairing. However, for understanding unconventional superconductors the phase of the gap is particularly important while it is notoriously complicated to get this information. Only neutron scattering or, very recently, tunneling spectroscopy in an applied magnetic field or in the presence of impurities provide some - still debated - indications of the phase of the ground state gap. Raman spectroscopy, similarly as all other spectroscopies, sees primarily the magnitude of the gap. However, there may be various additional features in the spectra which augment the lowest-order information. In all materials sharp in-gap modes are expected either having their origin in the band structure or resulting from anisotropies in $V_{\mathbf{k},\mathbf{k}'}$. In single-band superconductors the exciton-like modes predicted by Bardasis and Schrieffer (BS) are the leading higher order contribution encoding sub-dominant pairing tendencies above the ground state. When visible in the Raman spectra the BS modes directly show the symmetries of the sub-leading channels. They were identified in $Ba_{1-x}K_xFe_2As_2$ and analyzed using spin fluctuation (RPA) or renormalization group (fRG) schemes [2]. The spectra in $CaKFe_2As_2$ corroborate these results [3]. In multi-band superconductors there are various other contributions such as phase-number fluctuations between the bands (Leggett modes [4]) which were first observed in MgB_2 [5]. The energies of these modes depend crucially on the ratio of interband *versus* intraband coupling and are pushed to the gap edge when the interband interaction prevails [6]. All modes have characteristic features which by and large allow their identification. Once pinned down useful information for the pairing in unconventional superconductors can be derived from the properties of these collective modes.

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   The work was supported by the DFG via SPP 1458, SFB 1170 and TRR 80, by the DAAD, BaCaTeC, the ERC through ERC-StG-Thomale-TOPOLECTRICS, the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, and the Serbian Ministry of Education, Science and Technological Development. The RPA calculations were conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility. The work in China was supported by the National Key Research and Development Program of China and the National Natural Science Foundation of China (NSFC).
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Tensorial (d-wave) superconducting order in Luttinger semimetals

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Abstract.
We will discuss unconventional superconductivity in three-dimensional electronic systems with the chemical potential close to the quadratic band touching point in the band dispersion. The latter arises when the bands are inverted due to strong spin-orbit coupling, in materials such as mercury telluride or half-Heuslers, for example. Featureless contact interaction can then lead to either a familiar s-wave, or an unconventional d-wave state, with five complex components that transform as irreducible symmetric second-rank tensor under rotations. The general structure of the Ginzburg-Landau free energy for such a three-dimensional d-wave state with an emphasis on its unusual features that stem from the complex tensorial nature of the order parameter will be further elucidated. The computation of the coefficients in the Ginzburg-Landau free energy implies that in the isotropic limit there remains a large residual symmetry-unrelated accidental degeneracy at the quartic-term level between different d-wave configurations, which is ultimately resolved only by the higher-order terms. For a vanishing chemical potential the ground state is the superconducting analogue of the uniaxial nematic, which features two parallel circular line nodes in the quasiparticle spectrum. At finite chemical potential and at weak coupling, however, time-reversal-symetry-broken superconducting states which contain fermi points and surfaces are energetically preferred. Some phenomenology of various superconducting states and possible connections to the penetration depth measurements in YPtBi will be explored.

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Concepts for Understanding Nonlinear Second Harmonic Generation of Bulk Silicon

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Abstract. We have recently realized an experimental setup capable of measuring the polarization state of the outgoing frequency doubled (second harmonic generation- SHG reflected) radiation as a function of the polarization state of the incoming fundamental[1]. A sketch of this setup, allowing also to rotate the sample azimuthally with an angle of incidence of 45°, is shown in Fig.1. In Fig. 2 typical data exhibiting an amplitude as well as a phase variation are shown as a function of the azimuthal rotation angle for different polarizer and analyser setting (incoming 60°; outgoing SHG: p, 60°, 30°, s) for a Si(111) sample with native oxide.

In this contribution the focus is on presenting the concepts to understand the physical differences between linear optics and polarization sensitive nonlinear (spectroscopic) ellipsometry (NL-SE), especially NL-SHG, and to a smaller extent sum frequency generation (SFG). The main differences, besides the intensities and surface sensitivity, are:

1. In linear optics the Maxwell equations, respectively the Helmholtz equation "disguise" the fact that the sources of the polarization are inside the sample by deriving the Fresnel coefficients through the boundary conditions (cp. Ewald Oseen theorem). For NL-SE it is clear that the outgoing radiation is due to the anharmonic motion of the dipole sources inside, inducing a time dependent current, which generates via a vector potential the coherently superimposed fields of the single dipoles.
2. The linear Fresnel relations become unimportant for NL-SE, they are only used to calculate the field direction and strength $E_j(\omega)$ inside the material. The NL polarization is then given by $P_i(2\omega) = \varepsilon_0 \sum_{j,k} \chi^{(2)}{}_{ijk}(\omega) E_j(\omega) E_k(\omega)$. The nonlinear permittivity tensor $\chi^{(2)}{}_{ijk}(\omega)$ (using Clausius Mosotti also called hyperbolarizibility tensor) can also be complex, however, its imaginary part **does not determine extinction** during propagation, just a (rather noninteresting) relative phase shift between fundamental and SH.
3. Despite NL ellipsometry cannot be used to measure the amplitude and phase of the first element of $\chi^{(2)}{}_{111}(\omega)$ relative to the fundamental, it is able to determine the relative phases between this single element and all – up to 26- others.
4. The Simplified Bond Hyperpolarizibility Model (SBHM), proposed by D. E. Aspnes,[2] reduces these 27 parameters to one, and until now it can describe all experimental findings well, cp. Fig. 2. For rather many systems (e.g. zincblende)

this *a- priori* assumption can be proven by group theory[3]. However, one has to be aware that 3rd and 4th rank tensors are never isotropic and even NL permittivity tensors with one element show direction dependent properties. Finally we will present a method to test in the simplest nontrivial case the SBHM *ansatz*.

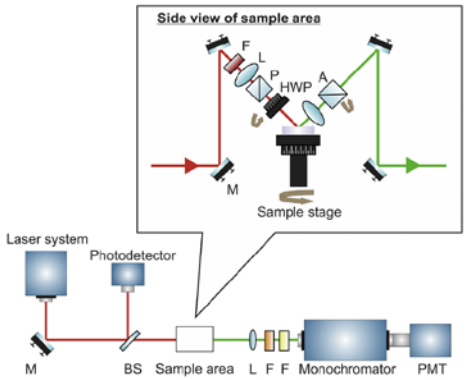

FIGURE 1. Top view of setup for polarization sensitive rotational SHG experiments; tunable laser system, mirror (M), beamsplitter (BS), photodetector,filter (F), lens (L), Glan-laser prism (P), rotatable half-wave plate (HWP), rotatable analyzer (A), monochromator, photomultiplier tube (PMT). Insert: Side view of sample stage.

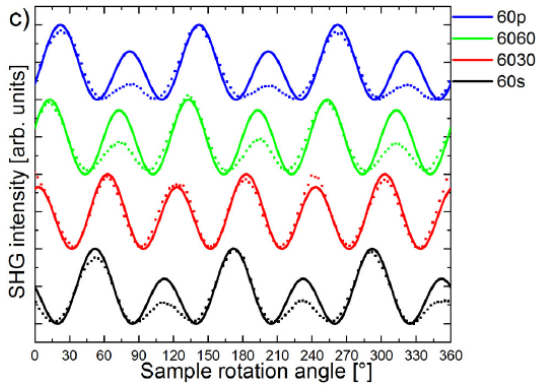

FIGURE 2. Experimental (dotted) and simulated (SBHM Model, solid line) data for 4 different polarization states measured on a Si(111) surface at a SHG wavelength of 400 nm. Plots are vertically shifted for clarity.

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Engineering the Electronic and Chemical Properties of Graphene via Functionalization and Intercalation.

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Abstract. Extensive control of the electronic and chemical properties of graphene on Ir(111) is available through chemical functionalization [1] and intercalation. Combined Scanning Tunneling Microscopy, (Standing Wave) X-ray Photoemmission Spectroscopy and Density Functional Theory calculations show how on one hand, functionalization structures can be controlled via intercalation, while conversely, intercalation can be hindered via chemical functionalization. Furthermore, unique oxygen functionalization structures [2] and molecular hydrogen dissociative adsorption pathways [3] are available in this system. Overall this allows for extensive control of electronic properties for band gap engineering [1], as well as control of the graphene-substrate interaction, providing proof-of-principle pathways to e.g. enhance the coating properties of graphene on metal surfaces [4].

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Searching For Quantum Scars In Constrained Bosonic Models

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Abstract. Recent experiments on arrays of Rydberg atoms have shown that preparing a system in a certain initial state can lead to unusually slow thermalization and persistent density oscillations [1]. This type of non-ergodic behavior has been attributed to the existence of "quantum many-body scars", i.e., atypical, weakly-entangled eigenstates of the system that have high overlaps with a small subset of vectors in the Hilbert space. Periodic dynamics and many-body scars are believed to originate from a "hard" kinetic constraint: due to strong interactions, no two neighbouring atoms are both allowed to be in an excited Rydberg state. Here we investigate quantum many-body scars in a 1D bosonic lattice model with a "soft" constraint: there are no restrictions on the allowed boson states and the particles can hop freely, but the amplitude of a hop depends on the occupancy of the hopping site. We find that this model exhibits similar phenomenology to the Rydberg atom chain, including weakly entangled eigenstates at high energy densities and the presence of a large number of exact zero energy states, with distinct algebraic structure. We discuss the relation of this model to the standard Bose-Hubbard model and possible experimental realizations using ultracold atoms.

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Electronic Structure Engineering Of SiGeSn(C) Alloys For Optoelectronic And Thermoelectric Applications

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Abstract. The electronic band structure of binary and ternary group-IV SiGeSn alloys is first briefly reviewed, and different aspects of their optoelectronic applications discussed, and the computational analysis is then extended to the dilute carbon-containing alloys. Furthermore, calculations of thermoelectric properties of group-IV SiGeSn alloys are presented and discussed.

With the advances in group-IV photonics a reliable knowledge of the electronic band structure of CSiGeSn alloys, including their ternary and binary subsets, is increasingly important. The eventual target is the integration of group-IV alloy based (opto)electronic components on silicon substrate, with all the benefits coming from mature and cost-effective fabrication. The directness of the band-gap is most important for optoelectronic devices, primarily lasers [1], but also for some purely electronic devices, e.g. by delivering a higher electron mobility. The values of direct and indirect gaps can be controlled by both the composition and strain. Some of the group-IV alloys have been studied in considerable detail, e.g. [2]. We first review the recent studies of the band structure of SiGeSn, and discuss the potential of these alloys for optoelectronic applications, and then present theoretical considerations of carbon-containing alloys, where different predictions of the effects of incorporation of carbon on the alloy band gaps have been made, e.g. [3,4].

Another possible application of SiGeSn alloys is for thermoelectrics. Calculations of their thermoelectric properties, for both n- and p-doped materials, are presented and, combined with the calculated thermal conductivity [5], the results indicate good prospects for applications of these alloys for thermoelectric power conversion.

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Spontaneous Emission In Metallodielectric Superlattices

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Abstract. Metallodielectric superlattices with ultrathin noble metal layers are known to exhibit interesting optical properties associated with the excitation of Bloch plasmons - bulk waves formed through the hybridization of single-interface surface plasmon polaritons [1]. Very large values of the photonic density of states (PDOS) [2] found in these systems, explicable in simple terms by analogy with hyperbolic media [3], have recently been of particular interest in view of developing novel light sources.

Here we consider the problem of spontaneous emission for emitters placed at locations where the discrete translational symmetry of the superlattice is broken: at interfaces with homogeneous media [4], as in recent experiments [5], and near defects inside the superlattice appearing when a layer slightly deviates from the periodic pattern, relevant for emitters embedded into the superlattice. Our results show that the PDOS spectra is strongly influenced by the contribution of localized states, which is of particular interest for quantum emitter-based light-emitting devices and photodetectors.

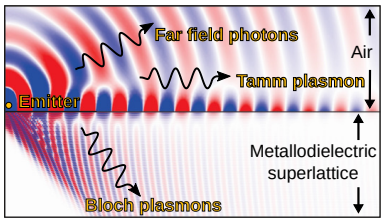

FIGURE 1. Electromagnetic field radiated by a vertical point dipole on top of a semi-infinite metallodielectric superlattice, illustrating the excitation of Bloch plasmons in the superlattice and a Tamm plasmon [4] localized at the interface.

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The effect of thresholding on interevent correlations

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Abstract. Systems that respond to external stimuli by bursty dynamics in the form of avalanches are ubiquitous. Subsequent avalanches in many systems with such dynamics are separated by waiting times whose distributions are of power-law type suggesting the existence of temporal correlations even when the original avalanche triggering is described by a random uncorrelated process. We show that such correlations may arise due to implementation of a finite detection threshold separating the avalanche events into subavalanches. This is demonstrated by the analysis of data from planar crack propagation experiments and numerical simulations of the related nonequilibrium crack-line model, as well as in the case of 3D nonequilibrium zero temperature random field Ising model.

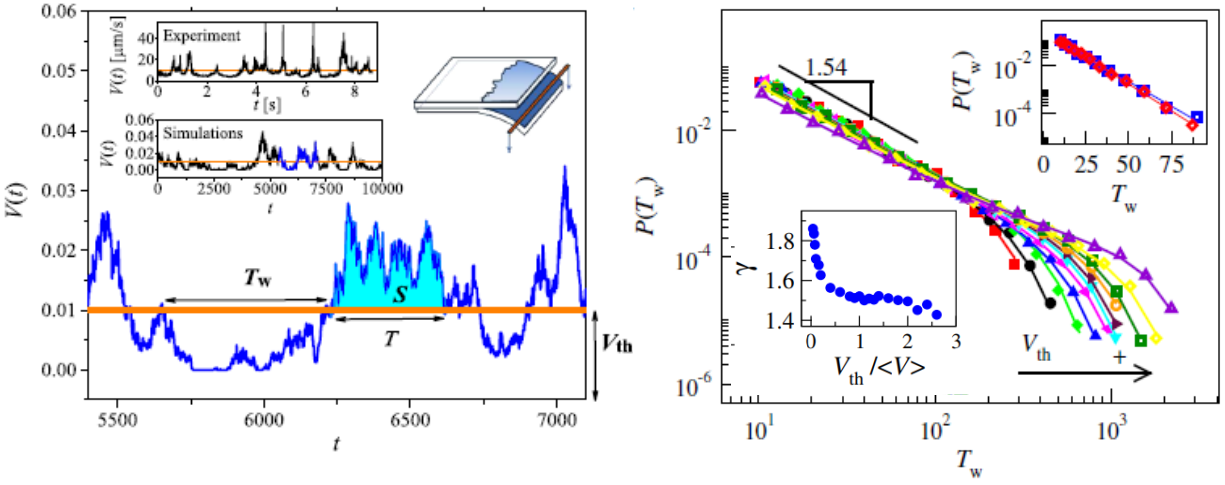

FIGURE 1. Left panel: Thresholding of a signal. Right panel: Power-law distributed waiting times between the events of interest.

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Light-To-Charge Conversion In Organic Photovoltaics: Mechanisms And Timescales

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Abstract. Recent years have seen an intense debate on the physical mechanisms and time scales of free-charge generation following photoexcitation of donor/acceptor organic solar cells, which initially produces strongly bound excitons in the donor material. The interpretation of ultrafast spectroscopic signatures suggests that free carriers are predominantly generated on a subpicosecond time scale following the excitation, the key role in this process being played by high-energy ("hot") delocalized interfacial charge transfer (CT) states [1]. However, other experimental studies indicate that the main precursor towards free charges is the strongly bound and localized ("cold") CT state, so that free-charge generation occurs on time scales ranging from tens to hundreds of picoseconds [2, 3].

We investigate charge separation in a one-dimensional model of an interface between two organic semiconductors, both on ultrashort and on much longer time scales. We conclude that free carriers present on a subpicosecond time scale following a pulsed photoexcitation are mainly directly optically generated from the ground state thanks to the resonant mixing between states of donor excitons and free charges [4]. However, on the same time scale, we find that the majority of photogenerated charges still remain bound in form of donor or CT excitons [5]. We obtain that their further separation on longer time scales is weakly electric field- and temperature-dependent and is enabled by the synergy between carrier delocalization and moderate disorder [6].

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A Step Towards A Comprehensive Steady-State Picture Of Photosynthetic Solar Energy Conversion

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Abstract. The interpretation of oscillating experimental signals observed in ultrafast nonlinear spectroscopies [1] has been motivating vigorous interest in quantum effects in photoinduced biological processes. However, electronic dynamics triggered by natural light, which is stationary and incoherent, is generally substantially different from the one observed in pulsed laser experiments. It has been suggested that the physically correct picture of photosynthetic excitation energy transfer (EET) should be in terms of a steady state [2], which is formed when the photosynthetic antenna is continuously photoexcited and continuously delivers the excitation energy to the reaction center, in which charge separation takes place.

We study EET triggered by a low-intensity photoexcitation of an initially unexcited molecular aggregate, which interacts with its environment and is coupled to the reaction center. We treat the aggregate–environment coupling in a numerically exact manner and extend previous theoretical treatments [3, 4] by formulating the hierarchy of equations of motion (HEOM) which explicitly takes into account the photoexcitation process. We investigate the properties of the steady state arising when the aggregate is subjected to a continuous-wave excitation, while the charge separation from the reaction center occurs at a constant rate. The developed theoretical formalism enables us to approach questions ranging from the influence of the short-time dynamics (which is accessible in pulsed laser experiments) on the steady state to the relevance of steady-state coherences for the EET process.

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Computationally intelligent estimation of properties for polymer microphone diaphragms by photoacoustic measurement

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Abstract. This paper presents the application of artificial neural networks for fast and precise characterization of electret microphones with polymer transducer (diaphragm) by photoacoustic measurements. The model consists of two neural networks: the first one for the classification of the microphone type and the second one for the determination of the detector parameters, related to its electronic and geometric features as well as to piezoelectric transducer properties. Obtained prediction has been used for estimation of polymer diaphragms properties by employment of Helmholtz model for sound propagation in small volumes.

Keywords: photoacoustic, artificial neural networks, microphone

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Fluctuations In $Ba(Fe_{1-x}Co_x)_2As_2$ Close To Quantum Criticality

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Abstract. Fluctuations arising from a quantum critical point (QCP) have been discussed to play a vital role in the pairing mechanism of unconventional superconductors. However, the very nature of the QCP as a phase transition at zero temperature renders it inaccessible to experiments. The associated quantum fluctuations on the other hand extend over a wide temperature range even above the superconducting transition temperature T_c and may therefore be probed by experimental means.

We present inelastic light scattering results on $Ba(Fe_{1-x}Co_x)_2As_2$ in extension of an earlier study tracking critical fluctuations from $x = 0.055$ to optimal doping ($x = 0.060$) into the overdoped regime at $x = 0.085$. While the thermal fluctuations present for the underdoped compounds are expected to vanish at optimal doping, we find a finite response from fluctuations for optimally doped $Ba(Fe_{0.94}Co_{0.060})_2As_2$. These fluctuations survive down to T_c in absence of any other phase transition such as nematic or magnetic ordering. To shed light on the nature of these fluctuations, they were analysed twofold: (a) on the real time axis by extracting the static susceptibility $\chi'(0)$ via a Kramers-Kronig transformation and (b) on the imaginary time axis by calculating the imaginary time-ordered correlation function $\tilde{\Lambda}(\beta/2)$ with β being the inverse temperature. $\tilde{\Lambda}(\beta/2)$ is a quantity measured by quantum Monte Carlo simulations and can be connected to the real frequency Raman response. This enables us to directly compare theoretical and experimental data in the vicinity of a QCP.

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Higher Order Topological Phases: General Principle of Construction and Their Realizations

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Abstract. Topological states of matter, featuring exotic robust boundary states, are at the forefront of research in the modern condensed matter physics. In this talk, I will focus on the topological phases in the electronic systems, which are characterized by a topological invariant of the corresponding band structure. The emergent gapless edge or surface states are protected by the bulk topological invariant and arise as a consequence of the so-called bulk-boundary correspondence, which is a hallmark feature of a topological state. More recently, the notion of topological states of matter has been extended to the so-called higher order topological (HOT) states featuring gapless surface states at boundaries of co-dimension higher than one, such as hinges and corners.

I will particularly discuss a general principle of construction for these states within the Dirac Hamiltonian framework [1]. As I will show, if a D-dimensional first-order or regular topological phase involves m Hermitian matrices that anticommute with additional p - 1 mutually anticommuting matrices, an nth-order HOT phase can be realized, where n = 1,…, p, with appropriate combinations of discrete symmetry-breaking Wilsonian masses. This principle will be illustrated on prototypical three-dimensional gapless systems, such as a nodal-loop semimetal possessing SU(2) spin-rotational symmetry, and Dirac semimetals, transforming under (pseudo)spin- 1/2 or 1 representations. The former system permits an unprecedented realization of a fourth-order phase, without any surface zero modes. The crystalline symmetries play an important for HOT states, but, as I will show, they can also be realized in amorphous solids [2]. Particularly, as long as structural disorder is confined by outer crystalline boundary, the system continues to host corner states, realizing an amorphous HOT insulator. However, as structural disorder percolates to the edges, corner states start to dissolve into amorphous bulk, and ultimately the system becomes a trivial insulator. Finally, I will discuss a realization of an out-of-equilibrium second order topological insulator, which is obtained from a quantum spin Hall insulator by using a particular kicking protocol [3].

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Wake Potential In Graphene-Sapphire-Graphene Composite Systems

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Abstract. We investigate the wake potential of different hybrid modes in the sy_1-Al_2O_3-sy_2 composites induced by charged particle moving parallel to the structure, as depicted in FIG. 1. This will be attained by exposing any wake patterns of the electrostatic potential in the surface closest to the incident particle. The three methods used in acquiring the effective dielectric function of the structure are based on the massless Dirac fermions (MDF), the extended hydrodynamic (eHD) model, and the *ab initio* approach. It is shown that in the low velocity regime (below graphene's Fermi velocity, v_F) transverse optical (TO) phonons in the Al_2O_3 layer give dominant contribution to the wake potential. In the intermediate velocity regime (above v_F) it is the hybridized plasmon-TO phonon modes on both surfaces that give rise to the wake potential with hybridized Dirac plasmons giving the dominant contribution. For the high velocities (well above v_F) only the symmetric hybridized Dirac plasmons are excited by the charged particle. It was found that *ab initio* approach agrees well with the MDF method at low and intermediate velocities for the pristine and doped graphene, and with eHD method at high velocities for pristine graphene layer.

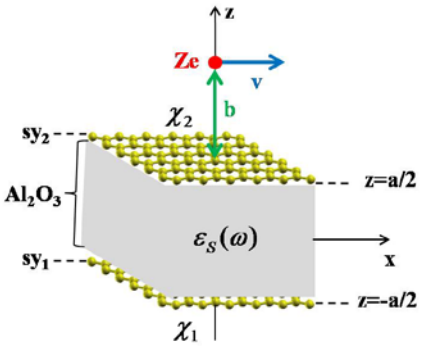

FIGURE 1. Diagram of a graphene-sapphire-graphene structure with point charge *Ze* moving parallel to the *x* axis with constant speed *v* at a fixed distance *b* above the top graphene with the polarization function χ_2.

Surface Tensions between Active Fluids and Solid Interfaces: Bare vs Dressed

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Abstract. We analyze the surface tension exerted at the interface between an active fluid and a solid boundary in terms of tangential forces. Focusing on active systems known to possess an equation of state for the pressure, we show that interfacial forces are of a more complex nature. Using a number of macroscopic setups, we show that the surface tension is a combination of an equation-of-state abiding part and of setup-dependent contributions. The latter arise from generic setup-dependent steady currents which "dress" the measurement of the "bare" surface tension. The former shares interesting properties with its equilibrium counterpart, and can be used to generalize the Young-Laplace law to active systems. We finally show how a suitably designed probe can directly access this bare surface tensions, which can also be computed using a generalized Virial formula.

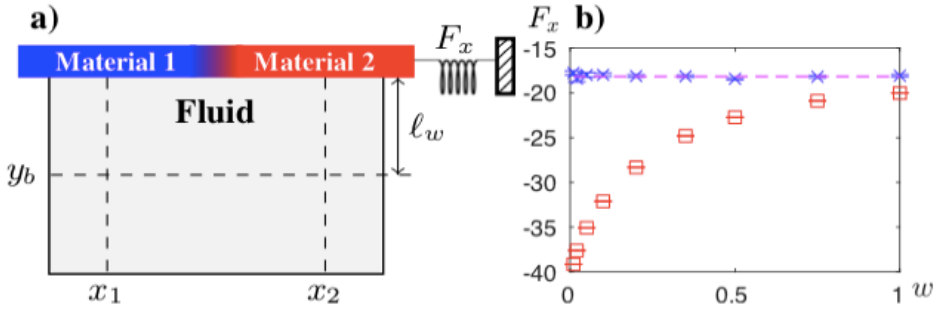

FIGURE 1. (a) Modified Langmuir setup. (b) Total tangential force F_x exerted on the upper wall as a function of the width w of the junction.

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Nanostructured $BiFeO_3$ thin films

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Abstract. Well defined structures at nanometric scale of multiferroic materials present an increasing interest due to their unique physical properties and potential applications. Fabrication of artificial nanostructures requires sophisticated technology and has been recognized as a hard-attainable issue. For these reasons the fabrication of ordered nanostructures, via spontaneous self-organization, is a topic of major relevance. Complex oxide thin films are often elastically strained 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 a self-assembled network of nanostructures (pits and grooves) in highly epitaxial $BiFeO_3$ thin films. As previously shown in the case of manganite thin films [1-2], the remarkable degree of ordering is achieved using vicinal substrates with well-defined step-terrace morphology. Nanostructured $BiFeO_3$ thin films show mixed-phase morphology, exhibiting the giant ferroelectric polarization close to the theoretical limit. These particular microstructures open a huge playground for future applications in multiferroic nanomaterials.

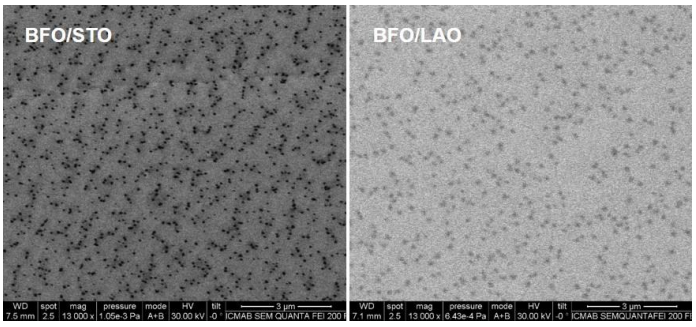

FIGURE 1. Scanning Electron Microscopy of nanostructured $BiFeO_3$ films grown on top of $SrTiO_3$ and $LaAlO_3$ substrates.

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Manipulation Of Organic Thin Film Growth By The Step Width Of Ion Beam Modified $TiO_2(110)$

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Abstract. In this study we attempt to manipulate the thin film morphology of the organic semiconductor para-hexaphenyl (6P) on rippled TiO2(110) surfaces. The rutile $TiO_2(110)$ surface is a highly anisotropic template for organic thin film growth due to it's atomic rows in [001] direction. [1] Further manipulation of the substrate can be accomplished by using ion bombardment under oblique angles, which results in nanometer size ripple structures that alter the morphology and stability of the 6P thin films. [2, 3] Defined by the projected ion beam direction, nanometer size ripples in either [001] direction parallel to the atomic rows or perpendicular to them in [1-10] direction can be induced. The ripples conserve the substrate's crystallinity with short (110) terraces separated by atomic steps as confirmed by low energy diffraction (LEED) and scanning probe microscopy (SPM). Depending on the parameters of the ion bombardment, the terraces' widths can be well adjusted which allows to tune the 6P film properties.

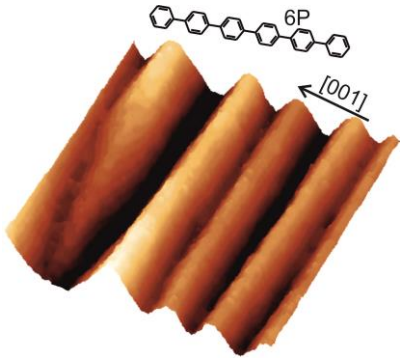

FIGURE 1. 3D representation of a rippled $TiO_2(110)$ surface (65 x 65 nm^2 , z~4 nm) and a structural model of the 6P molecule (not to scale).The substrate atomic rows run along the [001] direction.

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Electron-Phonon Interaction in Room and High Temperature Superconductors – The Current State and Perspective

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Abstract. The role and importance of electron-phonon interaction (EPI) in High and Room Temperature Superconductors (HRTSC) is discussed. The following superconductors(SC) with high critical temperature (T_c) are analyzed. (i) HTSC-cuprates (T_c~100 K) - with very anisotropic EPI and forward scattering peak; (ii) Bulk Fe-based SC (T_c~50 K) - with giant magneto-elastic effects; (iii) Interface SC in FeSe on the $SrTiO_3$ substrate – with dominant forward scattering peak in EPI; (iv) RTSC in H_3S and LaH_{10} with T_c~200-250 K at high pressure P~150-170 GPa – strong EPI with high frequency phonons. It is argued that the pairing in HTSC is due to a subtle interplay between Coulomb and EPI interaction (with forward scattering peak), while in RTSC the pairing is dominated exclusively by EPI with high frequency phonons. We argue that at very high pressure, very high T_c ~ 600 K can be reached in metallic hydrogen dominated by EPI with high frequency transverse phonons. Possibilities for reaching RTSC in metastable hydrogen-systems at low pressure are discussed.

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Raman Spectroscopy Study of Primary Mesenchymal Stem Cells

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Abstract. Cells possess specific dynamic biochemical structure and by analyzing (inter)molecular vibrations with Raman spectroscopy, correlation between biochemical composition to specific cell lineages is established, as well as to disorders of their physiologic state. In regenerative medicine and tissue engineering, mesenchymal stem cells, as adult stem cells, are of crucial importance, due to self-renewal, multi-lineage differentiation potential and undemanding isolation procedure. These cells are widespread in the adult organism and no ethical issues are related to their isolation. However, they need to be well characterized and purified before further application, having in mind their intrinsic heterogeneity. Raman spectroscopy was used for analyzing the influence of two most frequently used chemical fixatives, methanol and formaldehyde, on Raman spectra of primary mesenchymal stem cells isolated from periodontal ligament. Further, this vibrational spectroscopy technique was applied for probing differentiation status of these cells, after stimulating towards chondrogenic, adipogenic, and osteogenic lineages.

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Frustrated Spin Order and Fluctuations in FeSe: A Raman Scattering Study

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Abstract. FeSe is the simplest and yet the most controversial member of the iron based superconductors whose charge and spin dynamics may hold key information on the physics of high temperature superconductors. As opposed to the related iron pnictides and FeTe, no long range magnetic order is found down to lowest temperatures. Here, we present the results of the inelastic light scattering experiments on FeSe as a function of temperature and polarization. In agreement with numerical simulations of a spin-1 Heisenberg model, several peaks in all Raman active symmetries can be assigned to spin excitations. The dominating feature is a peak in B_{1g} symmetry around 500 cm^{-1} which shows distinct temperature dependence. Further comparison of the simulations to neutron scattering data furnishes evidence for FeSe hosting nearly frustrated stripe order of local spins.

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Magnetic Topological Semimetals with Kagome Lattices

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Abstract. The origin of anomalous Hall effect (AHE) in magnetic materials is one of the most intriguing aspect in condensed matter physics and has been a controversial for a long time. Recent studies indicate that the intrinsic AHE is closely related to the Berry curvature of occupied electronic states. In a magnetic Weyl semimetal with broken time-reversal symmetry, there are significant contributions to Berry curvature around Weyl nodes, which would lead to a large intrinsic AHE. On the other hand, the kagome lattice is known to host exotic quantum magnetic states. Theoretical work has predicted that kagome lattices may also host topological electronic states. In this work, we introduce two kind of materials Fe_3Sn_2 and $Co_3Sn_2S_2$ with Kagome lattice, which show large AHE, and it can be ascribed to the existence of Weyl or Dirac fermions in these systems. It indicates that magnetic kagome metals provide a new platform to study on the emergent topological electronic properties in a correlated electron system.

Increasing Endurance and Retention in HfO_2-based ReRAM: a Microscopic Picture

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Abstract. Resistive Random Access Memory (ReRAM) is based on defective oxides: within an initially insulating oxide material, conductive oxygen-deficient filaments are made during the so-called forming step. when local heating in a strong electric field enables ionic transport; this leads to a strong deviation of the stoichiometry in the active area of the device, and, possibly, to formation of multiple phases and/or extended defects. Due to the forming conditions which are far from equilibrium, theoretical investigations that have the purpose of optimizing the ReRAM are quite complicated and linked across multiple length scales. Here, I will present our Density Functional Theory-based study of oxygen-deficient hafnia, which, in combination with an evolutionary algorithm, shows that formation of phases with properties optimal for the resistive switching is possible under specific conditions. I will discuss the structural and electronic properties of these phases as well as to what extent the conclusions are transferable to other oxide materials.

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Gold/MoS_2 Interface Engineering Using Self-Assembled Monolayers

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Abstract. This study aims at finding strategies for avoiding the high contact resistance between gold electrodes and the two-dimensional semiconductor molybdenum disulfide. We demonstrate that tuning the work function (WF) of gold by pyrimidine-containing self-assembled monolayers (SAMs) can be used to eliminate the high injection barrier at the interface between gold electrodes and MoS_2. Exfoliated single-crystalline flakes of MoS_2 have been used in this study. The flakes were transferred onto pre-fabricated substrates suitable for the fabrication of field effect transistors (FET) comprising SAM-functionalized gold electrodes that act as bottom contacts for MoS_2. Through combining the electrical characterization of the MoS_2-based FETs with various SAM treated electrodes and Kelvin probe force microscopy (KPFM) investigations of the devices during operation, the strong influence of the injection barrier on the device performance is revealed. In cases, where the SAMs induce a suitable alignment of the transport levels of the semiconductor flakes with the WF of the electrodes, the contact resistance becomes irrelevant and intrinsic properties of MoS_2 are accessible. In contrast, high injection barriers lead to a sizable contact resistance, and almost the entire bias voltage drops at the carrier injection contact. In addition, KPFM was employed to reveal – frequently omitted – asymmetric, non-linear, and bias-dependent components of the contact resistances. As a consequence, the device performance is deteriorated and the drain current drops by over two orders of magnitude
Acknowledgement: *M. Kratzer, C. Teichert, Institute of Physics, Montanuniversität Leoben, Austria; A. Petritz, G. Schider, B. Stadlober, Joanneum Research MATERIALS Weiz, Austria; M. Krammer, K. Zojer, E. Zojer, Institute of Solid State Physics, Graz University of Technology, Austria; M. Gärtner, A. Terfort, Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Germany.*

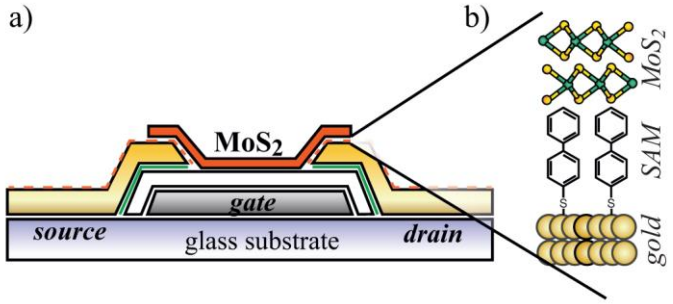

FIGURE 1. (a) Schematic cross-section of the device. (b) Schematic structure of the electrode interface.

Preparing and monitoring photoacoustic response measurements of two-layer PLLA samples of different crystallinity levels

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Abstract. In this work, specially prepared and characterized PLLA samples are covered by a thin polymer layer of acrylic dye in order to be made opaque, thus forming a protection layer which prevents incident light from penetrating the acquisition chain (i.e. the microphone). Uniformity and thickness of the deposited layer are confirmed, and then frequency photoacoustic (PA) response of the obtained two-layer system is recorded using a transmission configuration minimum volume PA cell. Multiple recordings are performed at two thickness levels, for each side separately, until the repeatability is confirmed.
Herein, preprocessed measurement results are presented, confirming the validity of using two-layer theoretical model of PA response for their interpretation. The correlation between the recorded response and the samples' crystallinity level is observed and discussed. Further processing methods are suggested for the obtained data, aimed at quantitative characterization of the investigated polymer samples using artificial intelligence based procedures (neural networks).

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Lattice dynamics and phonon anomalies in FeS

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Abstract. Crystal structure, magnetic ordering and nematic phase are closely interrelated in the iron-based superconductors. Although isostructural and isoelectronic, properties of 11 chacogenides, FeSe, FeTe and FeS, differ significantly. Whereas FeSe undergoes a nematic and structural phase transition at 90 K, togeather with superconductivity below 9 K, and no traces of long-range magnetic ordering, FeTe is not superconducting but exhibits magnetostructural phase transition at temperature of 67 K. The last member of the familly, FeS, have a superconducting transition at 5 K, and remains tetragonal down to lowest temperatures.

Here, we present results of Raman scattering experiment on tetragonal FeS, and analysis of vibrational properties close to potential instabilities [1]. Besides A_{1g} and B_{1g} modes assignation, which is in a good agreement with DFT calculations, third peak whitin a gap of calculated phonon density of states can be indentified as a result of second order scattering process. Both, selection rules for two-phonon processes, based on modified group projector technique and energy are in a good agreement with the experiment. A fourth mode, close to A_{1g} could originate from either deffect-induced scattering or second order scattering as well. The temperature dependence of all four modes is governed by the contraction of the lattice, with anomalies at 50 K and below 20 K. The anomaly observed at 20 K has a correspondence with previously reported results of short-range magnetic ordering. The presence of two-phonon scattering indicates strong phonon-phonon scattering, which is likely to originate from an electron-phonon interaction being enhanced in comparison to other pnictides and chalcogenides.

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Liquid-phase Exfoliation of Graphene and Chemical Doping of Langmuir-Blodgett Assembled Graphene Films

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Abstract. In current optoelectronic devices transparent conductive (TC) electrodes are widely used [1]. Graphene films as new TC material can be used to overcome shortcomings of the exited TC electrodes especially using graphene films as an active electrode. They offer advantages such as higher transparency over a broad range of light wavelengths, higher flexibility, excellent electrical conductivity and chemical stability. Using graphene films as an active electrode, band-structure alignment at the interface can be achieved with an appropriate work function (WF). Therefore, appropriate WF can enhance the charge injection and improve device performances. Chemical doping is an effective method for tuning of the WF by charge transfer between the graphene sheet films and dopants [2, 3]. Liquid-phase exfoliation (LPE) via sonication was the method for the preparation of graphene sheet (GS) dispersion. The films were self-assembled from LPE few-layer GS dispersion by Langmuir-Blodgett (LBA) technique at the water-air interface. Chemical doping of the films was performed in two ways. In the first approach, chemical doping with nitric acid is introduced after the film was formed. Fivefold improvement of sheet conductivity was achieved, with no change in transparency [4]. In the second approach, chemical doping of the film was happening at the moment of its formation. To achieve doping, metal standard solutions were introduced instead of water. Au based salts increase the WF of the films (p-doping), while Li based salts decrease it (n-doping). A span of 0.7 eV in both directions was obtained. Formation of the graphene films and both procedures of their chemical doping are very simple, low-cost and extend their potential use in low-cost optoelectronic applications as well as using them as an active electrode.

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Symmetry Required Band Crossings in Low-dimensional Systems

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Abstract. Topological semimetals are characterized by valence and conduction band crossings which cannot be removed by a symmetry preserving perturbation. If there were no symmetry, the valence and conduction bands, when close in energy, would hybridize and a gap would be opened. However, in a system with symmetry, the bands can be assigned by different quantum numbers, and thus protected from hybridization. Unlike accidental band crossings, characterized by a local topological invariant, the symmetry required band crossings exhibit a global topological charge and they are stable under all symmetry preserving deformations. They are protected by the nonsymmorphic symmetries, which determine the band structure globally. When in addition to the nonsymmorphic symmetry, there are also other symmetries, more complex dispersion patterns with topologically nontrivial band connectivity can emerge. Here, we analyze the band connectivity and related symmetry enforced band crossings in mono- and di-periodic systems (line and layer groups), including spin-orbit interaction (double groups) and time reversal symmetry (gray groups).

A Phase Diagram of Fractional Quantum Hall Effect at Filling Factor 5/2 Without Disorder

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Abstract. Various paired states, Pfaffian (Moore-Read), anti-Pfaffian, and particle-hole symmetric Pfaffian – PH Pfaffian, are proposed for the explanation of the gapped state at the even-denominator filling factor 5/2. In this work [1], based on field theoretical arguments, the evolution and appearances of these states as a function of Landau level (LL) mixing are described. The phase diagram captures the dominance of (anti)-Pfaffian physics and the criticality of PH Pfaffian for small LL mixing, and predicts the relevance of the PH Pfaffian correlations for moderate LL mixing.

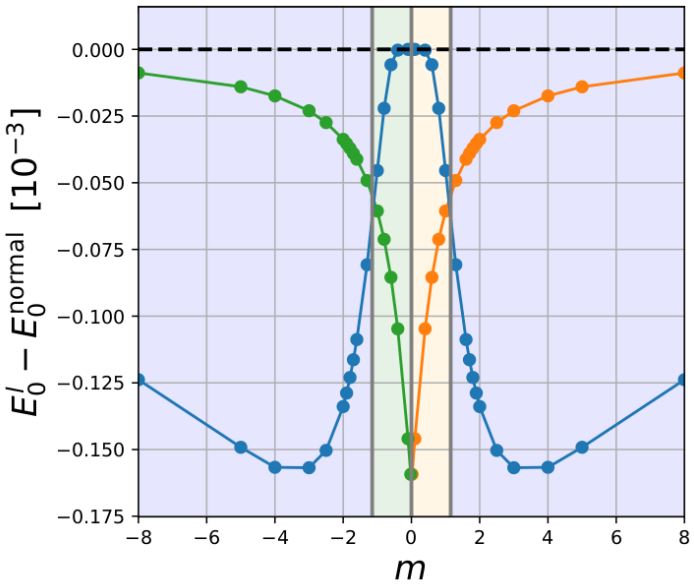

FIGURE 1. Energies of paired states: Pfaffian - green, anti-Pfaffian - orange, PH Pfaffian - blue, compared with the normal state energy, as functions of a measure of LL mixing (m).

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Double Moiré With A Twist: Super-Moiré In Encapsulated Graphene

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Abstract. When two-dimensional atomic crystals are brought into close proximity to form a van der Waals heterostructure, neighbouring crystals can start influencing each other's electronic properties. Of particular interest is the situation when the periodicity of the two crystals closely match and a moiré pattern forms, which results in specific electron scattering, reconstruction of electronic and excitonic spectra, crystal reconstruction, and many other effects. Thus, formation of moiré patterns is a viable tool of controlling the electronic properties of 2D materials. At the same time, the difference in the interatomic distances for the two crystals combined, determines the range in which the electronic spectrum is reconstructed, and thus is a barrier to the low energy regime. In this talk, we present a way which allows spectrum reconstruction at all energies. By using graphene which is aligned simultaneously to two hexagonal boron nitride layers, one can make electrons scatter in the differential moiré pattern, which can have arbitrarily small wavevector and, thus results in spectrum reconstruction at arbitrarily low energies. We demonstrate that the strength of such a potential relies crucially on the atomic reconstruction of graphene within the differential moiré super-cell. Such structures offer further opportunity in tuning the electronic spectra of two-dimensional materials.

Influence of Andreev Reflection on Zero Bias Conductance in DFD Junctions

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Abstract. Zero bias conductance (ZBC) in ballistic voltage-biased d-wave superconductor/ferromagnet/d-wave superconductor (DFD) junctions is studied theoretically, for various orientations of superconducting electrodes [1,2]. The time-dependent Bogoliubov-de Gennes equations which are associated with the relaxation time model for charge transport, through which the mean free path for inelastic scattering enters into calculation, have been solved. The current density and corresponding conductance is calculated from solutions within the barrier. We show that ZBC increases with exchange field h in the F barrier, up to some maximum value of h which is of the order of the pair potential in the superconducting electrodes. We find that for given exchange field, ZBC monotonically decreases with temperature. When the exchange field h is smaller or of the order of the superconducting gap Δ, ZBC has a distinct kink at some characteristic temperature T^*. It appears that for this temperature $\Delta(T^*)=h$. Thus, observing T^* where the kink in the ZBC temperature dependence occurs provides a reliable measurement method to determine exchange fields of the order of the superconducting gap.

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Energy losses and transition radiation produced by the interaction of fast charged particles with two-dimensional materials

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Abstract. Interactions of graphene and other two-dimensional (2D) materials with externally moving charged particles have been studied in the context of Electron Energy Loss Spectroscopy in Scanning Transmission Electron Microscope, a powerful technique for probing plasmons in nanostructures. Moreover, the need for a stable and tunable source of terahertz (THz) radiation has prompted recent studies of electromagnetic radiation from graphene, mediated by the excitation of its Dirac plasmon polariton (DPP) due to an incident electron beam. We have developed a fully relativistic theory of energy losses of a fast charged particle traversing single-layer graphene [1,2] and multi-layer graphene (MLG) [3-5]. The total energy loss of the external particle was found to consist of the energy absorbed in graphene (termed Ohmic loss) in the form of electronic excitations, which include its collective modes, and the energy emitted in the far field as transition radiation (TR). The dynamic response of graphene was described by means of a 2D conductivity tensor, which was modeled using *ab initio* calculations [6] or empirical models [7]. We have studied the effects of varying the charged particle energy and its angle of incidence [1,2], as well as the effects of hybridization between the DPPs in graphene layers within an MLG structure [3-5]. In the THz range of energy losses, we have observed intriguing asymmetry with respect to the direction of the incident particle, both in the Ohmic losses and in the TR spectra from an MLG. In a more recent work, we have applied our methodology to phosphorene, a single layer of black phosphorus, which exhibits strongly anisotropic in-plane optical properties, giving rise to hyperbolic plasmon polaritons at infrared frequencies.

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Spectral properties of hyperbolic nano-networks

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Abstract.
Cooperative self-assembly is a ubiquitous phenomenon found in various natural systems, including nanostructured materials. Knowledge about its origin and mechanisms can be used for designing nano-materials with new functional features. In these materials, nano-particles form networks with non-trivial topological properties [1]. Global, mesoscopic and local properties of complex networks are strongly correlated with spectral properties of Adjacency and Laplacian matrix of a given complex network [2]. We study topological and spectral properties of a large class of self-assembled structures or nano-networks consisting of monodisperse building blocks (cliques of size $n = 3,4,5,6$) which self-assemble via sharing the geometrical shapes of a lower order [3]. The topology of the network is tuned by varying the chemical potential ν which determines the size of shared sub-structure between two cliques. While hyperbolicity of the networks does not depend on ν, their spectral dimension d_s varies with clique size n and chemical potential. We find that spectral distribution of normalised Laplacian has a characteristic shape with peaks and a pronounced minimum which are related to the size of the network building blocks and self-assembly rules [4].

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Ruddlesden-Popper phases of 2D halide perovskites

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Abstract. Halide perovskites are promising candidates for solar cell applications due to their outstanding electronic and transport properties. However, their instability at finite temperature presents an unsolved issue that keeps them out of large-scale market. Addition of large organic spacers and reducing dimensionality of halide perovskites have been shown to have beneficial effects on their stability. In this work, we study electronic and structural properties of Ruddlesden-Popper phases 2D halide perovskites based on 5-ammonium valeric acid (AVA)[1,2]. In contrast to aromatic and aliphatic spacers without additional functional groups, the RP phases of AVA are characterized by the formation of a regular and stable H-bonding network between the carbonyl head groups of adjacent AVA molecules in opposite layers (Fig. 1), which may lead to an enhanced thermal stability. Additionally, we have developed a theoretical framework that can predict and correlate electronic and structural properties of any 2D halide perovskite system, which may serve as a guideline to design new compounds.

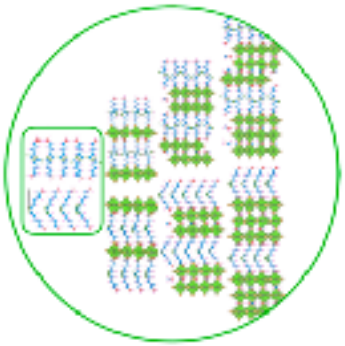

FIGURE 1. Structural model of Ruddlesden–Popper (RP) phases of $AVA_2(CH_3NH_3)_{n-1}Pb_nI_{3n+1}$ for n = 1, 2, and 3.

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Zinc Oxide Nanowire Field Effect Transistors For UV Photodetector And Non-Volatile Memory Applications

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Abstract. Transistor scaling is rapidly reaching its physical limitations and alternative device designs at the nanoscale are required for the "after Moore" regime. In particular, zinc oxide (ZnO) nanowires (NWs) are considered as excellent candidates for future nanoscale building blocks with applications ranging from optoelectronics to sensing. As-synthesized ZnO NWs are intrinsically n-type doped due to the presence of oxygen vacancies and/or zinc interstitials [1, 2]. ZnO NWs were reproducibly synthesized by thermal CVD and electrical characteristics of different ZnO NW field effect transistor (FET) configurations were studied. Parylene C passivated devices exhibited low power consumption and excellent field effect mobilities up to ~189.2 cm^2/Vs. Time-resolved drain current response to periodic ultraviolet illumination was evaluated for conventional and surface passivated back-gate ZnO NW FETs. The effects of surface passivation, gate voltage bias, temperature, and ambient pressure were examined with regard to the photosensitivity, photoconductive gain and the photocarrier relaxation dynamics of the ZnO NW FET based photodetectors. Non-volatile memory functionality of ZnO NW FETs has been previously demonstrated using ferroelectric nanoparticles [3] and mobile protons in the SiO_2 gate dielectric layer [4]. High performance ferroelectric non-volatile memory devices based on top-gate ZnO NW FETs were fabricated on glass substrates by spin coating the ZnO NW channel with a 200 nm thick poly(vinylidenefluoride-co-trifluoroethylene) (P(VDF-TrFE)) film acting as a top-gate dielectric [5]. Electrical conductance modulation and memory hysteresis are achieved by a gate electric field induced reversible electrical polarization switching of the ferroelectric thin film. Remarkably, the device exhibited a large memory window of ~16.5 V, a high drain current on/off ratio of ~10^5, a gate leakage current below ~300 pA, and excellent retention characteristics for over 10^4 s.

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An ultra-sensitive thermometer based on superconducting heterostructures

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Abstract. Due to its importance for understanding the basic principles of the nature as well as the technological development, the low temperature physics has reigned the interest since its foundation. One of the main issues in the experimental realizations is a need of a stable thermometer for low temperature calorimetry. An experimental realization of such a thermometer has been proposed by *Karimi et al.* [1]. It turns out that the zero-bias conductance of a proximitized normal metal-superconductor junction scales linearly with the temperature. Hereby we proposed a theoretical description of such a system done in the framework of the quasiclassical Green's functions in the dirty limit (the Usadel equation). We focus on the Cooper pair-mediated tunnelling current in a contact between a proximitized normal metal and a BCS superconductor. Since the main contribution comes from the low bias voltages, we are supposed to make use of the theory of single particle tunnelling which deals with electromagnetic environments coupled to the system. By combining the two theories we are able to provide IV characteristics of the system which qualitatively resemble the experimental ones.

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Friedel Oscillations of One-dimensional Correlated Fermions from Perturbation Theory and Density Functional Theory

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Abstract. We study the asymptotic decay of the Friedel density oscillations induced by an open boundary in a one-dimensional chain of lattice fermions with a short-range two-particle interaction. From Tomonaga-Luttinger liquid theory it is known that the decay follows a power law, with an interaction dependent exponent, which, for repulsive interactions, is larger than the noninteracting value -1. We first investigate if this behavior can be captured by many-body perturbation theory for either the Green function or the self-energy in lowest order in the two-particle interaction. The analytic results of the former show a logarithmic divergence indicative of the power law. One might hope that the resummation of higher order terms inherent to the Dyson equation then leads to a power law in the perturbation theory for the self-energy. However, the numerical results do not support this. Next we use density functional theory within the local-density approximation and an exchange-correlation functional derived from the exact Bethe ansatz solution of the translational invariant model. While the numerical results are consistent with power-law scaling if systems of 10^4 or more lattice sites are considered, the extracted exponent is very close to the noninteracting value even for sizeable interactions. The talk will be based on Ref. [1]

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Atomic Collapse and Flat Bands in Graphene

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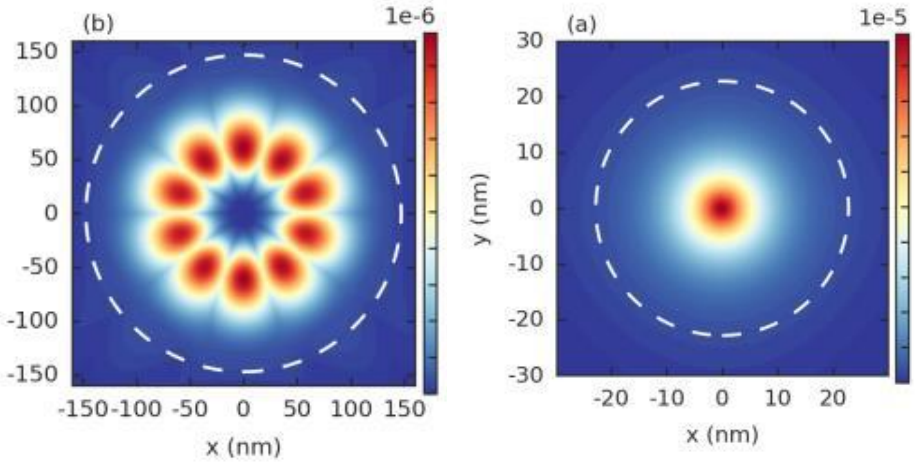
Abstract. Quantum electrodynamics predicts that heavy atoms ($Z > Zc \sim 170$) will undergo the process of *atomic collapse* where electrons sink into the positron continuum and a new family of so-called *collapsing* states emerges. This phenomenon has never been confirmed experimentally. The wonder material graphene has made it possible to investigate1 similar physics in two dimensions using vacancies with tunable charge where the 'atomic' collapse occurs at a much lower critical charge ($Zc \sim 1$).

The transition from sub-critical to the supercritical regime is accompanied by trapping of electrons in quasi-bound states which are the condensed matter analogue of the long sought after phenomenon of atomic collapse in super-heavy nuclei. The quasi-bound electron-states show up as a strong enhancement of the density of states within a disc centered on the vacancy site. We find that these states are surrounded by a circular halo of hole states which are interpreted as the analogue of positron production in atomic collapse. We further show that the quasi-bound states at the vacancy site are gate tunable and that the trapping mecanism can be turned on and off, providing a new paradigm to confine, control and guide electrons in graphene.

Recently[2], we found that a sharp STM tip is able to induce similar atomic collapse states (see Fig. a). For large tip potentials a sub-micrometer scale p-n junction is induced that exhibits *whisper gallery modes* (see Fig. b). Thus the STM tip allows us to tune a circular p-n junction in graphene from quantum confinement to optical guiding.

We realized[3] a periodic buckling structure of a single graphene layer. Because of the periodic strain the electrons are subject to a periodic *pseudomagnetic field* that does not break time reversal symmetry. Through a detailed STM spectrum mapping and tight binding calculations, we reveal the possibility of generating a robust flat band. This buckling method should enable us to design flat bands with different superlattice symmetry which is inaccessible by the moiré superlattices method that was recently realized for magic angle twisted bilayer graphene[4].



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Graphene on Nickel Surfaces: Theory and Experiments

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Abstract. The morphologic, electronic and chemical properties of epitaxial graphene layers are strongly determined by the substrate orientation and flatness. By combining extensive numerical simulations (DFT, MD, KMC) with a multi-technique experimental approach (STM, STS, XPS), we performed atomic-scale investigation of graphene grown both on single-crystal and polycrystalline Ni surfaces, unraveling also transient phenomena taking place during the growth process. The structural and bonding configuration of graphene overlayers varies from flat and uniform on Ni(111) [1] to corrugated and with variable strength in moiré patterns on Ni(001) (Figure 1a-f) [2]. Continuous regular 2D carbon layers can also form on stepped polycrystalline Ni surfaces, involving a rearrangement of the substrate and a peculiar steps dynamics [3]. We observed a temperature-driven change of the edge structure from substrate to hydrogen passivation in graphene flakes growing on Ni(111) [4]. On the same substrate, we followed the action of single nickel adatoms diffusing on the surface, which, temporarily attaching at kink sites along the graphene flake edges, facilitate the incorporation of new C atoms in the carbon network (Figure 1g) [5].

This work is partially supported by the Italian Ministry of Foreign Affairs and International Cooperation (PGR00795 SERBIA 2019) and the University of Trieste (FRA2018).

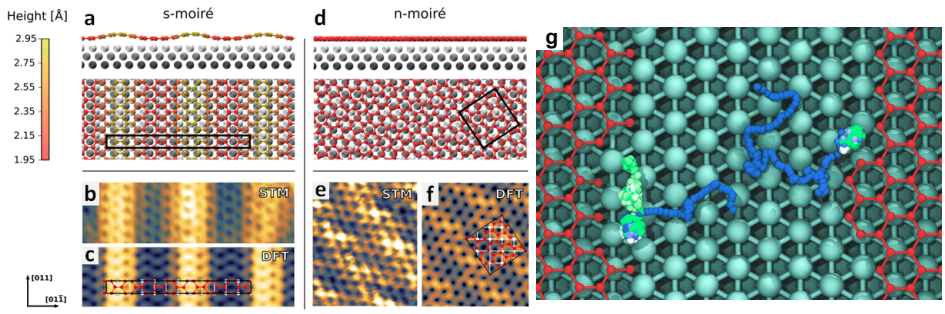

FIGURE 1. (a-f): DFT simulations of two different graphene moiré patterns on Ni(100) compared with experimental STM images (b,e) [2]. (g): MD trajectories of nickel adatoms at growing graphene edges on Ni(111): adatoms are diffusing on surface towards the graphene zigzag (right) and klein (left) edges and temporary attaching at kinks [5].

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Strain effects on vibrational properties in hexagonal 2D materials from the first principles – doped graphene and MgB2- monolayer study

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Abstract. We present computational study within the density functional theory framework of the effects of application of the (equi) biaxial strain on the two isostructural two-dimensional materials, Li-intercalated graphene and magnesium-diboride monolayer, both electron-phonon mediated superconductors [1-4]. The application of the tensile biaxial strain causes softening of the phonons, enhancing the total electron-phonon interaction and resulting in significantly a higher critical temperature. By application of the strain, we achieve the increase of the density of states at the Fermi level and softening of the modes [2,4,5]. Without drastically modifying the structure, with experimentally achievable strain [2,5], we significantly affect the electron-phonon coupling strength.

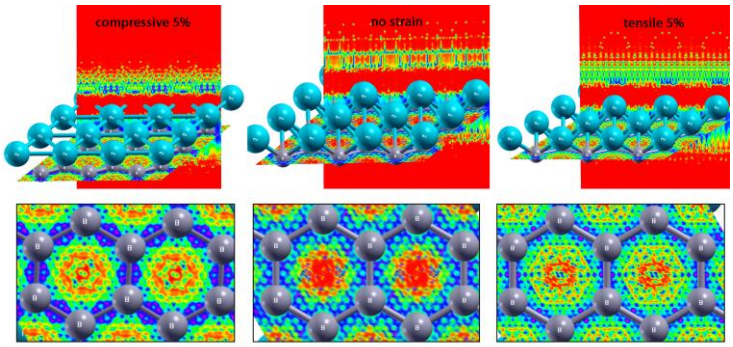

FIGURE 1. Electron localization function (ELF) for MgB2-mono nonstrained and compressively (left) and tensely (right) strained. Top: 3D projection of ELF with focus on the Mg layer. Bottom: ELF projection on the B layer.

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Defect-induced colossal thermopower in FeSb2

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Abstract. Recent interest in thermoelectric energy conversion stimulates search for new materials with high thermoelectric performance [1-2]. A narrow distribution or a large peak in the electronic density of states close to the Fermi level is considered favorable for high thermopower [3-4]. Such peak could be induced by the resonant level dopants in semiconductors [5-6] or by the magnetic interaction between the local magnetic moment and itinerant electrons [7-8]. Some strongly correlated materials show significant enhanced thermopower and power factor [9-10]. In this talk I will discuss FeSb2 [11-13], a correlated electron semiconductor similar to FeSi [14] that was found to host a record-high thermopower of up to 50 mV/K [15]. The mechanism of colossal thermopower in FeSb2 is presently not understood and moreover there is a wide variety in its reported values. In my talk I show how atomic defects create in-gap states of Fe orbital character that carry high electronic diffusion thermopower whereas phonon drag acting on such states – when crystal is engineered to have high phonon mean free path – enhances thermopower to colossal values. This reveals a subtle interplay of phonon and electronic diffusion mechanisms and points to relevant physics and crystal chemistry that can be exploited in predictive thermoelectric materials design.

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Dynamics and Spin and Charge Pumping of Noncollinear Magnetic Textures: A Multiscale Quantum-Mechanics/Classical-Micromagnetics Approach

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Abstract. This talk introduces recently developed [1,2] multiscale and self-consistent computational tool which combines time-dependent nonequilibrium Green function (TDNEGF) algorithms, scaling linearly in the number of time steps and describing quantum-mechanically conduction electrons in the presence of time-dependent fields of arbitrary strength or frequency, with classical description of the dynamics of local magnetic moments based on the Landau-Lifshitz-Gilbert (LLG) equation. Such TDNEGF+LLG approach can be applied to a variety of problems where current-driven spin torque induces the dynamics of magnetic moments as the key resource for next generation spintronics. Previous approaches for describing such nonequilibrium many-body system have neglected noncommutativity of quantum Hamiltonian of conduction electrons at different times and, therefore, the impact of time-dependent magnetic moments on electrons which can lead to pumping of spin and charge currents that, in turn, can self-consistently affect the dynamics of magnetic moments themselves including introduction of non-Markovian damping and magnetic inertia terms into the LLG equation [2]. Thus, TDNEGF+LLG can be viewed as "quantum-classical micromagnetics" which captures numerous effects missed by widely utilized purely classical micromagnetics. We use examples of current- or magnetic-field-driven motion of domain walls within magnetic nanowires (including their annihilation observed in very recent experiments [3]) to illustrate novel insights that can be extracted from TDNEGF+LLG simulations. In particular, TDNEGF+LLG as a nonperturbative (i.e., numerically exact) framework allows us to establish the limits of validity of simpler theories, such as the so-called spin-motive force theory [4] for pumped charge current by time-dependent noncollinear and noncollinear magnetic textures which turns out to be just the lowest order of the result predicted by TDNEGF+LLG.

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Synthesis And Characterization Of $Mo_{1-x}W_xS_2$ Nanotubes

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Abstract. Semiconducting MoS_2 and WS_2 nanotubes were studied in the last decades for their interesting electrical, optical and structural properties. Recently it has been shown that MoS_2 nanotubes can enhance performance of sodium-ion batteries and act as optical resonators while the WS_2 nanotubes have shown enhanced field emission properties. [1,2,3] Ternary compounds, such as $Mo_{1-x}W_xS_2$, could show different properties than pure MoS_2 and WS_2 and the tuning of some characteristics by changing the ratio of the transition metals [4]. Here we present the first $Mo_{1-x}W_xS_2$ nanotubes synthesized by the chemical transport reaction. The synthesized material has been characterized with SEM, TEM, EDS, XRD and Raman spectroscopy. The starting material contained MoS_2 and WS_2 in 50:50 atomic ratio. The transported material was composed of flakes, nanotubes (NT) and nanoribbons of $Mo_{1-x}W_xS_2$. The diameter of the nanotubes and nanoribbons ranges from 10 nm up to a few microns, and their length up to several 10 μm. EDS data revealed that both transition metals are homogeneously distributed in this ternary compound, but the atomic ratio is close to 60:40. The Raman spectra of the $Mo_{1-x}W_xS_2$ NTs is a superposition of Raman peaks attributed to MoS_2 and WS_2. The diffraction pattern on single flakes points to the stabilization of the rhombohedral 3R stacking, which is in pure MoS_2 or WS_2 stable only at high pressures [5]. The $Mo_{1-x}W_xS_2$ NTs grow in chiral growth mode with a chiral angle of 17.3° in the [100] direction. In contrary to the flakes, the existence of the (10*l*) peaks reveals that the nanotubes grow in the 2H stacking.

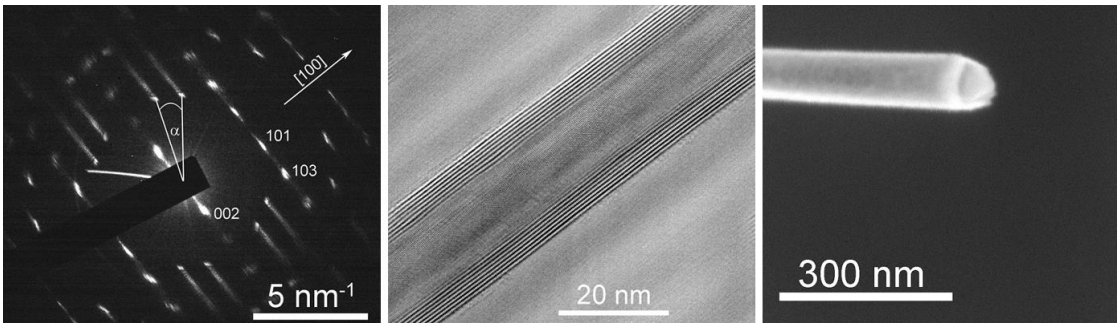

FIGURE 1. A $Mo_{1-x}W_xS_2$ nanotube: a) TED pattern showing the chiral growth; b) HR-TEM image revealing molecular layers separated by 6.7±0.1 Å; c) SEM image of an open end.

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Multifunctional Nanodevice Based on Ti_2O

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Abstract. Miniaturization of microelectronics, as integration of increasingly more transistors and hence functions per chip area, approaches its end due to the limits of the silicon technology. We propose a new concept of multifunctional nanodevices which multiple functionality is at the material's level, as replacements for common transistors. An example of such a multifunctional nanodevice based on a Ti_2O monolayer will be presented. In contrast to TiO_2 crystal, Ti_2O have not been intensively investigated even though the crystal was fabricated in 1953 for the first time. Our study based on density functional theory indicates that a Ti_2O layer is bistable for two lattice parameters, being metallic for one and semiconducting for another parameter. In a switching configuration, this provides a high current ON/OFF ratio of 10^3 when the layer is biased and stretched simultaneously. The electronic conductance of the layer is highly anisotropic. The high sensitivity of conductance to layer stretching can be utilized for electromechanical switching, the bistability provides potential for application as a nonvolatile memory bit, while the current-voltage characteristic of the material in its semiconducting phase indicates a possible use as a varistor – all in a single nanodevice.

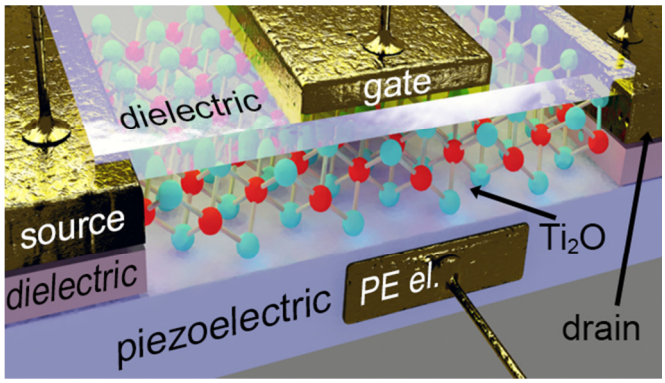

FIGURE 1. Illustration of the multifunctional device based on a Ti_2O monolayer

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Amplitudes Of Minima In Dynamic Conductance Spectra Of SnS Andreev Contact In The Framework Of KGN Theory

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Abstract. There is a lack of qualitative comparison between theoretical predictions and experimental practice for multiple Andreev reflection (MAR) effect manifestation at dynamic conductance spectra of ballistic ($l > d$) high transparent SnS contact (l-electron mean free path, d-the width of thin normal "n" layer or the constriction, S-thick superconductive banks) due to several reasons. The K***ü***mmel, Gunsenheimer and Nicolsky (KGN) theory [1] consider the finite ballistics of the contact along the current direction, which could be introduced as l/d ratio and used as an input parameter, instead of taking it infinite as it is a case in the majority of MAR theories. We made qualitative comparison between theoretical predictions of the extended KGN theory [2] and experimental data of "break-junctions" technique [3] for amplitudes of the subharmonic gap structure minima in the dynamic conductance spectra of ballistic SnS Andreev contact on temperature. The results for the numerical estimation of amplitude of dI/dV Andreev minima with l/d ratio variation are discussed.

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The Use of Complex Oxide Interfaces and Monoatomic Scale Defects in Controlling Transport Properties in ZnO Nanowires

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Abstract. Meeting the demands for sufficient supply of affordable and reliable energy that has a minimal impact on the environment requires exploring many different avenues of research and development. One of such avenues is the field of thermoelectric materials, which demonstrate the conversion of the temperature gradient into electric current, with potential applications in sensors, consumer electronics, medical devices, etc. Thermoelectric $M_2O_3(ZnO)_n$ nanowires, where M could be In, Ga, Fe, synthesized using solid-state diffusion, enabled us to control their defect structure at atomic level and to create an aperiodic superlattice structure, in which complex oxide interfaces are formed between ZnO wurtzite crystal structure and monoatomic indium (In) containing defect layers. Two kinds of defects: planar, parallel to basal wurtzite planes and zigzag, parallel to pyramidal planes, facilitate decoupling of electrical and thermal properties. Both of these factors facilitate achieving a high figure of merit, used to rank thermoelectric materials. Atomic resolution scanning transmission electron microscopy of these nanowires confirmed the presence of In containing planar defects perpendicular to the [0001] direction. These defects separate wurtzite $GaZn_nO_{(n+1)}^+$ slabs of various thicknesses at nanoscale enabling quantum confinement effect to take place and act as obstacles for phonon propagation. Incomplete In monoatomic layers are associated with edge dislocations, providing fast diffusion paths for large indium atoms. In summary, $M_2O_3(ZnO)_n$ polytypoid nanowires were converted from pure ZnO nanowires by a simple preferential diffusion process along line defects, which can be used to produce a wide range of ZnO alloys with controllable alloy concentration and defect layers density. It is apparent that these two quantum mechanics tools, quantum confinement and phonon scattering, can be used for better control of thermoelectric properties, which could be the key in developing next-generation nanostructured materials.

Superconducting Nature of Elemental Bismuth Under Pressure

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Abstract. Elemental bismuth has a very rich pressure-dependent phase diagram. At room temperature, it undergoes a series of structural transitions. Upon cooling all phases become superconducting, but the superconducting nature between phases is very different. We report the superconductivity in the Bi-II phase of elemental bismuth (transition temperature $T_c \simeq 3.94$ K at $p \simeq 2.80$ GPa). It was studied experimentally by means of muon-spin rotation as well as theoretically using the Eliashberg theory in combination with Density Functional calculations. Experiments reveal that Bi-II is the type-I superconductor with the zero temperature thermodynamic critical field $B_c(0) = 32.07(2)$ mT. The Eliashberg theory provides an excellent agreement with the experimental critical temperature and magnetic field and the estimated value for the strong coupling parameter $T_c/\omega_{\ln}$ suggests that Bi-II is an intermediately-coupled superconductor. We also address the superconducting nature of Bi-I phase. We report the negligible electron-phonon interaction and possible signatures of exciton-mediated superconductivity.

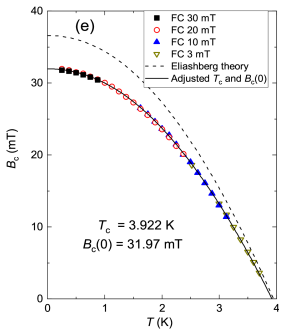

FIGURE 1. The temperature dependence of the thermodynamical critical field B_c for Bi-II phase obtained in μSR experiments and within the framework of *ab-initio* Eliashberg calculations using Density Functional Theory.

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Creating Emergent Phases in Transition Metal Oxides

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Abstract. Transition Metal Oxides (TMOs) exhibit unique and multifunctional physical phenomena (such as high-temperature superconductivity, colossal magnetoresistance, metal-insulator transitions, etc.) directly related to the spin and orbital degrees of freedom of the transition metal d-states and their interplay with the lattice. Importantly, the iso-structure of TMOs permits realization of hetero-structures generating at their surfaces and interfaces new physical matters that radically differ from those of the constituent bulk materials.
Through two examples, novel and fascinating properties emerged in TMO based hetero-structures and ways to control them will be presented:
1. **Altering orbital ordering and band filling of the 2DEG at titanates surfaces.** Employing Angle-resolved photoemission spectroscopy (ARPES) we found ways to manipulate the 2DEG and, consequently, to tune electronic properties of titanates surfaces (SrTiO3 in bulk [1,2] and film forms, TiO2-anatase [3] and CaTiO3 [4] films).
2. Tuning electronic phases in ultra-thin NdNiO3 (NNO) films via the strain and the proximity to a magnetic layer. The electronic structure of differently strained NNO films grown solely and in proximity to magnetically ordered manganite layers has been studied. Our study reveals that substrate-induced strain tunes the crystal field splitting, consequently changing the FS properties, nesting conditions, and spin-fluctuation strength, and thereby controls the Metal Insulator Transition (MIT) [5]. In addition, we found that the insulator anti-ferromagnetic (I-AF) ground state and MIT can be induced or quenched in ultra-thin NNO via the proximity to the magnetically ordered (AF or FM) manganite buffer layer [6].

Overall our studies establish different approaches to manipulate the properties of the two-dimensional electron gas and electronic phases in NNO signifying perspectives of TMO for novel applications.

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Self-Organization, Time Operator and Number Theory

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Abstract. Self-organization and complexity, representing some of the most important properties of complex systems, are quantified based on the Hidden Markov model (HMM) of wavelet coefficients. The model represents a versatile framework which concurrently addresses several important issues related to the nonlinear and multiscale phenomena involved in the dynamics of complex systems, namely it: 1.chooses the optimal template wavelet for the analysis of temporal or spatio-temporal dynamics; 2. detects parameter values at which bifurcations occur; 3. quantifies complexity and self-organization of the dynamics; 4. enables short-term prediction of nonlinear dynamics; 5. extracts coherent structures in turbulence by separating them from the incoherent component and 6. performs superior noise reduction.

An explicit expression for the internal time (expressed as an operator) of complex systems is derived by exploring classical statistical mechanics in the Hilbert space operator formalism and its relationship with self-organization of the wavelet based model is established. Furthermore, we prove the existence of the relationship between the HMM wavelet model and the real number system and implicitly with the problem of measurement .

Living on the edge: Model states for the interface of chiral topological orders

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Abstract. Interfaces between topologically distinct phases of matter reveal a remarkably rich phenomenology. To go beyond effective field theories, we study two prototypical examples of such an interface: Between two Abelian states (the Laughlin and Halperin states) or between an abelian and a non abelian states. Using matrix product states, we propose a family of model wavefunctions for the whole system including both bulks and the interface. We show through extensive numerical studies that it unveils both the universal properties of the system, such as the central charge of the gapless interface mode and its microscopic features. It also captures the low energy physics of experimentally relevant Hamiltonians. For the abelian/non-abelian case, we show that a Majorana mode is trapped at the interface. Our approach can be generalized to other phases described by tensor networks.

Controlling The Magnetic Anisotropy Of Van Der Waals Ferromagnet Fe_3GeTe_2 Through Hole Doping

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Abstract. Identifying material parameters that affect magnetic properties of ferromagnets is key to optimize materials better suited for spintronics applications. Magnetic anisotropy is of particular importance in a van der Waals magnet, since it not only influences the magnetic and spin transport properties, but also is essential to stabilizing magnetic order in the two-dimensional limit[1-2]. Here, we report that a simple hole doping effectively modulates the magnetic anisotropy of a van der Waals ferromagnet, and explore the physical origin of this effect. Doping and thickness dependent magnetic property measurements of a few nanometer thick $Fe_{3-x}GeTe_2$ show a significant suppression of the magnetic anisotropy with hole doping. Electronic structure measurements and calculations reveal that the chemical potential shift associated with hole doping is responsible for the reduction in the magnetic anisotropy energy by decreasing the energy gain from the spin-orbit induced band splitting. Our findings provide an understanding of the intricate connection between electronic structures and magnetic properties in a two-dimensional magnet and propose a method to engineer magnetic properties through charge carrier doping.

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Multy functional roles of microtubules in living cells

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Abstract. Biological cells have evolved biomechanical, mechanical, electrical and genetic networks aimed to perform basic living function across diverse length and time scales. Microtubules, as the most abundant proteins in cells are the main constituents of such networks. They are implicated in intracellular architecture, dynamics and signaling. Microtubules can play the roles of cellular pillars, levers, rods, strings, electric wires (cables) and railways (or streets) for cellular traffic. We will present our recent contribution regarding the biophysical mechanisms underlying some of above roles.

Wrinkle patterns in active viscoelastic thin sheets

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Abstract. We show that a viscoelastic thin sheet driven out of equilibrium by active structural remodelling develops a rich variety of shapes as a result of a competition between viscous relaxation and activity. In the regime where active processes are faster than viscoelastic relaxation, wrinkles that are formed due to remodelling are unable to relax to a configuration that minimises the elastic energy and the sheet is inherently out of equilibrium. We argue that this non-equilibrium regime is of particular interest in biology as it allows the system to access morphologies that are unavailable if restricted to the adiabatic evolution between configurations that minimise the elastic energy alone. Here, we introduce activity using the formalism of evolving target metric and showcase the diversity of wrinkling morphologies arising from out of equilibrium dynamics.

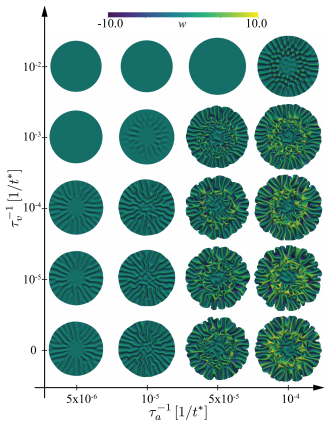

FIGURE 1. A snapshot of the out-of equilibrium shapes obtained by numerical integration of equations of motion for a viscoelastic thin sheet. Vertical axis represents the rate of viscous relaxation with increasing values designating faster residual stress relaxation. On the horizontal axis we plot the active structural remodelling rate, with larger values corresponding to faster changes of the local reference metric. Colours represent the height function measured from the x, y plane.

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Lattice dynamics and phase transitions in $Fe_{3-x}GeTe_2$

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Abstract. A new class of magnetic van der Waals bonded materials has recently become of great interest, as a suitable candidates for various applications. Whereas $CrXTe_3$ (X = Si, Ge, Sn) and CrX_3 (X = Cl, Br, I) classes maintain low phase transition temperatures even in a monolayer regime, $Fe_{3-x}GeTe_2$ has a high bulk transition temperature, between 220 and 230 K, making it a promising applicant.

Here we present DFT calculations of lattice dynamics and Raman spectroscopy measurements of the van der Waals bonded ferromagnet $Fe_{3-x}GeTe_2$ [1]. Four out of eight Raman active modes are observed and assigned, in agreement with numerical calculations. The energies and linewidths of the observed modes display an unconventional temperature dependence at about 150 and 220 K, followed by the nonmonotonic evolution of the Raman continuum. Whereas the former can be related to the magnetic phase transition, the origin of the latter anomaly remains an open question.

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Transparent Conductors and Gas Sensors from 2D Material Thin Films

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Abstract. Chemical sensors are an enabling tool across many industries, including the largest ones such as energy, transport, and construction. Low-cost, high performance sensors, especially ones compatible with flexible substrates, are becoming increasingly important with the development of mobile gadgets and wearable devices. Here we show chemical sensors produced in a facile way from inexpensive materials. The sensors, made of liquid-phase exfoliated (LPE) 2D materials deposited on a substrate with Langmuir-Blodgett assembly, are only several nanometers thick, with high optical transparency, high sensitivity to various chemicals, made with an inexpensive process that can be applied to any substrate, including flexible ones. The method that we demonstrate is scalable and consistently yields films of high quality. The sensors that we make from graphene are more sensitive to humidity than ones demonstrated with CVD graphene [1], with up to 30% change in sheet resistance upon exposure to water vapor. We also demonstrate chemiresistive sensing of nitric acid vapour and ozone gas with the same films. Using thin sheets of LPE PtSe2 we show NH3 and NO2 gas detection with unprecedented 200 ppb and 15 ppb detection limits, respectively. The physical mechanism for the high sensitivity is an abundancy of reactive edges that trap analyte molecules [2]. Our large-area low-cost films are also excellent candidates for use in transparent conductor applications, with a transparency higher than 80% at sheet resistances on the order of 10 kOhm, which result in a better figure of merit than films made with any other deposition method from liquid solutions of 2D materials. Finally, we present the use of ultrathin LPE hexagonal boron nitride films as a layer that protects CVD graphene from photochemical oxidative degradation.

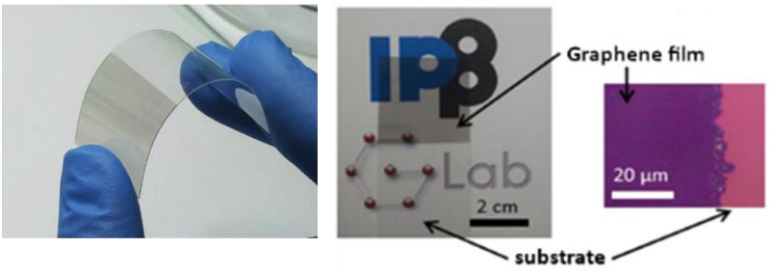

FIGURE 1. Large area, thin graphene film on flexible and hard substrate for transparent conductors and sensing

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On the 3D to 2D crossover in the nonequilibrium athermal random field Ising model

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Abstract. Theoretical studies of the 3D systems with small thickness and large lateral sides attracted recently a growing attention due to vast importance for modern science and technology. In particular, the question of whether to analyze and interpret their data like for the 2D or like for the (bulky) 3D systems remained open. Here we present the results about some aspects of criticality of such systems (namely, the critical disorder and critical field) within the nonequilibrium athermal random field Ising model playing the role of a paradigm in the theoretical studies of the nonequilibrium critical phenomena.

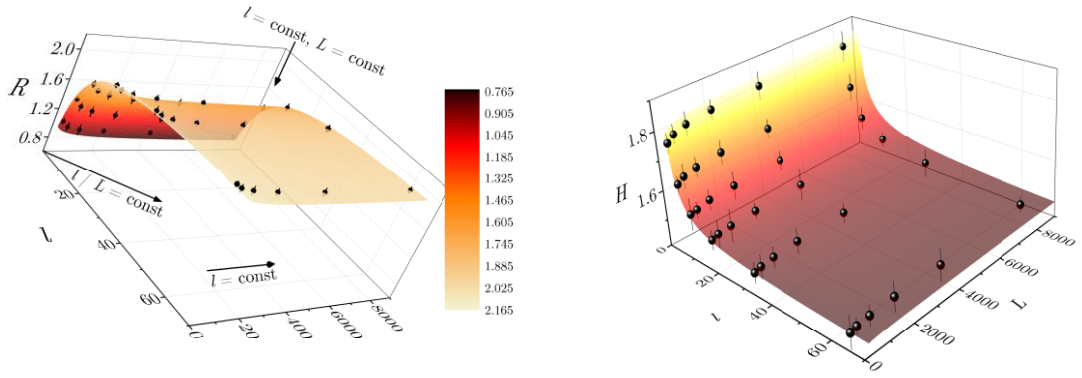

FIGURE 1. Left panel: effective critical disorder R vs lateral size L and thickness l for the 3D RFIM $L\times L\times l$ systems with closed boundary conditions along lateral sides and open boundary conditions along thickness. Right panel: same as in left panel, but for the effective critical field H.

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Assemblies of spherical and cuboidal magnetic particles: a laboratory for magnetic systems

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Abstract. Our system consists of structures created by the assembly of magnetic spheres and cubes [1-3]. From a fundamental point of view, by looking into the self-assembled structure, we can in-revers conclude about interactions present in the system. We will first discuss the dependence of cohesive energy on the structure of assemblies of magnetic particles [1,4]. Afterwards, we will demonstrate length-scale transcendent behavior in micro and macroscopic dipolar tubes. All magnetostatic properties found in continuous solid-state magnetic nanotubes, in which the dipolar interaction is comparable to or dominant over the exchange interaction, are reproduced by the dipolar tubes including an intermediary helically magnetized state. As far as the ground state is concerned, the dipolar tubes switch from circular to axial magnetization with increasing tube length. Besides, we will analyze the antiferromagnetic phase resulting from the square arrangement of the dipolar spheres and its interesting vortex state. The origin of observed ground states is traced back to a breakup of degeneracy observed in planar square and triangular packings [5].

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Understanding Trends In Lithium Binding At Two-Dimensional Materials

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Abstract. Layered structure and peculiar electronic properties of two-dimensional (2D) materials foster the concept of utilizing them as main components of lithium-ion batteries. Understanding basic physical mechanisms governing the interaction of Li with 2D crystals is of key importance to succeeding in a rational design of cathode and anode materials with superior functionalities. Study of Li atoms adsorbed at graphene clearly shows that Li atoms, featuring a long-ranged electrostatic repulsion, are individually dispersed across the surface [1]. This was a motivation for the further investigation of Li adsorption at a number of different 2D materials. In this study density functional theory was applied to reveal the microscopic picture of Li interaction with 15 2D crystals, including several transition metal oxides and dichalcogenides, carbides of Group XIV elements, functionalized graphene, silicene, and germanene, as well as black phosphorus and Ti2C MXene [2]. We found that the general trend in Li binding can be estimated from positions of conduction band minima of 2D materials since the energy of the lowest unoccupied electronic states shows a nice correlation with the strength of Li adsorption. At variance to the majority of studied surfaces where the electron transferred from Li is spread across the substrate, in monolayers of carbides of Group XIV elements the interaction with Li and the charge transfer are well localized. This gives rise to their capability to accommodate Li structures with a nearly constant binding energy of alkaline atoms over Li coverages ranging from well-separated adatoms to a full monolayer.

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$CeCu_2Si_2$: Unconventional Superconductivity Close To A Three-Dimensional Spin - Density - Wave - Quantum Critical Point

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Abstract. According to the so - called 'quantum critical paradigm' any antiferromagnetic quantum critical point (QCP) in a clean, stoichiometric heavy - fermion (HF) metal should give rise to *unconventional superconductivity (SC)*. In this talk, the first HF superconductor $CeCu_2Si_2$ [1] will be addressed as an exemplary material which exhibits SC close to a *conventional*, i.e., *three - dimensional spin – density - wave QCP* [2 – 5]. For a long time, $CeCu_2Si_2$ was considered a (single – band) *d* - wave superconductor [6, 7]. However, a few years ago its specific heat was found to exhibit two - band behavior with an exponential temperature dependence at very low temperatures [8], typical for a conventional BCS superconductor. Based upon atomic – substitution [9 - 11], neutron – scattering [3, 4, 12, 13], specific - heat and London penetration - depth [14] measurements it will be shown that $CeCu_2Si_2$ is a fully - gapped, two - band *d* - wave superconductor [14], rather than an isotropic (BCS – type) or anisotropic *s* - wave superconductor.

Work done in collaboration with O. Stockert, J. Arndt, M. Smidman, H. Q. Yuan, G M. Pang, L. Jiao, H. S. Jeevan, P. Gegenwart, G. Zwicknagl, E. M. Nica, R. Yu, J. X. Zhu and Q. Si.

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Effect Of The Laser Turning On and Off On The Optical Properties Of The Spherical Quantum Dot With Hydrogen Impurity

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Abstract. Investigation of the time response of the medium to the applied laser field is important for the application in all-optical switches and transistors [1], [2]. The goal of this paper is to study the temporal properties of the interaction of the GaAs spherical quantum dot with on-center hydrogen impurity with continuum wave laser driving the transition 1s→2p of the impurity. The model of two-level atom was used, along with density matrix approach, to obtain optical Bloch equations [3]. The equations were then solved numerically, as well as analytically in order to obtain the level populations and susceptibility in two cases: 1) the laser was the turned on for all the time of observation; 2) the laser was successively turned on and off. It was investigated how populations and susceptibility vary with the change of laser intensity, laser detuning, dephasing rate and time periods of the laser turning on and off. It was found that for the properly chosen values of the corresponding parameters, the absorption of the quantum dot in the case 2) could be smaller or larger, then in case 1), even for the resonant laser field.

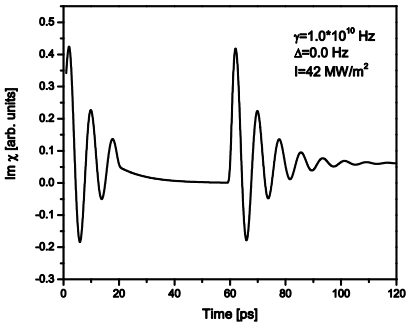

FIGURE 1. Imaginary part of the susceptibility of the spherical quantum dot with hydrogen impurity as the function of time.

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Cooperative Self-Assembly as a Modeling Framework for Programmable Materials

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Abstract. Computational materials science utilizes complex mathematical rules to guide the self-assembly of nanostructured materials [1]. Meanwhile, the synthesis of colloids with "valence" and directional bonding [2] opens a new avenue for the assembly of new functional materials. In this context, the cooperative self-assembly, where pre-formatted groups of nanoparticles join the growing structure, represents a challenging problem for theoretical and numerical modelling. Recently, we have introduced a model [3] for the aggregation of building blocks made of various groups of nanoparticles, which we describe by simplexes (triangles, tetrahedral, and higher-order cliques). The assembly rules take into account the geometrical compatibility of the added simplex with the growing structure (a nanonetwork [4]), as well as the chemical affinity towards the addition of the new group. In this lecture, we present the model details and describe the architecture of different classes of nanonetworks that we grow by varying the chemical affinity and the size of the building blocks. Further, by exploiting the long-range effects induced by tgeometrical compatibility in the assembly with defect simplexes, we show that nontrivial patterns of defects emerge and can be used to control the entire structure effectively.

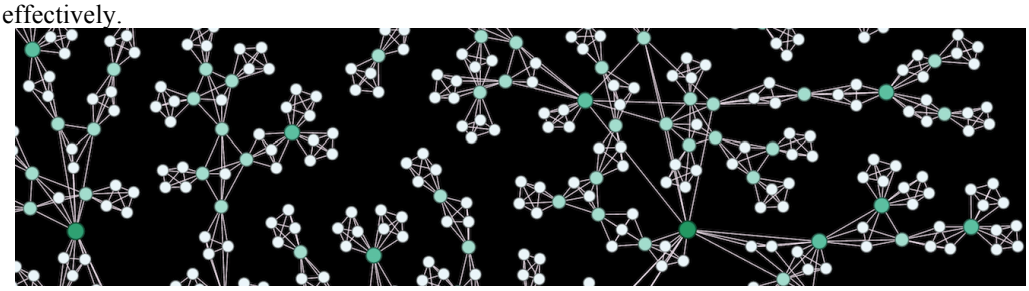

FIGURE 1. A segment of the mono-disperse assembly grown with strongly repulsive 5-cliques

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Pure Brookite Nanopowder: Photocatalytic Properties Before and After Annealing

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Abstract. TiO_2 nanopowder with pure brookite phase was synthesized using sol-gel hydrothermal method, with $TiCl_4$ as a precursor [1]. After this alkaline hydrothermal approach an annealing process at 860 K took place. The structural properties of the as synthesized and annealed nanopowders were analyzed by X-ray powder diffraction (XRPD). The structural, morphological and texture characteristics of both nanopowders were also investigated by Raman spectroscopy, Scanning Electron Microscopy (SEM) and N_2 physisorption at 77 K. Efficiency of photocatalytic degradation of Reactive Orange (RO16), one of the most toxic azo-dye among various types of dyes, was investigated for both nanopowders. As synthesized brookite nanopowder showed the fast photocatalytic degradation of RO16, whereas the annealed nanopowder was slower in degradation under the same conditions. Lower degradation efficiency could be related to decrease of the textural parameters (specific surface area, mesopore volume, and maximum pore diameter) of brookite nanopowder due to annealing.

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Magnetic-field dependence of the electronic and optical properties of hexagonal-shaped 2D HgTe quantum dots and quantum rings

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Abstract. The electron states and optical absorption in hexagonal-shaped 2D HgTe quantum dots and quantum rings in the presence of a perpendicular magnetic field are investigated theoretically. We use the $sp^3d^5s^*$ tight binding method within the nearest neighbor approximation to model the electronic structure [1,2]. Both bulk-like and edge states are found in the energy spectrum. Due to double connected topology bulk-like states in the quantum rings exhibit Aharonov-Bohm oscillations in magnetic field [3]. Most of the edge states in rings and dots are delocalized over all the edges and oscillate with magnetic field. However, some of the edge states are localized at certain spots confined to the ring edges and appear as nearly flat quasi-bands when magnetic field varies. The most intriguing part of the absorption spectra originates from transitions between the edge states and results in appearance of numerous absorption peaks which take place in the infrared part of the electromagnetic spectrum [4]. The optical absorption is found to be strongly dependent on the dot or the ring size. Moreover, it was demonstrated that the transition energy which corresponds to the highest absorption peak can be manipulated by perpendicular electric field, and that the varying perpendicular magnetic field could be employed to fine tune the transition energies and the optical absorption.

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Molecular mechanisms of anti-tumor action of TTFields determined by measurements and modeling of electro-conductive properties of microtubules

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Abstract. Biological effects of AC electric fields at frequencies between 100-300 kHz discovered a decade ago are being applied to cancer cells as a therapeutic modality in the treatment of glioblastoma multiforme (GBM). They are called Tumor Treating Fields (TTFields) as they disrupt cell division. Based on our electro-conductive measurements and modeling, we provide an assessment of possible molecular-level mechanisms. Computer simulations and experimental measurements carried out for microtubules and actin filaments are presented. Charge and dipole values for monomers and dimers as well as polymerized forms of these proteins are summarized. Continuum approximations for cable equations describing actin filaments and microtubules compare favorably to measurements in buffer solutions showing soliton waves and transistor-like amplification of ionic signals, respectively. AC Conductivity and capacitance of tubulin and microtubules have been measured and modeled in the range of frequencies between 100 kHz and 1 MHz. A dramatic change in conductivity occurs when tubulin forms microtubules. In living cells, this signals a conductive phase transition coinciding with mitosis in dividing cells. This process is allowed by TTField penetration into the cleavage furrow in dividing cells and provides the most significant mechanistic explanation of the observed effects. We provide estimates of the forces, energies and power involved in the action of TTFields on microtubules and kinesin motors. These calculations are compared and contrasted with typical values experienced at a cell level and provide strong arguments for real physical effects of TTFields in dividing cells. We also show results of DLS and TEM measurements on microtubules and tubulin oligomers in solution, which allow us to quantify these processes under controlled conditions. In conclusion, the most likely candidates to provide a quantitative explanation of these effects are ionic condensation waves around microtubules as well as dielectrophoretic effects on the dipole moments of microtubules.

Nanoscale electrical and mechanical control of resistive switching in iridates and manganites

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Abstract. Resistive switching (RS) is an electrically induced change of the resistance of various thin metal-oxide films [1]. Research on RS is mainly motivated by possible applications in new data storage devices. In addition, RS can be induced by strain engineering [2] which does not depend on film thickness, while biasing is not needed. In this talk the main focus will be on the nanoscale RS induced and characterized by atomic force microscopy (AFM) based methods. In the first part, the relation between the electrically induced RS in semimetallic $SrIrO_3$ thin films and metal-insulator transition (MIT) triggered by film thickness reduction will be discussed [3]. It is shown that thin films are insulating and characterized by hysteretic I-V curves. The threshold voltage indicating the transition from high- (HRS) to low-resistance state (LRS) is well defined due to a band gap opening as a result of MIT. On the other hand, thicker films are semimetallic, while the transition from HRS to LRS is characterized with a smooth increase of the current without a threshold voltage. In the second part, mechanically induced switching of surface electrical properties of $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) thin films covered by magnetic nanoparticles is discussed [4]. The local pressure applied by AFM tip leads to a drop of the electrical conductivity, finally inducing an electrically insulating state for high enough normal load as shown in Fig. 1. Subsequent electrical characterization suggests that the RS is mainly governed by the flexoelectric field induced at the sample surface.

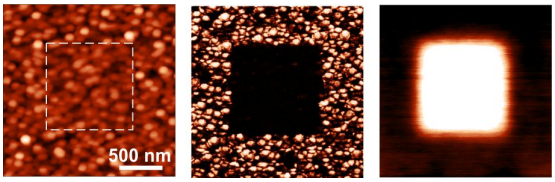

FIGURE 1. Morphology (left), current map (middle) and electrical surface potential (right) measured after the rubbing of the inner square domain of LSMO thin film.

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Optical Properties Of WS_2 Nanotubes

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Abstract. Strong coupling of electric transition dipoles with optical or plasmonic resonators modifies their light-matter interaction and, therefore, their optical spectra. Semiconducting WS_2 nanotubes intrinsically provide the dipoles through their excitonic resonances, and the optical cavity via their cylindrical shape. We investigate the non-equilibrium light-matter interaction in WS_2 nanotubes in the time domain using femtosecond transient extinction spectroscopy. We develop a phenomenological coupled oscillator model with time-dependent parameters to describe the transient extinction spectra, allowing us to extract the underlying non-equilibrium electron dynamics. We find that the exciton and trion resonances shift due to many-body effects of the photogenerated charge carriers and their population dynamics on the femto- and picosecond time scale. Our results show that the time-dependent phenomenological model quantitatively reproduces the non-equilibrium optical response of strongly coupled systems.

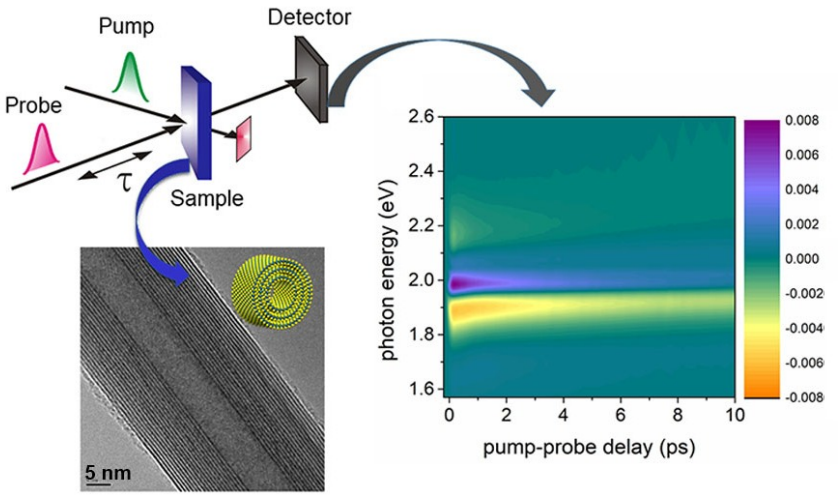

FIGURE 1. A schematic representation of femtosecond transient extinction spectroscopy setup used for measuring the nonequilibrium dynamics of strongly coupled resonances in the intrinsic cavity of WS_2 nanotubes, with the resulting 2D spectrum

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Dynamical Mean-Field Theory of Strongly Correlated Electron Systems

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Abstract. Electronic correlations in solids give rise to dynamical features such as heavy quasiparticles, transfer of spectral weight, and Mott insulating behavior. They can neither be explained within a single-electron picture nor by Density Functional Theory (DFT). Here the Dynamical Mean-Field Theory (DMFT) – a novel kind of mean-field theory for interacting lattice fermions – has proved to be a breakthrough which opened new perspectives for the investigation of correlated electron systems. The derivation of DMFT makes use of the fact that diagrammatic perturbation theory for quantum lattice models with an on-site interaction greatly simplifies in the limit of infinite dimensions or coordination number, without becoming trivial. In particular, the self-energy becomes local in this limit. Therefore DMFT may be constructed by mapping an electronic correlation problem onto a single-impurity Anderson model with a self-consistency condition. In contrast to single-particle theories the mean field of the DMFT is dynamical, whereby local quantum fluctuations are taken into account exactly.

DMFT makes it possible to investigate the dynamics of correlated electron systems non-perturbatively at all interaction strengths, electron densities and temperatures. In particular, the computational scheme obtained by merging approximate treatments of DFT, e.g. the Local Density Approximation (LDA), with the many-body DMFT has developed into a powerful method for the calculation of the electronic, magnetic, and structural properties of correlated electron materials from first principles. This approach, referred to as LDA+DMFT or DFT+DMFT, has already been very successful in the investigation of typical correlated electron materials such as transition metals and their oxides, f-electrons and Heusler alloys.

Extensions of DMFT using clusters or diagrammatic methods opened the possibility to include non-local correlations and thereby study, for example, interfaces and heterostructures, unconventional superconductivity, or the critical behavior at thermal and quantum phase transitions. Furthermore, generalizations of DMFT to non-equilibrium states make it possible to explore the real-time dynamics of correlated systems.

In my talk I will review the foundations of DMFT and discuss recent results obtained with this approach for correlated electrons in models and materials [1].

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1. For a recent series of lectures on DMFT and its applications and extensions see *DMFT: From Infinite Dimensions to Real Materials*, eds. E. Pavarini, E. Koch, A. Lichtenstein, D. Vollhardt; Modeling and Simulation, Vol. **8** (Forschungszentrum Jülich, 2018); OpenAccess: https://www.cond-mat.de/events/correl18/manuscripts/.

A large family of triangular lattice spin liquid candidates

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Abstract. Quantum spin liquid (QSL), theoretically proposed over 40 years ago, is a novel spin-entangled phase exhibiting many exotic excitations. It remains a major challenge in the field to search for ideal QSL materials. Recently, we revealed a large family of triangular lattice QSL materials named rare-earth chalcogenides. The existing measurements down to milikelvins, like inelastic neutron scattering, muSR and thermodynamics, consistently point to a QSL ground state. The high symmetry, the simple structure and the rich diversity enable the family as a model platform exploring QSL physics. In this talk I will introduce the family and share our developments in materials and experiments.

Kondo Effect in Unconventional Host Materials

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Abstract. The Kondo effect is the screening of impurity local moments by itinerant quasiparticles of the non-magnetic host material. This leads to marked anomalies in thermodynamic and transport properties at low temperatures, such as the presence of the resistivity minimum at a finite temperature. Traditionally the host material is a regular metal and the screening is done by the Landau quasiparticles (dressed electrons) of the Fermi liquid ground state of the system. Recently, the fate of magnetic impurities has been investigated in a range of unconventional host materials. I will discuss two notable cases: impurities in superconductors and impurities in quantum spin liquids.

Magnetic impurities in superconductors produce an attractive spin-dependent potential for the Bogoliubov quasiparticles and generate sub-gap states (Yu-Shina-Rusinov states). For sufficiently strong exchange coupling, a Bogoliubov quasiparticle is trapped by the magnetic impurity and the impurity local moment is effectively screened. Such transitions can now be studied in very controlled setting in hybrid semiconductor-superconductor devices where a quantum dot plays the role of a fully tunable magnetic impurity. In addition, reliable theoretical tools are available for this class of problems. In this domain, precision experiments are now possible even in more complex multiple-impurity situations, and they show remarkable agreement with theoretical modelling.

Since the charge degree of freedom is not relevant for the Kondo effect, the screening can also occur in materials that are charge insulators. This is the case for quantum spin liquids with spinon excitations. These materials remain paramagnetic down to very low temperatures in spite of strong exchange interactions. Spinons are fermionic quasiparticles that carry no charge, but they do have a spin degree of freedom. They may form a Fermi surface and resemble, in many respects, electrons in a regular metal. In particular, they are predicted to Kondo screen the magnetic impurities in close analogy to the regular Kondo effect. Recently, this has been observed in Zn-brochantite. In this domain, the theory is less much less developed and even clean host materials are not well understood. In fact, studying impurity effects represents a powerful tool to study the spin liquid state.

Kondo physics is thus found to be very generic, occurring in any material with itinerant quasiparticles carrying spin, be it insulators, metals or superconductors.

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