# **Solid-State Physics**

# Frontiers in science and scientific policy

# Lifetime of transitions between Landau levels

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In a magnetic field, band electrons become confined to Landau levels. There is a clean link between the material's band structure, and the energy spectrum of these Landau levels. Since the early 1950s, excitations from one Landau level to another—Landau level spectroscopy—has been abundantly employed as an extremely sensitive probe of semimetal and semiconductor band structure. From it, we obtain band parameters: effective mass, or Fermi velocity, the band gap. However, we rarely consider the width of inter-Landau level transitions, a parameter that tells us about the lifetime of inter Landau level transitions. The purpose of this work is to explore how this lifetime depends on the magnetic field, for a number of topological materials. We employ new analysis strategies on highly detailed maps of Landau levels, obtained in extreme magnetic fields.

# **Exciton Manipulation and Transport in 2D Semiconductor Heterostructures**

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The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS<sub>2</sub> and other layered semiconducting materials. They have a wide range of interesting fundamental properties and potential applications. New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarization. I will show here how by using MoS<sub>2</sub>/WSe<sub>2</sub> van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. On the other hand, the weak interlayer interaction and small lattice mismatch in MoSe<sub>2</sub>/WSe<sub>2</sub> heterostructures results in brightening of forbidden optical transitions, allowing us to resolve two separate interlayer transitions with opposite helicities and meV-scale linewidths. These have opposite helicities under circularly polarized excitation, either preserving or reversing the polarization of incoming light. By using externally applied electrical fields, we can control their relative intensities and polarization by different regions in the moiré pattern, characterized by different local symmetries and optical selection rules. Our more advanced excitonic devices now also offer the way to manipulate the motion of valley (spin) polarized excitons.

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# High-T<sub>c</sub> superconductivity in strongly overdoped cuprates

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For over three decades, research on superconducting cuprates has been focused on the underdoped and optimally doped regions of the electronic phase diagram, where these materials display an unconventional normal state – or "strange metal" – properties. It is widely accepted that, in the overdoped region at p > 0.27 hole/Cu, where superconductivity disappears, the properties are conventional, i.e. Fermi-liquid like. In fact, until recently, this region has been little studied owing to the difficulty of overdoping the CuO<sub>2</sub> plane, so such conventional scenario for overdoped cuprates has never been verified experimentally in a systematic manner.

Here we present recent results that give evidence of high- $T_c$  superconductivity in a number of cuprates, such as Cu<sub>0.75</sub>Mo<sub>0.25</sub>Sr<sub>2</sub>YCu<sub>2</sub>O<sub>7.54</sub> [1], Ba<sub>2</sub>CuO<sub>4-y</sub> [2] and La<sub>2-x</sub>Ca<sub>x</sub>CuO<sub>4</sub> [3], where strong overdoping, p > 0.4 hole/Cu, is achieved using high-pressure oxygenation during synthesis. In order to investigate the superconducting properties in this unusual region of the phase diagram, we studied the local structure of the above compounds by means of Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy. To our surprise, we found huge (~1 Å) dynamical distortions of the lattice at  $T_c$  that involve the apical oxygen [4,5], which suggests the existence of a lattice-driven change of the electronic structure in the superconducting state. The above unexpected results put into question the validity of the current phenomenological description of cuprates [6,7]. Specifically, we shall discuss the possibility of multi-orbital superconductivity [8] and the consequences of the nonadiabatic scenario suggested by our experiments on the description of the electron-lattice dynamics [5].

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# Global band topology: Classification of Dirac points and nodal planes

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The concept of global band topology refers to the fact that a given topological band feature (e.g., a Weyl point) does not exist in isolation, but is part of a global network of band degeneracies, that extends through the entire Brillouin zone [1,2]. The composition of this topological network is strongly constrained by the symmetries of the lattice and the fermion doubling theorems [3]. For example, a single Weyl node at the  $\Gamma$  point of a chiral nonsymmorphic space group must necessarily be accompanied by topological nodal planes [1,2]. In this talk we apply this concept to classify (i) Dirac points in general 2D systems and (ii) nodal planes in 3D magnets.

First, we derive in an algorithmic fashion the principle building blocks, out of which all twodimensional nodal systems are built [3]. This includes in particular, Dirac semimetals, nodal superconductors, as well as non-Hermitian systems with exceptional points. We discuss a number of physical examples of topological 2D materials, e.g., p2mm boron, to demonstrate the usefulness of our classification approach. Second, we enumerate all magnetic space groups whose symmetries enforce the existence of topological nodal planes [1]. Using database searches, several materials with nodal planes are identified, including ferromagnetic MnSi. We discuss experimental consequences of the nodal planes in the surface spectra and de Haas-van Alphen measurements of MnSi and CoSi [1,2].

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# FROM NANOSCALE STRUCTURE TO NANOSCALE FUNCTION

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As we gain ever-greater control of materials on a very small scale, so a new world of possibilities opens to be studied for their scientific interest and harnessed for their technological benefits. Nanoscale structures must be understood in terms of the positions of individual atoms and electrons, and the behaviour of individual quantum states.

We can take a single molecule, attach two wires to it, and use it as the active element in a transistor with graphene electrodes.<sup>1</sup> We can use this as a testbed for quantum interference in single-electron transport, for example in porphyrin nanoribbons.<sup>2</sup>

In a similar but slightly larger device we can use a suspended carbon nanotube as a tiny guitar string,<sup>3</sup> and thereby investigate how thermodynamics applies to a single object in which information could play a measurable entropic role.<sup>4</sup> A vibrating membrane has enabled us to demonstrate the thermodynamic cost of timekeeping within an order of magnitude of the theoretical limit.<sup>5</sup>

A basic challenge in quantum computing is to tune and characterise qubits on an ever-expanding scale.<sup>6</sup> We have developed machine learning methods for quantum technologies, which are able to learn how to do this more efficiently than even experienced humans.<sup>7</sup>

As scientists we have the responsibility and the privilege of advocating the responsible use of the progress to which we contribute. This calls for insight from science and wisdom from other disciplines to learn how together we can seek to promote human flourishing in times which seem to be increasingly subject to uncertainty.<sup>8</sup>

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# New exact theoretical methods for transport properties of quantum paraelectrics SrTiO<sub>3</sub>, KTaO<sub>3</sub>, and PbTe.

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Transport properties of quantum paraelectrics, including such famous perovskites as SrTiO<sub>3</sub>, KTaO<sub>3</sub>, and PbTe, were always treated basing on the assumption that the origin of anomalies of carrier movement in these compounds is the electron-phonon interaction. Historically, only linear coupling to the lattice vibrations was considered. However, recent studies [1,2] highlighted the fact that the temperature dependence of mobility cannot be explained in the framework of linear electron-phonon interaction paradigm and quadratic coupling to the lattice plays crucial role in explanation of transport anomalies in quantum paraelectrics.

Recent development of the Diagrammatic Monte Carlo (DMC) methods resulted in creation of the approximation-free machinery for theoretical description of the transport and optical properties of the models with linear electron-phonon interaction [3,4]. However, there was no exact approximation free approach to the treatment of the quadratic interaction.

We present two different novel approximation-free techniques valid for study of quadratic electron-phonon interaction. These DMC and path integral techniques pave the way to exact studies of the interplay between linear and quadratic couplings to lattice and theoretical interpretation of the puzzling transport and optical properties of quantum paraelectrics SrTiO<sub>3</sub>, KTaO<sub>3</sub>, and PbTe. We show our first data on the temperature dependence of the mobility in these cases.

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# Exotic localization properties in one-dimensional quasiperiodic models

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Transport properties of quantum systems crucially depend on how ordered they are. Periodic order favours extended Bloch waves that generate metallic bands, whereas disorder is known to localize the motion of particles, especially in lower dimensions. In this context, quasiperiodic systems, which are neither periodic nor disordered, reveal exotic transport properties, self-similar wavefunctions, and critical phenomena. In this talk, I will present a theoretical study of localization in a particular one-dimensional quasiperiodic model, dubbed the interpolating Aubry-André-Fibonacci (IAAF) model [1]. This model interpolates between two paradigmatic quasiperiodic examples: the Aubry-André model, known for a metal-to-insulator transition at finite potential strength, and the Fibonacci model, which is always critical. In a single-particle case, contrary to what one would naively expect, we find that the IAAF model has a non-monotonous and non-uniform behaviour of the spectrum. More precisely, we discover that by controllably evolving an Aubry-André into a Fibonacci model, a cascade of localization-delocalization transitions take place before the spectrum becomes critical. In a many-body IAAF model [2], we find that the cascade of localization transitions found in the single-particle case is destroyed even for weak interactions between particles. Moreover, in the region of the parameter space where the single-particle spectrum contains a non-trivial mobility edge, we observe an anomalous effect with tuning the interaction strength; namely, weak interactions localize the system, whereas stronger interactions enhance ergodicity. Our findings offer a unique new insight into understanding the criticality of quasiperiodic chains as well as a controllable knob by which to engineer band-selective pass filters. Furthermore, our model serves as a rich playground for studying the interplay between many-body interactions and tunable potentials.

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# Cellulose nanocrystals: from self-assembly to optical properties

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Cellulose is the most naturally abundant polymer on the planet and represents an ideal choice for sourcing materials. In its native form, it is usually found as part of plant cell walls arranged in highly crystalline microfibrils, which can be further processed to produce, after chemical treatment, stable suspensions of slender, splinter-like particles, termed 'Cellulose Nanocrystals'. [1] These biosourced and highly polydisperse suspensions (with dimensions of *ca*.  $200\pm100$  nm in length and  $15\pm10$  nm in width) present fascinating properties: above a critical concentration, they form cholesteric colloidal liquid crystalline suspensions, with a pitch in the micron range. When these suspensions are left to dry in a shallow dish, they lead to the formation of a film displaying strong reflection of left-circularly polarised light of specific wavelength adjustable within the visible range. While the use of these particles is promising for a variety of applications in effect pigments industry, the optical properties of these films are impacted by many parameters that remain still unclear. In this talk, I will present our recent progress on the understanding of the mechanisms of their self-assembly and how to control them to produce a variety of optically interesting effects. [2–5]

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# Quantum oscillations in Zr<sub>1-x</sub>Hf<sub>x</sub>SiS

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Dirac matter is a class of materials where the low-energy excitation spectrum can be described by the Dirac equation. They share a property of forming symmetry protected Dirac nodes (or lines) on valence and conductive bands crossings, with bands linear in close vicinity of nodes [1]. When magnetic field is applied to a system of free charged fermions, their energy states quantize into Landau levels. In a quantum oscillation experiment, the external magnetic field is varied, which causes Landau levels to pass over the Fermi surface. This in turn results in oscillations of the electronic density of states at the Fermi level, resulting in oscillations in various properties [2].

Using different angles of external field, we explored anisotropy of Dirac nodal line semimetal Zr1-xHfxSiS. Material is solid solution of ZrSiS and HfSiS and we managed to grow quality single crystals that show quantum oscillations. Here we present Shubnikov-de Haas and de Haas-van Alphen oscillations for external field along [001] for several x in  $Zr_{1-x}Hf_xSiS$ . Knowing the frequency of recorded quantum oscillations, as well as direction of applied field, we were able to reconstruct parts of Fermi surface for ZrSiS and HfSiS.

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# **Confining Layered Conductors**

### Carsten Putzke

Some of the most enigmatic correlated states in the field of quantum matter arise in lower dimensions such as guasi-2d and guasi-1d materials. The layered crystal structure in organic and high-T<sub>c</sub> superconductors is an example of these materials, where a quasi-2D electronic structure gives rise to several unconventional electronic instabilities. The layered crystal structure allows exfoliation in some materials allowing to uncover transport properties such as the quantum Hall effect as well as enables spectroscopic probes in single layer and few layer systems. It is the same crystallographic anisotropy that hinders the study of interlayer electrical transport and spectroscopic probes such as angle resolved photoemission spectroscopy (ARPES) of the states and Fermi surface warping relevant for interlayer conductivity. In this poster we will demonstrate the novel physical phenomena as well as experimental capabilities that focused ion beam microstructuring enables. Confining the in-plane dimension of quasi-2D high purity metals of the Delafossites to length scales smaller than the electron mean free path gives rise to a novel realization of the particle-wave duality. In the ballistic regime the intra-layer resistivity becomes directionally dependent<sup>1</sup> which is absent in bulk single crystals. The same effect leads to the observation of 1D-modes in magnetic field, which propagate through the material like a light would through a gird, leading to constructive and destructive interference<sup>2</sup>.

Beyond these exciting physical phenomena of finite size confined pillars, novel experimental possibilities will be presented which enable previously inaccessible insight into layered materials.

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Scanning electron microscope image of a 3D PdCoO2 micro-structure enabling to study the interplay between inter- and intra-layer electrical transport.

# SCANNING PROBE STUDIES OF CHARGE DENSITY WAVES - RECENT PROGRESS AND CHALLENGES.

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Charge density waves (CDWs) are the subject of renewed interest to understand their structure, their formation mechanism and their interplay with other quantum phases such as superconductivity and magnetism. Many models developed over the years often fail to fully describe specific experimental data sets, with embodiments of the classic Peierls Fermi surface nesting scenario being the exception rather than the rule. Scanning tunneling microscopy (STM) is a prime technique to investigate the CDW ground state, with a couple of pitfalls we will discuss based on recent high-resolution topographic STM images. Firstly, the correct identification of the CDW gap in tunneling conductance spectra is highly controversial, as evidenced by the large spread in gap amplitudes reported in the literature. Secondly, not all periodic charge modulations observed by STM are CDWs. We will present detailed analysis of the CDW modulation amplitudes and phases in real space [1], which offer unprecedented insight into the CDW gap in the band structure [2], including evidence for its multiband nature [3]. We find in particular that the CDW gap can open significantly below the Fermi level [2] and shift as a function of the local carrier concentration [4], providing an original insight into the cDW and superconducting ground states. We will also discuss possible orbital order and CDW chirality based on topographic STM images.

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# **TOPOLOGICAL SOLITONS IN CHIRAL QUANTUM MATTER**

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Topological solitons and quantum mechanics have been intertwined for the past 60 years. Even before the term soliton had been coined, Abrikosov's theory predicted the formation of twodimensional vortices in the phase field of superconductors, an exemplar exposition of macroscopic quantum coherence. Recent work shows that solitons are in fact a timely and promising platform for quantum operations. I will demonstrate the viability of using spin topology to influence a superconductor at selective length scales [1]. This includes adaptable recipes towards fluxonics and chiral superconductivity, as well as quantum processes such as non-perturbative, non-contact Majorana braiding. Time permitting, I will also introduce a new class of building blocks for realizing quantum logic elements [2]. Namely, nano-skyrmions in triangular magnets developing quantized helicity excitations with well-separated energy levels and distinct out-of-plane magnetizations.

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# Nanoscale self-organisation in Mott insulators: a pathway see to metastable metallicity see

#### <u>Claudio Giannetti</u>

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The interplay between electronic and lattice degrees of freedom in correlated materials often leads to spontaneous nanoscale architectures, which can favour and stabilize photoinduced emergent states with no counterpart at equilibrium. State-of-the-art light excitation protocols offer space-integrated information, which are insufficient to link and control the temporal and real-space dynamics of non-equilibrium states. We will present results [1] of time-resolved photoemission microscopy experiments on a  $V\Box O\Box$  thin film, which at equilibrium undergoes a transition at T≈140 K from intrinsically nanotextured monoclinic insulator to homogeneous corundum metal. We demonstrate that the excitation with infrared light pulses turns the low-T insulating phase into a non-thermal metallic state that retains the monoclinic in-plane shear strain. Mean-field modelling shows that the topology of the monoclinic nanotexture is key for stabilizing the emergent photo-induced metal state. Engineering the nanotexture of insulating strained domains may thus constitute a new tool to control non-thermal phases in correlated materials.

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# **OPTICAL CONDUCTIVITY OF CUPRATES IN A NEW LIGHT**

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Understanding the physical properties of unconventional superconductors as well as of other correlated materials presents a formidable challenge. Their unusual evolution with doping, frequency, and temperature, has frequently led to non-Fermi-liquid (non-FL) interpretations. Optical conductivity is a major challenge in this context. Here, the optical spectra of two archetypal cuprates, underdoped HgBa<sub>2</sub>CuO<sub>4+ $\delta$ </sub> and optimally-doped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+ $\delta$ </sub>, are interpreted based on the standard Fermi liquid (FL) paradigm. At both dopings, perfect frequency-temperature FL scaling is found to be modified by the presence of a second, gapped electronic subsystem. This non-FL component emerges as a well-defined mid-infrared spectral feature after the FL contribution determined independently by transport is subtracted. The evolution of the mid infrared feature with temperature, frequency, and doping indicates a gapped rather than dissipative response. In contrast, the dissipative response is found to be relevant for pnictides and ruthenates. Such an unbiased FL/non-FL separation is extended across the cuprate phase diagram, capturing all the key features of the normal state and providing a natural explanation for, why the superfluid density is attenuated on the overdoped side. Thus, we obtain a unified interpretation of optical responses and transport measurements in all analyzed physical regimes and all analyzed compounds. Our work presents a major advance in the analysis and interpretation of the optical spectra of high-temperature superconducting cuprates and other correlated systems. The first unambiguous experimental determination of the non-conducting part of optical responses gives rise to an overall simplification of our understanding. For the cuprates, in particular, it proves that the conducting part is always an ordinary FL, while the non-Fermi liquid character is entirely due to the non-conducting part. This insight has been employed to understand the optical responses of superconducting pnictides as well as strontium ruthanate; the success of this approach represents a breakthrough in understanding entire classes of what are currently the most interesting functional materials.

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# Studies of iron pnictide superconductors using XAS and XLD techniques

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Results of measurements on iron pnictide high-temperature superconductors using synchrotron radiation (Solaris and Elettra synchrotrons) and XAS (X-ray absorption spectroscopy) and XLD (X-ray linear dichroism) techniques will be discussed. XLD results on  $L_{3,2}$  Fe edge on compounds from Eu(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> family indicate that there is an uneven occupation of Fe  $d_{xz}$  and  $d_{yz}$  orbitals, which is related to nematicity observed in these materials [1]. Additionally, comparison of XANES results (Fe and As edges) on compounds from so called 122 and 112 families, as a function of Ni and Co doping, will be presented.

This work was supported by the National Science Centre of Poland grant no 2018/30/E/ST3/00377.

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# Magnetoconductivity of a metal with a closed Fermi surface reconstructed by a biaxial charge density wave

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We investigate quantum dynamics and kinetics of a 2D conductor with a closed Fermi surface reconstructed by a biaxial density wave, in which electrons move along a two-dimensional periodic net of semiclassical trajectories coupled by the magnetic breakdown tunneling under a strong magnetic field [1, 2]. We derive a quasiparticle dispersion law and magnetoconductivity tensor. The quasiparticle spectrum is found to be the alternating series of two-dimensional magnetic energy bands with gaps between them. The longitudinal magnetoconductivity shows giant oscillations with change of magnetic field, while the Hall coefficient changes sign and is absent in a wide range of the magnetic fields in between.[3] Preliminary estimations show that the suggested magnetic field, as observed in experiments in materials with analogous topology of the Fermi surface, such as the high-Tc superconducting cuprates.

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# The Ruđer Bošković Institute, Today and Tomorrow: Croatian Science and Beyond

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The Ruder Bošković Institute (RBI) in Zagreb is the largest pubic research institute in Croatia. With a multidisciplinary focus, activities at the RBI span physics, chemistry, biology, marine and environmental research, molecular medicine, and informatics. Recent years have seen increasing success in securing competitive projects from both national and international funding agencies. This has been complemented with an increased effort for more direct relevance to society. The presentation will highlight selected past activities and outline future directions, all within the context of the ever changing domestic and foreign research landscapes.

# Murunskite: A Bridge Between Cuprates and Pnictides

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Exploring novel materials as the candidates for unconventional superconductors can help to understand the mechanism of this exotic phenomenon but also lead to synthesis of compounds with important technological applications. The main compound of interest is murunskite (K<sub>2</sub>FeCu<sub>3</sub>S<sub>4</sub>), a material isostructural to iron-based superconductors with iron and copper occupying the same crystal site. I will discuss the synthesis methods and measurements of structural, electronic and magnetic properties. [1] The current study shows that murunskite is a Mott insulator with sulfur orbitals partially open and electronically active, similar to oxygen orbitals in cuprates. Measurements indicate the conduction band is cuprate-like while the valence band is pnictide-like, positioning murunskite as an interpolation compound.

We have successfully modified murunskite structure by substitution and doping on all three crystallographic positions. Effects on the electronic and magnetic properties leading towards the metallization will be discussed.

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# **Cuprate Superconductivity: Perfect Match of Ionicity and Metallicity**

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A recent comprehensive synthesis of observational and theoretical insights in cuprate superconductors is reviewed [1]. The evolution of the Fermi arcs and pseudogap with doping, and the concomitant evolution of superconductivity itself, are understood on an equal footing, within a simple picture of a Fermi liquid against an ionic background. The evolving background determines the relative proportion of the localized (ionic) and itinerant (Fermi liquid) components in the total charge. The transition from a low-density superconducting to a high-density non-superconducting Fermi liquid is related to the disappearance of the localized component at overdoping. It is understood microscopically as a transition from an ionic to a covalent Cu-O d-p bond. This transition is first-order, like an orbital transition, and does not entail a quantum critical point or any dissipative mechanism. A fast virtual local mechanism of Cooper pairing is proposed.

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# Magnetotransport and supercurrents in HgTe-based topological nanowires

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Topological insulator (TI) nanowires in proximity to conventional superconductors have emerged as a tunable platform to realize topological superconductivity and Majorana zero modes [1]. The tuning is done using an axial magnetic flux  $\phi$  which allows transforming the system from trivial at  $\phi = 0$  to topologically nontrivial when half a magnetic flux quantum  $\phi = \phi_0 / 2 = h / 2e$  threads the crosssection of the wire.

Our system of choice is wires made from strained HgTe layers, known to be a strong topological insulator. This material is characterized by high electron mobilities, enabling ballistic transport, and featuring pronounced quantum effects [2,3]. Besides magnetotransport properties, I focus on the properties of Josephson junctions engineered by placing superconducting Nb contacts across the wires, thus inducing superconductivity in the surface states of the HgTe wires. On the one hand, we investigate the evolution of the supercurrent in HgTe wire based JJs as a function of an axial magnetic field, on the other we probe the periodicity of the superconducting phase utilizing microwave irradiation and probing the Shapiro steps. From the suppression of odd Shapiro steps, we extract the  $2\pi$ - and  $4\pi$ -periodic portion of the supercurrent where the latter is a required signature for Majorana zero modes present. Suppressed odd Shapiro steps herald the existence of  $4\pi$ -periodic supercurrents even at low magnetic fields, i.e., in the trivial regime, indicating that trivial mechanisms like Landau-Zener transitions are the origin. Our data suggest further that this  $4\pi$ -periodic supercurrent of trivial origin can be suppressed by an in-plane magnetic field oriented perpendicular to the wire, but that at magnetic fields above  $\phi_0 / 4$ , topological  $4\pi$ -periodic supercurrents take over [4].

Work done in cooperation with

Ralf Fischer, Wolfgang Himmler, Johannes Ziegler, Jordi Picó-Cortés, Gloria Platero, Milena

Grifoni, Dmitriy A. Kozlov, N. N. Mikhailov, Sergey A. Dvoretsky, Michael Barth, Jakob Fuchs,

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# **METASTABILITY - A LIFE FORCE IN QUANTUM MATERIALS**

# <u>Dragan Mihailovic,</u> Jaka Vodeb, Viktor Kabanov, Yaroslav Gerasimenko, Igor Vaskivskyi, Tomaz Mertelj, Jan Ravnik, Rok Venturini and Anže Mraz

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Nonequilibrium processes are prevalent everywhere from life systems to cosmology. The study of nonequilibrium systems requires not only temporal, but also spatial and spectral resolution that is tailored to the system under study. Unfortunately achieving all these requirements is usually very difficult, and often impossible. Quantum systems offer an opportunity to study non-equilibrium processes and associated metastable states in detail all the way to the atomic level with a combination of state-of-the-art nonequilibrium time-resolved and microscopy techniques [1]. Here we will present an investigation of prototype charge ordered quantum materials in which emergent properties, and metastability in particular, are accessed through non-equilibrium routes [2–5]. Apart from advancing our understanding of nonequilibrium quantum matter, the emergent metastable systems also have a useful application for ultrafast, ultra-efficient cryomemory devices [6,7], addressing the energy consumption problem of future big data systems head on.

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# Far-infrared *ab*-plane optical conductivity of La2-xBaxCuO4 single crystals

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Kramers-Kronig analysis of the *ab*-plane reflectance of ten La<sub>2-x</sub>Ba<sub>x</sub>CuO<sub>4</sub> single crystals, with x ranging from undoped to optimally doped, yields the optical conductivity  $\sigma_1(\omega)$  at temperatures from 10–300 K. The influence of stripe order around x = 0.125 appears in the spectra below T = 50 K, observed both as a reduction in the free-carrier (normal state) and superfluid (superconducting state) density and by the appearance of a relatively narrow conductivity band near 25 meV. Away from this band, the low-frequency conductivity follows the Drude function, with a *T*-linear scattering rate,  $\hbar/\tau = \alpha k_B T$ . The prefactor  $\alpha$  varies with x, exceeding the conjectured Planckian bound ( $\alpha = 1$ ) on inelastic scattering by more than a factor of two near optimal doping.

\*With Luyi Yan and Genda Gu

# Transcutaneous electrical nerve stimulation via deep-red light transduced by implanted thin film photocapacitors

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Great demand exists for minimally-invasive neuromodulation technologies to enable next-generation bioelectronic medicine. We report on our developments of ultrathin (opto)electronic devices for neurostimulation. All of these devices rely on far red/near infrared irradiation in the tissue transparency window to actuate nanoscale organic semiconductor components. Our flagship technology is the organic electrolytic photocapacitor (OEPC) – a device that mimics biphasic current-pulse neurostimulation and thus transduces an optical signal into directly-evoked action potentials in neurons. These devices are not only wireless, but also 100-1000 times thinner than existing technologies. We will discuss examples of chronic implants capable of stimulating peripheral nerves, the cortical surface, as well as deeper brain structures. Light power can be safely and effectively transmitted to implants up to 15 mm below the skin surface, and effectively penetrates the scalp and skull. We believe that the combination of deep red light and ultrathin photovoltaic devices can account for a new paradigm in wireless bioelectronic medicine.

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# High-Pressure Hydrides: Experimental Questions and some Theory

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Room-temperature superconductivity was reported in October, 2020, after 5 years of discovery of superconducting hydrides in the 200 - 250 K range. This talk will first critically review the experimental evidence for superconductivity. At the time of this writing, there are big resistivity drops, but no compelling measurements of the Meissner effect or flux trapping. We also provide a basic review of our current understanding of the electron-phonon interaction in relation to superconductivity. We revisit the age-old question (once thought settled) of whether or not the electron-phonon interaction can produce high-temperature superconductivity.

# MAGNETO-OPTICAL DETECTION OF TOPOLOGICAL CONTRIBUTIONS TO THE ANOMALOUS HALL EFFECT

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Recently, the topology of the electronic band structure has attracted much attention in materials with broken time-reversal symmetry as these compounds may host non-trivial features such as Weyl fermions. One of the most profound manifestation of the non-trivial topology is the emergence of the anomalous Hall effect (AHE). When the spin degeneracy of the bands is lifted by the exchange splitting, their spin-orbit mixing leads to a finite Berry curvature, which, as a fictitious magnetic field, deflects electric currents. However, identifying the band structure features responsible for the AHE is difficult based on magnetotransport experiments alone, since the response is a sum of multiple bands as well as intrinsic and extrinsic contributions with sometimes identical dependence on the longitudinal conductivity.

Here, we demonstrate that the energy resolved measurement of the infrared Hall-effect via the detection of the magneto-optical Kerr-effect (MOKE) spectrum can provide the necessary information. We studied kagomé magnets such as Fe<sub>3</sub>Sn<sub>2</sub> and Co<sub>3</sub>Sn<sub>2</sub>S<sub>2</sub>, showing large AHE, which is attributed to Dirac and Weyl fermions. Using MOKE spectroscopy, we identified the inter-band excitations responsible for the intrinsic AHE. In Fe<sub>3</sub>Sn<sub>2</sub>, we found that low-energy transitions, tracing "helical volumes" in momentum space reminiscent of the formerly predicted helical nodal lines, substantially contribute to the AHE, which is further increased by contributions from multiple higher-energy interband transitions [1]. Our study also reveals that local Coulomb interactions lead to band reconstructions near the Fermi level. Whereas in Co<sub>3</sub>Sn<sub>2</sub>S<sub>2</sub>, we identified enhanced infrared Hall conductivity at the electronic excitation in the vicinity of a nodal-loop.

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# Is there a Native Oxide for Intrinsic Magnetic Topological Insulator MnBi<sub>2</sub>Te<sub>4</sub> Thin Films?

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Understanding the effects of interfacial modification on the functional properties of magnetic topological insulator thin films is crucial for developing novel technological applications from spintronics to quantum computing. Here, we report a large electronic and magnetic response that is induced in the intrinsic magnetic topological insulator MnBi<sub>2</sub>Te<sub>4</sub> by controlling the propagation of surface oxidation [1]. We show that the formation of the surface oxide layer is confined to the top 1-2 unit cells but drives large changes in the overall magnetic response. Specifically, we observe a dramatic reversal of the sign of the anomalous Hall effect driven by finite thickness magnetism, which indicates that the film splits into distinct magnetic layers each with a unique electronic signature. These data reveal a delicate dependence of the overall magnetic and electronic response of MnBi<sub>2</sub>Te<sub>4</sub> on the stoichiometry of the top layers. Our study suggests that perturbations resulting from surface oxidation may play a non-trivial role in the stabilization of the surface may open new routes for engineering novel topological and magnetic responses in this fascinating material.

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# **Transfer of Graphene under Ultra-High-Vacuum**

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Current graphene transfer techniques most often require drop-coating of a supporting layer on top of graphene and immersion in an etching solution to remove the growth substrate, followed by removal of the supporting layer in another solution post-transfer, making them incompatible with ultra-high vacuum (UHV). We present a novel technique for graphene transfer fully compatible with UHV, based on the chemical etching of a Cu growth substrate, using teflon (PTFE) as a supporting layer combined with a wafer-bonding approach. We demonstrate successful transfer to both Ir(111) and Cu(100) crystals. The STM image shows UHV transferred graphene on Ir(111) after annealing to 1270 K (1000 Å x 1000 Å,  $V_t = 0.3$  V,  $I_t = 10$  nA, T = 300 K).





# SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> – a Deep Purple crystal

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The insulating quantum magnet SrCu2(BO3)2 is a unique material realization of the theoretical Shastry-Sutherland model, which has become an arena for developing and testing quantum many body methods in 2D. Using extreme conditions of magnetic field and pressure to drive the system across quantum phase transitions, we report on the quantum phases and quantum excitations. I will summarize a couple of intriguing results: correlated decay of triplons [1]; existence of a plaquette singlet phase [2]; discovery of a critical point as the quantum equivalent of the vapour-liquid transition in water [3].

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# STOCHASTIC RESONANCE SWITCHING IN A CORRELATED SPIN GLASS

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The interplay between spin-orbit interaction (SOI) and magnetic order is currently one of the most active research fields in condensed matter physics. Famous examples of this interplay are skyrmions and spin waves, but also the search for Majorana zero modes and magnetic topological insulators fit directly in this field and have gained much attention in recent years. The full spectrum of possibilities is unleashed in combination with breaking the symmetry of the system, either at interfaces or in the crystal structure itself. This makes multiferroic materials, where symmetry breaking in the form of ferroelectric order and magnetics. Here we will show that starting from a ferroelectric system with strong spin orbit interaction and doping this with magnetic impurities is indeed a promising pathway to achieve magnetic order with tuneable dynamics. The switching mechanism in this correlated spin glass system will be explained based on stochastic resonance.

In  $\alpha$ -GeTe the combination of the ferroelectric order and large SOI yields a switchable Rashba-type spin structure of the bulk states [1]. When doped with up to 20% Mn a magnetic order is induced while the ferroelectric order remains present, rendering it a multiferroic material [2]. Moreover, the strong magnetoelectric coupling in the system [1] ensures a coupling of the magnetisation and polarisation axes, resulting in the opening of a Zeeman gap in the Rashba split bands around the Brillouin zone centre [3]. This unique combination of properties creates a large bulk Rashba-Edelstein effect and allows for current driven magnetisation switching [4]. Here we will present X-ray magnetic circular dichroism (XMCD) and muon spin resonance (muSR) results supported by theory showing that the system orders in a correlated spin glass state with topological spin textures and spontaneously switches its magnetisation direction without changing any of the typical external parameters.

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# Measuring and tailoring anisotropies in skyrmion and antiskyrmion hosts

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As known for long, in centrosymmetric crystals magnetic anisotropy plays a key role in the formation of magnetic bubbles, including topologically trivial and non-trivial ones. In contrast, in non-centrosymmetric crystals, where the Dzyaloshinskii-Moriya interaction is the key player in stabilizing magnetic skyrmions, systematic studies on the effect of anisotropy have been virtually non-existing. However, recent theoretical predictions and experimental observations show that the quantitative description of the (anti)skyrmion stability range, the formation of distinct high- and low-temperature skyrmion lattice phases and other emergent exotic mesoscale spin patterns all require the treatment of magnetic anisotropy on equal footing with the Dzyaloshinskii-Moriya interaction. Here we provide a short overview, from an experimental point of view, on the vital role of magnetic anisotropy in various skyrmion and antiskyrmion host materials, via the spectroscopic determination of relevant anisotropy terms in non-centrosymmetric cubic (O, T) and axial ( $C_{nv}$ , S<sub>4</sub>) magnets as well as in centrosymmetric skyrmion hosts [1-6].

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# New interpretation of a phonon dispersion relation in Nd<sub>2-x</sub>Ce<sub>x</sub>CuO<sub>4</sub>

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The discovery of a high-temperature phonon anomaly in double-layer cuprate HgBa<sub>2</sub>CaCu<sub>2</sub>O<sub>6+ $\delta$ </sub> (Hg1212) [1], as well as the observation of dynamical charge correlations in its single-layer equivalent, HgBa<sub>2</sub>CuO<sub>4+ $\delta$ </sub> (Hg1201) [2], raised a question concerning the character of the interplay between lattice dynamics and the CDW correlations, both static and dynamic. Interestingly, it was reported for a wide range of hole-doped cuprates [3,4] that the dispersion of acoustic phonon modes is modulated around the CDW order wave vector,  $q_{CDW}$ . However, it remains unclear whether the effect can also be observed at higher energies, for optical modes. To solve these issues, we performed studies of the phonon dispersion relation in electron-doped cuprate Nd<sub>2-x</sub>Ce<sub>x</sub>CuO<sub>4</sub> (NCCO), around the momentum transfer  $q_{CDW} \approx 0.23$  which corresponds to the CDW wave vector. Our detailed temperature and doping-dependent inelastic X-ray scattering (IXS) studies resulted in a new interpretation of the bond-stretching mode dispersion and revealed broadening of this mode at the momentum where the two highest optical modes anticross. Our experimental results are complemented by density functional theory (DFT) calculations performed for an undoped compound.

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# UNIVERSAL PROPERTIES OF FLUORESCENCE INTERMITTENCY IN NANOSCALE EMITTERS

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Virtually all known fluorophores exhibit mysterious episodes of emission intermittency. A remarkable feature of the phenomenon is a power-law distribution of on- and off-times observed in colloidal semiconductor quantum dots, nanorods, nanowires and some organic dyes. More recently, fluorescence intermittency has also been detected in a quasi-two dimensional material: reduced graphene oxide.

For nanoparticles, the resulting power law extends over an extraordinarily wide dynamic range: nine orders of magnitude in probability density and five to six orders of magnitude in time.

Exponents hover about the ubiquitous value of -3/2. Dark states routinely last for tens of seconds practically forever on quantum mechanical timescales. Despite such infinite states of darkness, the dots miraculously recover and start emitting again. Although the underlying microscopic mechanism responsible for this phenomenon remains a mystery and many questions persist, I argue that substantial theoretical progress has been made. Within a single phenomenological framework[1] we succeeded to capture the universal behavior of a wide range of nanoscale emitters and, in some cases, to reveal microscopic scenarios that could lead to emission intermittency and optical 1/f noise in these systems.

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# (ANTI-)SKYRMIONS IN CRYSTALS WITH S4 SYMMETRY

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Magnetic skyrmions are nowadays found in a variety of different material classes, ranging from single crystals to sputtered films. They often emerge on length scales much larger than the atomic lattice where they appear as vortex-like, rotationally symmetric whirls. Their anti-vortex-like partners, consequently dubbed anti-skyrmions, naturally break this rotational symmetry which leads to a plethora of new effects. However, only a limited number of antiskyrmion-hosting materials are known and, previously, they all belonged to the D2d symmetry class, even though crystals with S4 symmetry were predicted to also host antiskyrmions.[1]

In my talk, I will present our recent works on antiskyrmions in crystals with S4 symmetry. Combining experiments and theory, we studied antiskyrmions, skyrmions, and other textures in the S4-symmetric family of schreibersites (Fe,Ni)3P with heavy element doping.[2,3,4] The competition between the dominant demagnetization energy and small Dzyaloshinskii-Moriya interaction stabilizes both antiskyrmions and skyrmions in the transition region from the stripe phase to the field-aligned ferromagnet and, moreover, renders antiskyrmions square-shaped and skyrmions elliptical.[2] In general, antiskyrmions form in thicker samples and samples with larger uniaxial anisotropy where the bulk DMI can compete with dipolar interaction. Vice versa, skyrmions form in thinner samples where they profit from the strong dipolar interaction.[3] Moreover, I will show how the ellipticity of skyrmions in these systems can be used to estimate the magnitude of the DMI[4].

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# Spin proximity effects in 2D materials

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Graphene has weak spin-orbit coupling and no magnetic order. But when placed in contact to a strong spin-orbit coupling material, such as a TMDC, or a ferromagnet, such as Cr2Ge2Te6, Dirac electrons acquire strong spin-orbit or exchange coupling, respectively. Such proximity effects render graphene suitable for spintronic applications that require spin manipulation [1]. In addition, graphene with strong proximity spin interactions can host novel topological states [2]. Fascinating new phenomena appear when bilayer graphene gets encapsulated by a TMDC from one side, and a ferromagnet from another. The resulting, so called ex-so-tic structure [3], offers spin swap functionality: switching spin-orbit and exchange coupling on demand by gate. In this talk I will review the recent developments in the proximity spin-orbit and exchange coupling by twisting the van der Waals layers. I will show that the signature proximity spin-orbit coupling in graphene----valley Zeeman coupling---can be efficiently tuned by the twist angle [4], and that proximity exchange coupling can be switched by the twist angle, and even morph from ferromagnetic to antiferromagnetic [5]. Support from DFG SPP1244, SFB 1277, and EU Graphene Flagship is acknowledged

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# Nature and symmetry charge order in cuprate superconductors

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I will present recent synchrotron experiments on the problem of charge order in cuprate superconductors [1-5]. Improvements of energy resolution has led to a wave of new resonant inelastic x-ray scattering (RIXS) results on the cuprates. In particular, new grounds have been gained on the understanding of electron-phonon coupling and its role for charge ordering. Another string of experiments has explored the tunability of charge order in the presence of uniaxial pressure.

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# Selected universal properties of high-temperature superconducting cuprates

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One of the fundamental problems od condensed matter physics is to explain the nature of electron states and microscopic pairing mechanism in the strongly correlated systems. Their specific characteristic is the circumstance that superconductivity appears in the systems, in which the reference state is either the Mott insulating state or that of magnetic metal, with specific exchange interaction surviving in the paired state. In our group we have constructed a unified theoretical model of these systems, which contains both the strong correlations and magnetic fluctuations. The model has been applied to the description of high-temperature superconducting cuprates [1,2,3], heavy fermions, and to the twisted graphene bilayer systems. The aim of our presentation is to summarize selected properties of those systems, that is: (i) to discuss evolution from the antiferromagnetic Mott insulator to high temperature superconductor and to provide its universal features in the latter case [1,3]; (ii) to describe the dynamic (paramagnons) and plasmon excitations across the phase diagram [4]. One should underline that pairing in all above systems is regarded as taking place in real space, what distinguishes them in a principal manner from the corresponding description in the BSC and Eliashberg theories. The theoretical results are compared with experiment in a quantitative manner.

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# NEAR-FIELD INFRARED MICROSCOPY ON CARBON NANOSTRUCTURES

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Scattering near-field optical microscopy (s-SNOM), based on the combination of atomic force microscopy and frequency-dependent light scattering, is an emerging method that combines high spatial resolution with high sensitivity even at long illuminating wavelengths. I will present results in the infrared frequency range obtained on various aspects of carbon nanostructures. The most obvious task, identifying individual molecules, is also the most difficult due to the weak scattering from molecular vibrations. Free (Drude) electrons in metallic carbon nanotubes [1] or encapsulated metal clusters [2] are more easily detected. The intense field under the tip can also be used to launch and detect the charge distribution inside nanotubes caused by interference of quasiparticles: plasmon-polaritons [3] or phonon-polaritons [4]. The interaction of phonon-polaritons with vibrational modes of molecules confined in the tubes [5] brings the capabilities of the method full circle, enabling to reach a detection threshold of a few hundred molecules and follow their chemical reactions by infrared spectroscopy.



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# EuFe<sub>2</sub>As<sub>2</sub>-BASED COMPOUNDS INVESTIGATED BY <sup>57</sup>Fe AND <sup>151</sup>Eu MÖSSBAUER SPECTROSCOPY

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The EuFe<sub>2</sub>As<sub>2</sub>-based compounds exhibiting 3*d* and/or 4*f* magnetic order were investigated with <sup>57</sup>Fe and <sup>151</sup>Eu Mössbauer spectroscopy [1-3]. It was found that spin-density-wave order of the Fe itinerant moments is suppressed by the chemical doping and in many cases the superconductivity is achieved. The Eu localized moments usually order regardless of the dopant concentration x, but undergo spin reorientation with increasing x from the alignment parallel to the *a*-axis in the parent compound, toward the crystallographic *c*-axis. The change of the 4*f* spins ordering from antiferromagnetic to ferromagnetic occurs simultaneously with a disappearance of the 3*d* spins order. The Fe nuclei experience the transferred hyperfine magnetic field due to the Eu<sup>2+</sup> ordering for sufficiently substituted compounds, while the transferred field is undetectable in EuFe<sub>2</sub>As<sub>2</sub> and for compounds with a low substitution level. It seems that the 4*f* ferromagnetic component arising from a tilt of the Eu<sup>2+</sup> moments to the crystallographic *c*-axis leads to the transferred magnetic field at the Fe atoms, even in the superconducting state.

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# Sublattice extension of the Rashba nanowire model

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Interplay between superconductivity, spin orbit coupling and magnetic field can lead to realization of the topological phase. Majorana bound states (MBS) emerging at the ends of a one dimensional nanowire are one of its manifestations[1,2]. Signatures of these states have been observed, e.g. in superconductor-semiconductor hybrid nanostructures or adatom chains.

During this talk, We will present a few cases where the MBS can emerge outside of the usual topological regime, due to the impact of the sublattice on the topology of Oreg-Lutchyn model of Rashba nanowire. It is done by expanding the Rashba nanowire model with dimerized sublattice similar to SSH model[3] or with antiferromagnetic sublattice[4].

In the first case, the dimerization-induced topological superconductivity allows for forming of additional topological *branch*. We provide an analytical justification based on the symmetry and parity considerations and discuss feasible spectroscopic methods for its empirical observation.

In the second case, an additional topological *branch* emerges due to the antiferromagnetic order allowing Majorana bound states to exist close to half-filling, obviating the need for either doping or gating the nanowire to reach the low density regime.

Additionally, we show the emergence of the Majorana bound states in the absence of the external magnetic field, which is also a result of inherent antiferromagnetic order.

We will discuss results in context of topological phase diagrams showing the beneficial impact on the robustness of MBS. Furthermore, we will demonstrate how these topological phases could be probed experimentally within the non local transport measurements.

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# Photoluminescence and optically detected magnetic resonance map of single-walled carbon nanotubes

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While the photoluminescence of semiconducting single-walled carbon nanotubes (SWCNTs) has only been observed first 20 years ago [1], these materials show high promises for applications of future technologies, such as light-harvesting, quantum computing, and optoelectronics. Thanks to this, they are being intensely studied ever since, with our group specializing in their investigation via optical spectroscopy by the usage of a self-developed spectrometer [2]. This device is equipped both with a tunable laser source as the excitation source and a spectrograph able to detect in the near-infrared range. Thanks to them, not only the photoluminescent (PL) spectrum of SWCNTs can be recorded, but their optically detected magnetic resonances (ODMR) as well. This can be performed for a range of exciting wavelengths, thus creating so-called PL and ODMR maps both at room temperature and at 77 K.

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# The role of the electron-phonon interaction strength in shaping spectra of phonon-plasmon systems

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We provide a systematic analysis of phonon-plasmon coupled excitations in polar systems [1] through the complementary lens of electron energy loss spectroscopy (EELS) and phonon spectra [2]. The whole experimentally relevant parametric space, spanned by the adiabaticity parameter and the electron-phonon interaction (EPI) strength, is covered by referring to several real materials [3] that are of particular interest. Excitations' dispersions evolutions, damping, and various limiting behaviours are qualitatively and quantitatively discussed.

We find that the EPI strength plays a determining role in distributing spectral weights among coupled excitations, which opens the possibility of estimating its value directly from experimental EELS spectra, even in cases of very limited energy resolution.

The projection of the excitations onto the phonon degree of freedom reveals for strong couplings large phonon production contributions, which are of very different origins depending on the adiabaticity parameter. In particular, in the adiabatic regime the additional phonon spectral weight is a consequence of the phonon softening effects, while in the antiadiabatic regime it arises due to a cloud of phonons that accompanies plasma oscillations.

We also comment on phonon properties of phonon-plasmon coupled systems within the static screening and the static polarization approximation, where the former is being frequently used in studying the impact of non-adiabatic effects on phonon spectra in *ab initio* modelling [4-6].

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# Green and rational synthesis of porous MOFs and their non-conventional forms via mechanochemistry

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Porous metal-organic frameworks (MOFs)[1] have become a highly researched area of modern materials science. MOFs are modular coordination materials whose structure and properties can be altered by a careful choice of metal nodes and suitable organic linkers. They are now widely studied for storage, separation, catalysis, sensing, light-harvesting, and other applications.[2] Microporous MOFs are now commercialized, but the standard synthetic procedures, involving an excess of organic solvents and harsh reaction conditions, still prevent their wider industrial application.

Here we present how mechanochemical reactions,[3], i.e. reactions between solid reactants induced by mechanical force, can be used for a rapid, sustainable, and controllable transformation of environmentally safe precursors into relevant microporous MOFs, such as MOF-74[4] or zirconiumbased MOFs of UiO[5], NU-[6], and PCN-[7] families. It is particularly suitable for the preparation of their multi-metal or amorphous derivatives by using only a catalytic amount of green liquids, such as alcohols or water. Direct monitoring by powder X-ray diffraction [8] revealed that the mechanochemical formation of MOFs often proceeds through intermediate phases, most of which are inaccessible from solution procedures. It is possible to isolate and characterize these intermediates and use them for the controllable synthesis of non-conventional MOFs, such as various bimetallic MOF-74 materials,[9] with interesting magnetic properties and strong potential for new catalytic reactivity.

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## The optical response of the quantum material family BaCoS<sub>2</sub>-BaNiS<sub>2</sub>

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BaCoS<sub>2</sub> and BaNiS<sub>2</sub> are the end members of a solid solution that shows a vast array of quantum properties. The Co material is a strongly correlated insulator with an antiferromagnetic transition, as well as a structural phase transition, around room temperature. At 28% Ni doping the solution undergoes an electronic metal-insulator phase transition to a Drude metal. The metallicity persists all the way to the pure Ni compound, where in addition to the Drude metal, we observe a strong contribution from bands with linear dispersion at the Fermi level. These will give origin to dispersive Dirac nodal lines. We performed optical conductivity measurements combined with abinitio calculations to reverse engineer the role of each band in the physical response of these materials. We explained uncommon features in their optical response such as a linear dispersion of the optical conductivity [1] and the existence of an isosbestic line separating a spectral-weight transfer across Dirac nodal states [2].

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# Mott Quantum Critical Points at finite doping

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We demonstrate that a finite-doping quantum critical point (QCP) naturally descends from the existence of a first-order Mott transition in the phase diagram of a strongly correlated material.

In a prototypical case of a first-order Mott transition the surface associated with the equation of state for the homogeneous system is "folded" so that in a range of parameters stable metallic and insulating phases exist and are connected by an unstable metallic branch.

Here we show that tuning the chemical potential the zero-temperature equation of state gradually unfolds. Under general conditions, we find that the Mott transition evolves into a first-order transition between two metals, associated to a phase separation region ending in the finite-doping QCP. This scenario is here demonstrated solving a simple multi-orbital Hubbard model relevant for the Iron-based superconductors, but its origin - the splitting of the atomic ground state multiplet by a small energy scale, here Hund's coupling - is much more general. A strong analogy with cuprate superconductors is traced. [1]

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# Harmonic Nanoparticles: from Multiorder Nonlinear Mixing to Blood Flow Imaging at GHz Pixel Rate

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Whereas most of the reports on the nonlinear properties of micro- and nanostructures address the generation of distinct signals, such as second or third harmonic, we recently demonstrated that the novel generation of dual output lasers developed for microscopy can readily increase the accessible parameter space and enable the simultaneous excitation and detection of multiple emission orders such as several harmonics and signals stemming from various sum and difference frequency-mixing processes.[1] This rich response, which in our case features 10 distinct emissions and encompasses the whole spectral range from the deep ultraviolet to the short-wave infrared (SWIR), is demonstrated using various metal-oxide nanomaterials (harmonic nanoparticles, HNPs) while being characterized and simulated temporally and spectrally. Together with spectral flexibility, the quasi-instantaneous response of parametric signals by HNPs can be exploited to increase imaging speed attaining dwell times shorter than fluorophore lifetimes. In this context, we demonstrate the detection and in-flow imaging of cells labelled by HNPs within whole, unfiltered blood by high-speed SLIDE [2] microscopy at the disruptive speed of 16'000 images per second (1 GHz pixel rate). This novel approach is presented in the context of stem cells monitoring for regenerative medicine procedures.

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# Quantum Manipulation of Graphene Edge States in Atomically-defined Nanoribbons

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Magnetic states in graphene nanostructures have undergone intense theoretical scrutiny, because their coherent manipulation would be a milestone for spintronic and quantum computing devices. In nanoribbons, experimental investigations are however hampered by lack of the required atomic control of the edges, and that the proposed graphene terminations are chemically unstable. Several questions remain thus unsolved: how can molecular spins be assembled into hybrid structures? What is the influence of the graphene environment on the spin? Can molecules be used to control coherent currents in graphene devices? Here we try to provide an answer to these questions, exploring spingraphene interactions by using molecular magnetic materials.

Here we show our results using bottom-up shaping of graphene, first by graphene nanoribbons made via molecular routes. We observe the predicted delocalized magnetic edge states, and comparison with a non-graphitized reference material allows clear identification of fingerprint behaviours.[1] We quantify the spin-orbit coupling parameters, define the interaction patterns, and unravel the spin decoherence channels. We then show how such molecular structures can be included into molecular devices, producing ultra-clean nanoscale devices[2] where single spin levels can be investigated[3] and where magnetoresistive effects run are opposite to non-molecular devices.[4] Even without any optimization, the spin coherence time is in the  $\mu$ s range at room temperature, and we perform room temperature quantum inversion operations between spins [5,6,7].

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## Atomic localization in many-particle reinterpretation of chemical bonding

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We analyze [1] two-particle binding factors of  $H_2$ , LiH, and HeH<sup>+</sup> molecules/ions with the help of our original exact diagonalization *ab intio* (EDABI) approach [2]. The interelectronic correlations are considered rigorously within the second quantization scheme with a restricted basis of renormalized single-particle wave functions, i.e., with their size readjusted in the correlated state.

We determine the many-particle covalency and ionicity factors in terms of the microscopic single-particle and interaction parameters, which are also predetermined within our method. We discuss limitations of those basic characteristics and introduce the concept of partial atomicity (*Mottness*), corresponding to the Mott-Hubbard criterion concerning the localization threshold in those many-particle systems. This addition introduces atomic ingredient into the collective electron states and thus eliminates a spurious behavior of the covalency with the increasing interatomic distance, as well as provides a physical reinterpretation of the bonding.

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# THIN FILMS OF SOLVATOMAGNETIC CN- BRIDGED COORDINATION POLYMERS: FROM MICRO TO NANOSCALE

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Molecular magnets exhibit many properties not found in conventional metallic magnetic materials, such as sensitivity to external stimuli e.g. light, pressure, temperature, magnetic field, or chemical modifications. A particularly interesting group of molecular magnets are solvatomagnetic compounds, in which magnetic properties are altered under the influence of the removal, introduction, or exchange of solvent molecules in the crystal lattice [1-2]. Porous magnets and magnetic sponges are potential chemosensitive switches and provide valuable insight into magneto-structural correlations.

In this report, two types of thin films of microporous CN-bridged hybrid organic-inorganic  $\{[Ni^{II}(cyclam)]_3[M^{III}(CN)_6]_2 \cdot nH_2O\}_n$  (M= Cr or Fe, cyclam= 1,4,7,11-tetraazacyclotetradecane) coordination networks will be presented. The films were obtained by using physical and chemical deposition techniques. In the first approach, the pre-formed nano-sized crystallites from water suspension were deposited on the PET/ITO substrate. As a result, films of 1-2 µm thickness composed of 40-200 nm size particles were obtained. As an alternative, the chemical sequential growth method was implemented, in which the coordination framework is anchored to the gold surface and built directly on the substrate from cationic and anionic building blocks. Finally, the films of reduced thickness (ca. 100 nm) and drastically improved morphology were obtained. Both types of thin films show solvatomagnetic behavior characteristics for bulk compounds and change magnetic characteristics, including the shape of the magnetic hysteresis, under different humidity conditions.

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## Nodal-line driven anomalous susceptibility in ZrSiS

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We shall present our recent study on the nodal-line Dirac system ZrSiS and our unique approach to test the signature of the nodal-line physics by thermodynamic methods. By measuring magnetic susceptibility in ZrSiS, we found an intriguing step-like temperature-driven transition from dia- to paramagnetic behavior. We show that the anomalous behavior represents a real thermodynamic signature of the underlying nodal-line physics through the means of chemical pressure (isovalent substitution of Zr for Hf), quantum oscillations, and theoretical modelling. The anomalous part of the susceptibility is orbital by nature. It arises due to the vicinity of the Fermi level to a degeneracy point created by the crossing of two nodal lines. Furthermore, an unexpected Lifshitz topological transition at the degeneracy point is revealed by tuning the Fermi level. The present findings in ZrSiS give a new and attractive starting point for various nodal-line physics-related phenomena to be tested by thermodynamic methods in other related materials.

# Interplay of various order parameters and disorder in iron chalcogenides

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Since the discovery of iron-based superconductors over a decade ago large efforts are directed towards uncovering the primary order parameter determining the properties of these materials. However, the abundance of various low-temperature phases observed experimentally suggests that there may be no single order parameter, instead, many degrees of freedom, including nematic, spin, charge, or orbital degrees of freedom, are strongly intertwined. In addition, these materials are prone to various forms of disorder, which influences the nature of the ground state.

In this talk, I will summarize several years of our studies of iron chalcogenide system, FeTe<sub>1-x</sub>Se<sub>x</sub>, in which the disorder is introduced intentionally by two different methods, substitution of transition metal element, Ni, into Fe-site, and by changing the crystallization rate during the crystal growth. This last method introduces either excess, or deficiency of the Fe, what affects both the crystal quality, and superconductivity, with the surprising result that the superconductivity is enhanced in crystals of inferior crystallographic properties [1].Over the years, we have used various experimental probes to understand this behavior, including transport [2], photoemission [3], and, most recently, magnetization and angular magnetoresistance experiments. I will combine the results of these experiments and discuss how the interplay of nematicity, spin fluctuations, and disorder-induced doping affects ground state properties of this system.

The work done in collaboration with I. Zajcewa, K.M. Kosyl, A. Lynnyk, and D. J. Gawryluk. Supported by Polish NSC grant 2014/15/B/ST3/03889. The research was partially performed in the laboratory co-financed by the ERDF Project NanoFun POIG.02.02.00-00-025/09.

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#### Gate tunable supercurrent in the epitaxial superconducting shell in Ta/InAs nanowires

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Integrated circuits with superconducting building blocks would have several benefits, such as high speed and low power consumption. In recent years, surprisingly, gate control of the supercurrent in all-metallic transistors has been observed. This phenomenon can be used to fabricate gate controlled transistors from superconducting materials, analogous to the field effect transistors. The suppression of the supercurrent was investigated in several materials however there is no scientific consensus on the microscopical explanation [1-3]. In this work, we studied gate tunable supercurrents in Ta superconducting shells epitaxially grown on the top of of InAs nanowires. The investigated device switches from superconducting state to normal state by applying  $\sim \pm 5$  V on the gate, which is really promising for standard electronical applications. Magnetic field dependence and switching current distribution measurements suggest that the gating effect does not stem from a simple thermal heating. Moreover, electric field driven collapse of superconductivity is not consistent with our experimental findings, however out of equilibrium phonon generation in the substrate is more likely to be the origin of this effect in our device.

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# Far-infrared and annealing studies of thermal donors in high-purity silicon

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We have measured the temperature-dependent infrared transmission of high-purity silicon samples having impurity concentrations of ~ $10^{15}$  /cm<sup>3</sup>. Measurements were made in a frequency range from 10–10,000 cm<sup>-1</sup> at temperatures from 10–300 K. At 10 K, silicon is transparent in the far infrared (10–600 cm<sup>-1</sup>) apart from narrow absorption lines caused by residual oxygen impurities known as thermal double donors (TDD). At higher temperatures, the electrons are ionized by the thermal energy in the crystal and become free electrons, causing a Drude-like response in the far infrared. There is also absorption caused by several vibrational modes of Si<sub>2</sub>O in the far and mid infrared regions. The oxygen is introduced by the amorphous silica crucible during the Czochralski growth process and occurs as an uneven distribution of oxygen throughout the boule. Samples were annealed between 450-700 C in vacuum and a significant effect on the TDD oxygen but not on the vibrational oxygen concentration was observed. This leads us to believe that the thermal history of the boule plays an important role in determining the structure of the oxygen impurity.

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# Tuning of charge density waves in correlated metals - New results and insights

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Transition metal compounds in which electrons from partially filled d-shells strongly interact with each other keep challenging the standard theory of solids as new, emergent exotic electronic orders are experimentally observed. Despite vastly different macroscopic properties, *e.g.* high temperature superconductivity (HTS), electronic nematicity or density waves to cite a few, the electronic phases encountered in these quantum materials can be almost degenerate and compete with each other within complex phase diagrams. The crystal lattice is more than a mere spectator. It can be used to tune the subtle interplay between charge, spin, orbital and lattice degrees of freedom that controls such competing electronic states and thereby to learn more about the microscopic mechanisms underpinning their stabilization.

I will show how the combination of pressure (hydrostatic or uniaxial) tuning and x-ray spectroscopy has been used in the course of the last decade to gain fresh insights on the properties of charge density waves (CDW) in high temperature superconducting cuprates [1-3].

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# Spin chirality driven by thermal fluctuations in correlated paramagnets

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Chirality is an ubiquitous concept in the natural sciences, distinguishing left- and right-handed objects or processes. In magnetic solids, the chirality of spin textures is derived from the twisting habit of neighboring atomic spins [1-3]. I will discuss dynamical processes, specifically thermal fluctuation processes, which are transient but generate a net chiral habit in a magnetic solid. Through their coupling to local magnetic moments, conduction electrons feel this chiral habit; hence, (thermo-) electric transport coefficients, which are time-averaged quantities, allow us to distinguish two scenarios:



(1) Short-range spin correlations, where a small cluster of magnetic moments is sufficient to describe the physical properties of the thermally disordered solid [4,5] and

(2) Longer-range correlations, such as dynamically nucleating and decaying topological defects [6].

I introduce toy model systems which realize Kagome and triangular lattices of magnetic moments, and discuss the role of lattice geometry in promoting these fluctuation phenomena [7]. Finally, I will show that the thermal Hall effect of magnetic insulators can also have a contribution related to thermal fluctuations of spin-chiral nature [8].

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# Spin Centres in Crystals: Quantum Sensors and Quantum bits

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Spin centres in crystals are promising candidates for the creation of quantum sensing, computing, and communication technology [1].

Nitrogen-vacancy (NV) centres in diamond have risen to prominence as quantum sensors as they offer biocompatibility, bright photoluminescence, and long spin coherence at room temperature [2]. Developing these systems towards practical sensor devices is underway, but the collection of photoluminescence for optical readout remains too cumbersome and costly for many applications. Recently, it has been shown that their quantum state can also be read out electrically, which constitutes a large step towards compact, integrated devices. This method has been used to measure the state of a single electronic spin, and even to observe the spin state of a single atomic nucleus [3,4].

Communication between such spin centres can be used to build quantum networks and quantum computers. The optical transitions of NV centres are not ideally suited for this purpose, mainly because of their emission in the visible domain which leads to scattering losses and is not compatible with optical fiber networks [1]. Other spin centres are therefore under investigation which may be better suited for such applications, such as the vanadium centres in silicon carbide (SiC). This family of defects is of great interest because of their telecom-range optical transitions and their rich spin structure [5]. The presentation will cover progress on investigation of the optical and spin properties of vanadium in SiC, with a view towards spin polarization and control, integration into photonic structures such as high-finesse microcavities, and the creation of long-distance quantum networks [6–8]. A long spin relaxation lifetime is one of a set of advantageous features which make vanadium a strong contender for such applications [9].

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# **MAGNETO-OPTICS OF VAN DER WAALS ANTIFERROMAGNET FEPS3**

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Research on magnetic materials currently constitutes a significant part of current activities in condensedmatter physics. Both experimental and theoretical studies are motivated by the scientific curiosity to uncover new phenomena, and also, triggered by the possible design of novel spintronic devices. Among current trends in the spintronic developments, there are many attempts to exploit antiferromagnetic materials (instead of ferromagnets), to work with 2D systems rather than with bulk crystals, as well as attempts to control the magnetic order in solids by means of light. These ideas have stimulated our magnetooptical studies of largespin (Fe<sup>2+</sup>, S=2) quasi-2D antiferromagnet FePS<sub>3</sub>. In this material, magnetic excitations (one-magnon gaps) have relatively large energies, and therefore, their interaction with light may be explored using techniques of THz and infrared magneto-spectroscopy.

In the present work, we report on THz/infrared magneto-spectroscopy and magneto-Raman studies of FePS<sub>3</sub>. Applying a magnetic field, we tune the one-magnon-gap excitation to coincide with the phonon modes. Hybrid magnon-phonon modes, the magnon polarons are unveiled with the demonstration of a pronounced avoided crossing between the otherwise bare magnon and phonon excitations. At higher photon energies, our data reveal a novel magnetic excitation. When a magnetic field is applied, it closely resembles semi-classical antiferromagnetic resonance in easy-axis antiferromagnets, nevertheless, the observed Zeeman splitting is four-times larger. We interpret this mode in terms of a longitudinal magnon excitation. This corresponds to a full reversal of a single iron spin in the magnetic lattice and thus carriers a total angular momentum of  $S_z = 4$ . We argue that condensation of such longitudinal magnons may lead to new and exotic multipolar states.

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# Size-dependent Electronic Properties of Strongly Confined Graphene Quantum Dots

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Laboratory for Advanced Materials (LAM) is a newly established research laboratory at the Faculty of Natural Sciences at Comenius University in Bratislava, Slovakia, supported by the European Commission under the Horizon 2020 program, the ERA Chair scheme. In the first part of my presentation, I will give a brief overview of the laboratory and the research areas the laboratory focuses on. In the second part of my talk, I will discuss in more detail our progress in one of the research areas, namely studies of strongly-confined graphene quantum dots (GQDs). I will present a new method for preparation of uniform ensembles of small (<2 nm) GQDs, using a systematic bottom-up step-wise synthesis. The new approach facilitates quantitative investigation of the effect of quantum confinement effect on the electronic structure of the GQDs using readily accessible ensemble level techniques. Using these techniques, we experimentally show how the bandgap, valence and conduction band offsets, exciton binding energies and densities of states systematically vary with the size in these strongly confined GQDs. The interpretation of the experimental results is supported by detailed DFT modelling. Experimental results indicate that the standard Dirac fermion model and tight-binding modelling approach do not adequately describe the electronic properties of GQDs in the strongly confined regime, which is attributed to stronger carrier-carrier interactions in the GQDs compared to the bulk graphene. Raman spectroscopy studies reveal that even the small GQDs show key D and G spectral features characteristic for periodic graphene structures and that the variation in the ratios of the corresponding band intensities (ID/IG) with the GQD size is in good agreement with previous studies of highly defected large area graphenes. This work was financially supported by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 810701 and by the Los Alamos Laboratory Directed Research and Development (LDRD) Program.

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## Dual character of the cuprate strange metal

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In this presentation, I will describe my group's recent studies of the (magneto)-transport properties of hole-doped cuprates across the strange metal regime in high magnetic fields up to 70 Tesla. By investigating three distinct families of hole-doped cuprates -  $Tl_2Ba_2CuO_{6+\delta}$ ,  $La_{2-x}Sr_xCuO_4$  and  $La/Pb-doped Bi_2Sr_2CuO_{6+\delta}$  – a common picture begins to emerge of two charge sectors coexisting within the strange metal phase of overdoped cuprates, one harboring coherent Landau quasiparticles, the other incoherent 'Planckian' dissipators. Curiously, as the contribution from the latter grows with reduced doping, so too does the superconducting condensate. Finally, a link is established between the quadrature scaling of the magnetoresistance at high field strengths and the so-called separation of lifetimes seen at low-fields.

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# **DESIGNING SUPERCONDUCTIVITY IN NANOWIRES**

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As the diameter of a superconducting nanowire approaches the coherence length, its superconducting state becomes increasingly sensitive to factors such as the disorder, texture, non-equilibrium effects and details of the interfaces with other materials. While this may present a difficulty for some applications, it also provides an opportunity for controlled manipulation of quantum states that is essential for creating tunable quantum devices. Full understanding and control of the physics at the interfaces is essential to understanding and control of the quantum state of a nanowire that may by dominated by such interfaces. I will describe a nanoprinting method for fabrication of ultranarrow nanowires with unprecedented control over their physical texture and will show how tunable interfaces with graphene and topological materials lead to unusual transport properties.

## Exploring polar order in oxide heterostructures by optical second harmonic generation

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Oxide heterostructures hosting ferroelectric materials have emerged over the last decade as a promising platform for energy-efficient electronics. However, determining the polarization direction, magnitude and domain configuration, as key properties in applications, remains a challenge in ultrathin layers and multilayers. We seek to illuminate polar order arising in oxide heterostructures using a non-invasive nonlinear optical method – second harmonic generation (SHG). With this approach, we facilitate the integration of BaTiO<sub>3</sub>-based superlattices on technologically relevant silicon by detecting the polarization state in the ferroelectric layer in dependence of its environment. We find that the out-of-plane polarization of BaTiO<sub>3</sub> is substantially enhanced in an asymmetric environment of tricolor superlattices in comparison to BaTiO<sub>3</sub> single films and standard bicolor superlattices. Using SHG, we identify the phase coexistence of the multi-domain phase with in-plane ordering and the vortex phase [2]. We furthermore find interlayer coupling between ferroelectric layers leading to an antiparallel alignment of local polarization in neighboring layers. Our findings pave the way towards using non-invasive techniques for monitoring the evolution of polar order operando.

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# Reversing the brain drain to promote scientific excellence in Eastern Europe

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Despite numerous measures on EU level to fight brain drain many intellectuals in Eastern European countries are still leaving to the West. The main problem is not that scientists and intellectuals are leaving to go abroad to work under better conditions — that is certainly beneficial for science as a whole. Rather, the problem occurs when they do not return.

For many years, EPFL has been participating in the so-called "Tenure Track Pilot Program" [1], which is administered by the Croatian Science Foundation and offers young talents the opportunity to build their careers as assistant professors at a Croatian academic institution. The program is based on the EPFL tenure track model and is adapted to local needs. Initial results and findings from the mid-term evaluation will be discussed in the presentation.

Recently, EPFL together with ETHZ helped creating a new institute called INSAIT on computer science and artificial intelligence as part of Sofia University in Bulgaria [2]. INSAIT's mission is to transform the world through excellence in science, research, and education by offering outstanding working conditions. The Bulgarian government supports INSAIT with 85 M€ over ten years. Key components, thoughts and hopes of INSAIT will be discussed during the presentation.

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# ZEEMAN DRIVEN SUPERCONDUCTOR INSULATOR TRANSITION IN STRONGLY DISORDERED MoC FILM. STM AND TRANSPORT STUDIES IN TRANSVERSE MAGNETIC FIELD.

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Low temperature STM and transport studies on ultrathin polycrystalline MoC films provide evidence that, in contrast to the previously studied TiN, InO<sub>x</sub> and NbN films, where the bosonic scenario of the superconductor-insulator transition is found upon increased disorder, unambiguous signs of the fermionic scenario are present [1].

In this presentation we study the transverse magnetic field induced superconductor-insulator transition in strongly disordered 3 nm thin MoC thin films, where the level of disorder approaches its critical value [2]. Surprisingly, the Zeeman paramagnetic effects dominate over orbital coupling on both sides of the transition. In superconducting state it is evidenced by a high upper critical magnetic field  $B_{e2}$ , by its square root dependence on temperature, as well as by the Zeeman splitting of the quasiparticle density of states (DOS) measured by scanning tunneling microscopy. At  $B_{e2}$  a logarithmic anomaly in DOS is observed. This anomaly is further enhanced in increasing magnetic field, which is explained by the Zeeman splitting of the Altshuler-Aronov DOS driving the system into a more insulating or resistive state.

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# Numerical Modeling of an Optoelectronic Stimulation Device in Contact with a Single Neuron

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In this work we electrically characterise an organic optoelectronic stimulation device and construct a realistic equivalent circuit model that reproduces important device parameters such as the dependence of open circuit potential and short circuit current on illumination intensity. The device is based on two organic pigments, metal-free phthalocyanine (H<sub>2</sub>PC) and N,N'-dimethyl perylenetetracarboxylic diimide (PTCDI) thermally deposited on the semi-transparent ITO back electrode. We use the constructed equivalent circuit to test the ability to stimulate a single CA3 pyramidal neuron cultured on top of the optoelectronic device. For that purpose, we developed a 3D FEM model of the CA3 pyramidal neuron along with realistic voltage-gated ion channels governed by Hodgkin–Huxley equations on the neuron membrane. We explore important parameters that determine the probability of successful stimulation including the distance from the device to the neuron and the illumination intensity.

# Evolution of the Hall-coefficient, dc-resistivity and Fermi-surface in Cuprates

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Cuprates exhibit a number of unusual properties, including the highest superconducting transition temperatures at ambient pressures known today. Despite tremendous research efforts, there is no consensus regarding the understanding of these compounds, except in two limits: at zero doping (parent compounds) and in the highly overdoped regime. The parent compounds are charge-transfer insulators, while at high doping levels they behave as a Fermi liquid with 1 + p itinerant carriers.

Only recently it has been revealed that the itinerant charges preserve their Fermi-liquid nature across the phase diagram, without a change of the scattering rate and effective mass [1]. Consequently, the complexity of cuprates is due to a gradual (de)localization of exactly one hole per  $CuO_2$  unit [1, 4]. Such an evolution implies the opening of a partial gap at the Fermi surface, not its reconstruction.

Here we show that the transport coefficients correspond to the ungapped parts of the Fermi surface, which are directly observed by photoemission spectroscopy. We use tight-binding parametrisations of measured ARPES spectra of HgBa<sub>2</sub>CuO<sub>4+ $\delta$ </sub>[2, 6], Tl<sub>2</sub>Ba<sub>2</sub>CuO<sub>6+ $\delta$ </sub>[3, 5] and La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> (LSCO)[7] to calculate the Hall-coefficient and dc-resistivity, where we consider only those parts of the Fermi surface which are not gapped. We find an excellent agreement between our model and measured values. This is particularly interesting in the case of LSCO which exhibits a complex evolution of the Fermi surface topology. Namely, LSCO undergoes a Lifshitz transition thereby strongly altering the Hall-response, an effect which is fully captured by our approach.

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## Synthesis, structural, magnetic and optical properties of (Bi<sub>1-x</sub>Ho<sub>x</sub>)-ferrites

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Magnetoelectric multiferroics, due to simultaneous ferroelectric and ferromagnetic ordering, have attracted wide attention in recent years, offering a wide range of potential applications in data storage media, spintronics and multi-state memories [1]. One of the wellknown materials exhibiting such properties is bismuth ferrite (BFO) BiFeO<sub>3</sub>. Because of the technological progress in the direction of nanotechnologies our interest is to obtain this compound in a form of nanoparticles. Since those particles are thermodynamically stable only in a very narrow temperature interval, the main challenge is to obtain a high-quality, uniform, single-phase material. Here we report the hydrothermal synthesis of BFO and Bi<sub>1-x</sub>Ho<sub>x</sub>FeO<sub>3</sub> ultrafine nanopowders, with a diameter of ~ 300 nm with no tendency to agglomerate. The diffraction patterns show that all obtained particles belong to the R3c space group. Regularity of the particle's geometric shape was demonstrated by Scanning electron microscopy (SEM), while the high-resolution transmission electron microscopy (HRTEM) reveals an excellent crystallization with non-fragmented surfaces. Individual grain analysis confirmed the existence of an ultra-fine crystal structure, with an interplane distance of 0.297 nm (d = 0.297 nm), which corresponds to (012) crystal planes. Magnetometry revealed a magnetic phase transition at  $T_N$ = 220 K, from a paramagnetic to canted antiferromagnetic phase. Doping with Ho increased the value of magnetization showing that weak ferromagnetic moment grows with the introduced defects, originating from the non-compensated magnetic moments due to the distortions of both the spin-cycloid order and the super-exchange bridges. Both distortions promote the additional spin-canting and increase the magnetization. The optical properties of the material were examined by the spectroscopic ellipsometry method and the energy gap was found to be 2.71 eV. Using the structure prediction method, which is based on the bond valence calculations, 11 additional perovskite-related structure candidates in different space groups were obtained, including a novel tetragonal BiFeO<sub>3</sub> phase which has never been reported before. With this, we have demonstrated that the hydrothermal method has good potential in obtaining BFO, for achieving better properties for the multiferroic application and offers an overall conclusion that the local magnetic properties of nanoparticles mainly depend on the particle size and their diverse morphology due to the different preparation methods and annealing temperatures.

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# DETECTION AND MANIPULATION OF ANTIFERROMAGNETIC ORDERS VIA THE MAGNETOELECTRIC EFFECT

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The concept of utilizing antiferromagnets (AFMs) in spintronic devices has attracted much attention recently. AFMs are appealing as the absence of net magnetization eliminates crosstalk between neighboring domains, the rich variety of antiferromagnetic orders offers new possibilities to encode information and their THz dynamics enables much faster manipulation compared to ferromagnets. However, the detection and manipulation of AFMs are notoriously difficult with the conventional methods that are based on the magnetization.

When the antiferromagnetic order breaks not only the time-reversal but also the spatial inversion symmetry, the magnetoelectric (ME) effect becomes allowed. This cross-coupling provides a new handle on the antiferromagnetic state. Moreover, in these compounds, the electric and magnetic dipoles are entangled at finite frequencies as well, thus, intriguing optical effects such as non-reciprocal light absorption and polarization rotation also emerge.

In this talk, we present our efforts to use these optical ME effects to detect antiferromagnetic orders. Using THz spectroscopy, we studied the antiferromagnetic resonances of LiCoPO4, an antiferromagnet with finite toroidal moment [1,2]. We found that some of the spin excitations are simultaneously electric and magnetic dipole active and show strong non-reciprocal light absorption. By cooling the sample in crossed electric and magnetic fields, we switched between the antiferromagnetic domains exhibiting different light absorption. In the easy-plane AFM, Ba2CoGe2O7, we also detected strong non-reciprocal light absorption in the THz frequency range [3]. The soft antiferromagnetic structure of this compound allowed us to demonstrate the in situ electric field control of the antiferromagnetic state.

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#### Low-dimensional materials: from lab to industry

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Current and emerging trends in social media, virtual and augmented reality, autonomous vehicles, big data and artificial intelligence are driving inflections in the semiconductor industry, which requires materials enabled 3D NAND, innovations in transistors and interconnects for advanced node devices and sophisticated circuit patterning approaches that use materials engineering to shrink devices. For the continuous innovation of advanced materials, an integrated development of chemistry, process and equipment has become imperative. In this talk, we will discuss our recent efforts on the implementation of novel nanomaterials – including two dimensional (2D) ultrathin films, one dimensional (1D) nanowires/nanotubes, and zero dimensional (0D) nanocrystals – into real-world applications.

First, I will discuss recent initiatives within the Applied Materials-NUS Advanced Materials Corporate Lab that combines Applied Materials' leading expertise in materials engineering and semiconductor technologies with NUS' world-class and multi-disciplinary R&D capabilities that span applied chemistry, materials science and microelectronics process engineering. This collaboration focuses on R&D in advanced materials engineering with the intent to create innovations that can be quickly transferred into commercial applications and serves as a model of collaboration between industry and academia. Furthermore, we will discuss a new type of freestanding down-conversion color filters based on colloidal 1D quantum dots for the next generation of high-resolution displays. Finally, I will discuss our efforts to tailor nanomaterials ondemand and with the atomic precision using highly focused ion- and electron-beams.

## Super exchange in artificial molecule coupled to a ferromagnet

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Exchange interaction is a key ingredient of strongly correlated electron systems. It plays important role in various fields of solid state physics like magnetic ordering, high temperature superconductivity or qubit operation. The magnetic ordering induced by exchange coupling depends on several parameters like the level position of atoms, their tunnel coupling to the neighbouring sites or coordination, which are fixed parameters in a crystal. Realizing artificial atoms and coupling them to ferromagnet opens a unique opportunity to modify these parameters and study the induced magnetic order on an individual atoms. In this contribution first we discuss the magnetic state of a single artificial atom coupled to a bulk ferromagnet: how the magnetic state of the atom can be measured and varied by parameters of the atom. Then we present our recent experimental results on an artificial molecule coupled to ferromagnet and show the presence of superexchange interaction. [1]

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# Designing opto-bioelectronic interfaces: from in-silico to in-vivo

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Designing effective bioelectronic devices such as neurostimulators or recording interfaces requires a multi-disciplinary integrative approach involving experts from materials science, electrical- and bio-engineering and medical science due to the complex nature of the problem. To bridge the gaps in understanding between those fields, we propose using integrated realistic numerical models of the bioelectronic device and the biological system as a non-biased mediator and as an alternative to expensive and sometimes ethically dubious in-vivo experiments.

State of the art in computing power and software development currently enables the integration of numerical 3D models of the stimulation device and the stimulation target. Such models could speed up the device development and reduce the costs involved with the repetitive invivo experiments. We will show a numerical model of an opto-bioelectronic stimulation device coupled with Hodgkin-Huxley's numerical model of a single neuron to study the suitability of our devices for single-cell stimulation. Based on the model's results, we will show guidelines and requirements for the successful stimulation of single cells, especially relating to the electrode material and electrochemical parameters. We will show how our simulation toolset can be applied to a more general class of bioelectronic interfaces.



Na channel conductivity during the firing of the action potential along the axon of a model neuron stimulated by a model organic electrolytic photocapacitor.
## The Role of Thermodynamic Confusion in Coarsening of Nanostructures

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The size distribution of particles, which is essential for many properties of nanomaterials, is equally important for the mechanical behavior of alloys whose yield and ultimate tensile strength are related to nanoscale precipitates. However, size distribution of particles formed by solid-state reactions is generally poorly controlled. This presentation will demonstrate an approach to forming highly monodisperse particle size distributions by simple solid-state reactions, involving the use of two-step heat treatment, whereby the core formed at high temperatures provides a template for growth of the shell at lower temperatures. If the core is allowed to grow to a sufficient size, the shell develops in a 'size focusing' regime, where smaller particles grow faster than larger ones. These results suggest new strategies for manipulating precipitate size distributions in similar systems through simple variations in chemical composition and thermal treatment. Formation of highly monodisperse particles can be perceived as a consequence of thermodynamic confusion of an alloy system and the delay of Gibbs-Thomson capillarity effect, contributing to high stability and resistance to coarsening of nanostructures. These phenomena have been studied by atomic resolution microscopy in tandem with first principal modeling and simulation applied to AlLiSc model system.

# Charge order and the Fermi surface reconstruction in cuprate superconductors

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A major difficulty in understanding high- $T_c$  systems is the complexity of the materials, the presence of strong electron-electron interactions, and their rich phase diagrams. We have employed synchrotron X-ray scattering to explore the electronic and structural degrees of freedom of complex materials, with the particular focus on the self-organized charge modulation, so called the charge density wave (CDW) order. Although its presence has been demonstrated within the CuO<sub>2</sub> plane of each family of cuprate superconductors [1], the extent of the CDW order as a function of doping, temperature, or magnetic field remains controversial.

I will present our results of the resonant X-ray scattering experiments in the model cuprate HgBa<sub>2</sub>CuO<sub>4+ $\delta$ </sub> (Hg1201). While resonant X-ray scattering (RXS) allowed us to establish the doping-temperature range of the static CDW or-der in this compound [2,3], resonant inelastic X-ray scattering (RIXS) enabled the discovery of the short range CDW correlations at temperatures exceeding the onset of the static correlations observed by RXS. Such coexistence of static and dynamic CDW correlations is consistent with theoretical predictions [4]. The following electronic transport measurements in magnetic fields up to 70 T allowed us to investigate the reconstruction of the Fermi surface by the CDW order. We found, that at low temperatures, the moderately doped cuprates undergo a phase transition to a reconstructed state, when sufficiently strong magnetic field is applied. This transition is associated to the folding of the Fermi arcs into an electron pocket [5].

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# MIXED COUPLED PLASMON MODES IN DIRAC ELECTRON SYSTEMS WITH DIFFERENT DIMENSIONALITIES

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We study the coupling between plasmon modes by the long-range Coulomb electron-electron interaction for a system consisting of a two-dimensional system of Dirac electrons embedded in threedimensional Dirac semimetal for various separations of the subsystems [1]. The plasmon mode in the three-dimensional Dirac semimetal has the optic dispersion, while the plasmon mode in the twodimensional system of Dirac electrons has the characteristic acoustic square-root dependence on the momentum. The mixing of the plasmon modes is achieved as the two-dimensional acoustic plasmon mode dispersion crosses the bulk plasmon mode. We find that the upper coupled plasmon mode increases from the bulk plasmon mode as the momentum increases and tends to the bare twodimensional plasmon at large momenta, while at the same time the lower coupled plasmon mode increases linearly from zero as the momentum increases and approaches the bare bulk plasmon mode at large momenta. The coupled plasmon modes become more separated with decreasing the separation between two subsystems as the coupling increases due to the enhanced Coulomb interaction between electrons from different subsystems. We also demonstrate how the coupling affects the spectral weights of the obtained modes in two subsystems for different separations. In addition, we study the effects of the Dirac cones tilts on coupled plasmon modes in both subsystems [2]. We show that the tilts of Dirac cones anisotropically increase the coupled plasmon mode energies and renormalize their spectral weights. The anisotropic effects of the tilt are more significant for larger separations of the subsystems.

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# Spin-Electric Coupling in Lead-Halide Perovskites

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Abstract body

Lead-halide perovskites enjoy a number of remarkable optoelectronic properties. To explain their origin, it is necessary to question how electromagnetic fields interact with these systems. We address this question here by studying two classical quantities: Faraday rotation and the complex refractive index in a paradigmatic perovskite CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub> in a broad wavelength range. We find that the minimal coupling of electromagnetic fields to the k·p Hamiltonian is insufficient to describe the observed data even on the qualitative level. To amend this, we demonstrate that there exists a relevant atomic-level coupling between electromagnetic fields and the spin degree of freedom. This spin-electric coupling allows for quantitative description of a number of previous as well as present experimental data. In particular, we use it here to show that the Faraday effect in lead-halide perovskites is dominated by the Zeeman splitting of the energy levels, and has a substantial beyond-Becquerel contribution. Finally, we present general symmetry-based phenomenological arguments that in the low-energy limit our effective model includes all possible couplings to the electromagnetic field in the linear order.

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## Spintronic Applications of Giant Rashba Effect in Bismuth Tellurohalides

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In the field of spintronics, efficient creation and manipulation of spin polarization without external magnetic fields is a key requirement for producing real-world devices, such as those based on spin-orbit torque (SOT), a potential technological successor of spin transfer torque.

Bismuth tellurohalides (BiTeX, where X is a halogen element), in addition to being layered semiconductors that can be used in 2D heterostructures, also exhibit giant bulk Rashba effect. The emerging spin texture allows for all-electric creation and manipulation of large spin polarization within the material by passing a bias current (the Rashba-Edelstein effect), a desirable feature for SOT applications. We experimentally demonstrate this in BiTeBr/graphene devices, using the graphene and conventional ferromagnetic contacts as nonlocal spin signal detectors.<sup>[1]</sup> The spin polarized carriers injected into graphene using a bias current can be confirmed to originate inside the BiTeBr crystal. In another work, BiTeI is successfully isolated in monolayer form and its stability in ambient conditions is confirmed.<sup>[2]</sup>

Tuning the carrier density in the material, by different growth techniques or by electrically gating few-layer devices, should enable significant enhancement of the achievable spin polarization. The inherent spin texture and electrically controllable polarization, without having to rely on proximity effects at the interface with another material, opens further avenues for applications in practical SOT-based devices.

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# DC and optical signatures of the reconstructed Fermi surface for electrons with parabolic band

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We study the main intra-band and inter-band transport properties at zero temperature of free electron-like system undergoing a topological reconstruction of the Fermi surface for the twodimensional and three-dimensional case. The calculated intra-band properties include the singleparticle density of states, the total and the effective concentrations of electrons and the thermopower. As for the inter-band case, the real part of the conductivity has been calculated within the vanishing inter-band relaxation approximation as a function of the incident photon energy. Within this approach, it is shown that the optical conductivity has a nonvanishing component parallel to the reconstruction wave vector and the shape which depends on the value of the Fermi energy. Each dimensionality has its particular features in the transport quantities which are discussed and compared with those in the free electron scenario. Finally, we identify the signature of the topological reconstruction of the Fermi surface in the intra-band and inter-band transport functions.

#### References

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