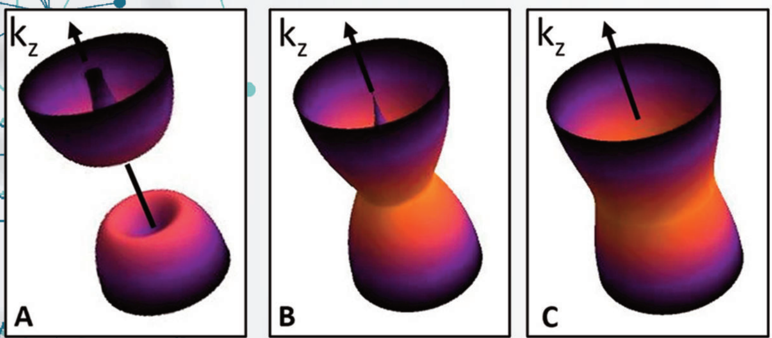
Topological Quantum Science



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* These authors presented the scientific reports collected in this book at the Topological Quantum Science Workshop – 76th Course of the Solid State Physics School, Erice, Italy on November 1-7, 2021

Papers presented at the
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Giorgio Benedek

EMFCSC President
Antonino Zichichi

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Topology and Ferromagnets

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Ferromagnetism breaks time reversal and inversion symmetries and can therefore substantially change the topological properties of electrons in materials. In addition, it introduces an additional type of quasi-particle, the spin wave, which itself can display interesting topological behaviour. Ferromagnetism can be induced through the Stoner mechanism or through proximity, the latter having been proposed as a method to produce the spin polarization needed for Majorana modes in semiconductor/superconductor heterostructures. There are thus numerous ways to engineer topological effects via ferromagnetism, and in this talk we describe some examples of such engineering.

Coupling Charge and Topological Reconstructions at Polar Oxide Interfaces

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In oxide heterostructures, different materials are integrated into a single artificial crystal, resulting in a breaking of inversion symmetry across the heterointerfaces. A notable example is the interface between polar and nonpolar materials, where valence discontinuities lead to otherwise inaccessible charge and spin states. This approach paved the way for the discovery of numerous unconventional properties absent in the bulk constituents. However, control of the geometric structure of the electronic wave functions in correlated oxides remains an open challenge. Here, we create heterostructures consisting of ultrathin $SrRuO_3$, an itinerant ferromagnet hosting momentum-space sources of Berry curvature[1], and $LaAlO_3$, a polar wide-band-gap insulator. Transmission electron microscopy reveals an atomically sharp $LaO/RuO_2/SrO$ interface configuration, leading to excess charge being pinned near the $LaAlO_3/SrRuO_3$ interface. We demonstrate through magneto-optical characterization, theoretical calculations and transport measurements that the real-space charge reconstruction drives a reorganization of the topological charges in the band structure, thereby modifying the momentum-space Berry curvature in $SrRuO_3$. Our results illustrate how the topological and magnetic features of oxides can be manipulated by engineering charge discontinuities at oxide interfaces[2].

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Magnetic field-induced non-trivial electronic topology in Fe_nGeTe_2

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Keywords: anomalous Hall, Nernst and thermal Hall, Bloch domain walls, Berry phase, anomalous and topological transport

The anomalous Hall, Nernst, and thermal Hall coefficients of the itinerant ferromagnet Fe_3GeTe_2 display several features upon cooling, like a reversal in the Nernst signal below $T = 50$ K pointing to a topological transition possibly associated to the development of bulk magnetic spin textures[1]. Since the anomalous transport variables are directly related to the texture of the Berry curvature, a possible topological transition might imply deviations from the Wiedemann-Franz (WF) law. This law has not yet been validated for the anomalous transport variables given that recent experimental studies yield contradictory, material-dependent results. Despite these features, the anomalous Hall and thermal Hall coefficients of Fe_3GeTe_2 are found, within our experimental accuracy, to satisfy the WF law for magnetic fields $\mu_0 H$ applied along its interlayer direction. Surprisingly, large anomalous transport coefficients are also observed for $\mu_0 H$ applied along the planar a-axis as well as along the gradient of the chemical potential generated by thermal gradients or electrical currents, a configuration that should not lead to their observation due to the absence of Lorentz force. These anomalous planar quantities are found to not scale with the component of the planar magnetization ($M_{\|}$), showing instead a sharp decrease beyond $\mu_0 H_{\|} = 4$ T which is the field required to align the magnetic moments along $\mu_0 H_{\|}$. We argue that locally chiral spin structures, such as skyrmions, and particularly spin spirals under planar fields, lead to a field dependent spin-chirality. In turn, this generates a novel type of topological transport in the absence of interaction between the magnetic field and elec-

trical or thermal currents. Locally chiral spin-structures are captured by our Monte-Carlo simulations incorporating small Dzyaloshinskii-Moriya and biquadratic exchange interactions. Our observations1 reveal not only a new way to detect and expose topological excitations, but also a new configuration for heat conversion that expands the current technological horizon for thermoelectric energy applications.
Time permitting, we will also discuss preliminary observations in the $Fe_{5-x}GeTe_2$ compound all the way up to room temperature[2].

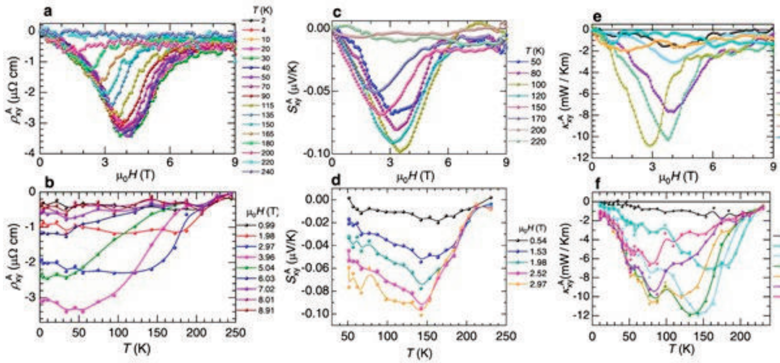

Figure 1: Field-induced maxima in the anomalous transport variables for currents and thermal gradients aligned along $\mu_0 H \parallel$ a-axis. (a) Anomalous Hall resistivity ρ^A_{xy} for a $Fe_{2.84}GeTe_2$ crystal as a function of $\mu_0 H$ applied along the a-axis and for several *T*s. ρ^A_{xy} displays a peak as a function of $\mu_0 H$ whose position is *T*-dependent. (b) ρ^A_{xy} as a function of *T* for several values of $\mu_0 H$ applied along a planar direction. (c) Anomalous Nernst effect SAxy as a function of $\mu_0 H$ along a planar direction for several *T*s. (d) S^A_{xy} as a function *T* collected under several values of the field applied along a planar direction. (e) Anomalous thermal Hall conductivity κ^A_{xy} as a function of $\mu_0 H$ applied along a planar direction and for several values of *T*. (f) κ^A_{xy} as a function of *T* and for several values of $\mu_0 H$ applied along a planar direction. The anomalous transport variables follow a similar dependence on magnetic field, which contrasts with the one followed by the magnetization.

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Measuring the Electron–Phonon Interaction in Two-Dimensional Superconductors and Topological Materials with He-Atom Scattering

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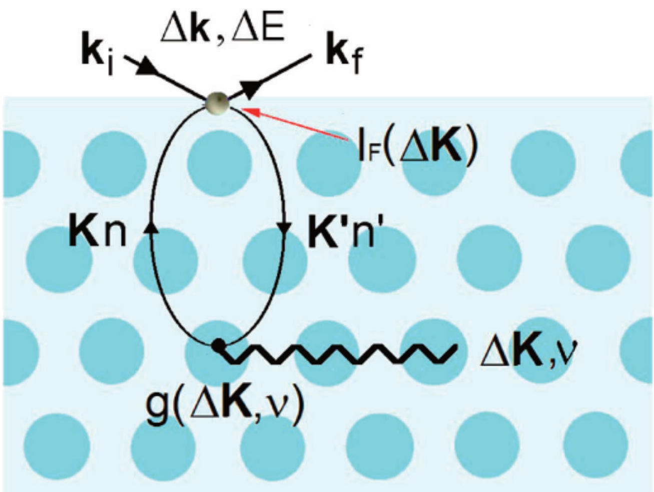
Helium-atom scattering (HAS) spectroscopy from conducting surfaces has been shown to provide direct information on the electron–phonon interaction, more specifically the mass-enhancement factor from the temperature dependence of the Debye–Waller exponent, and the mode-selected electron–phonon coupling constants from the inelastic HAS intensities from individual surface phonons. The recent applications of the method to superconducting ultra-thin films and layered topological chalcogenides is reviewed.



Resonant multi-gap room temperature superconductivity driven by Fano-Feshach resonance at Lifshitz electronic topological transition

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Tuning electronic topological transitions in complex materials generate novel electronic states of matter which are hot topics for new physics in Twistronics and in Superstripes, Supersolids and Supermetals [1-3]. We focus on the amplification of the superconducting critical temperature at a topological phase transition for the appearing of a new small Fermi surface with an energy dependent strong electron phonon coupling bacause of a Khon-anomaly or an incipient charge density wave instability [4-6]. Near the electronic topological transition the theory of superconductivity for overlapping BCS bands breaks down since multiple bands in the BCS regime, resonate with a single gap in the BCS-BEC crossover regime. The Bianconi-Perali-Valletta theory [7,8] proposed 25 years ago for hole doped cuprates [9,10] the material design of room temperature superconductors driven by a Fano-Feshbach resonance due to configuration interaction between multiple gaps in the BCS open pairing channel and the closed pairing channels in the BCS-BEC crossover, including the attractive Majorana or repulsive Heisenberg exchange interactions.
Here we propose that pressurized sulfur hydrides behave as a heterostructure made of a nanoscale superlattice of interacting quantum wires with a multicomponent electronic structure [4-6,9,10]. The high-order anisotropic van Hove singularity near the Fermi level observed in band

structure calculations of pressurized hydrides, typical of a supermetal, has been associated with the array of metallic hydrogen wires modules forming a nanoscale heterostructure at atomic limit called superstripes phase. We present a first-principles quantum calculation of the universal superconducting dome where T_c amplification reaches room temperature. The BPV theory predicts the top of superconducting domes in T_c versus pressure curves which is not predicted by standard superconductivity theories. In the proposed phase diagram, the critical temperature shows a three dimensional (3D) superconducting dome where T_c is a function of two variables (i) the Lifshitz parameter (η) measuring the separation of the chemical potential from the Lifshitz transition normalized by the inter-wires coupling and (ii) the effective electron phonon coupling (g) in the appearing new Fermi surface including phonon softening. Our results will be of help for material design of room temperature superconductors at ambient pressure.

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Topological effects in SnTe-class multilayers and nanowires

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Key words: SnTe nanowires, weak antilocalization

We investigate the topological properties of the low-energy states appearing at atomic steps [1,2] and magneto-transport across the topological transition in the multilayer Sn(Pb)Te(Se) compounds [3] as well as the (001) nanowires. We show that magnetic domain walls crossing atomic surface steps can support topological low-energy bound states that lead to similar tunneling conductance as Majorana zero-modes [2]. In this respect such steps behave similarly to the SnTe nanowires where we have also found topological end states at non-zero Zeeman magnetic field, both in the absence and in presence of superconductivity [4], see Fig. 1. In both cases topology is related with the non-trivial subspace degree of freedom, characteristic for the binary compounds, which can lead to in-gap end-states in one dimension [5]. For even SnTe multilayers we study quantization of the Berry phase along Fermi cross sections due to time-reversal and mirror symmetries to explain magnetoresistance in Pb(Sn)Se. We show by microscopic calculation of the Cooperon propagator that the Hikami-Larkin-Nagaoka formula can be generalized to account for mirror symmetry breaking to explain the emergent length scale present in samples covered by amorphous Se [3].

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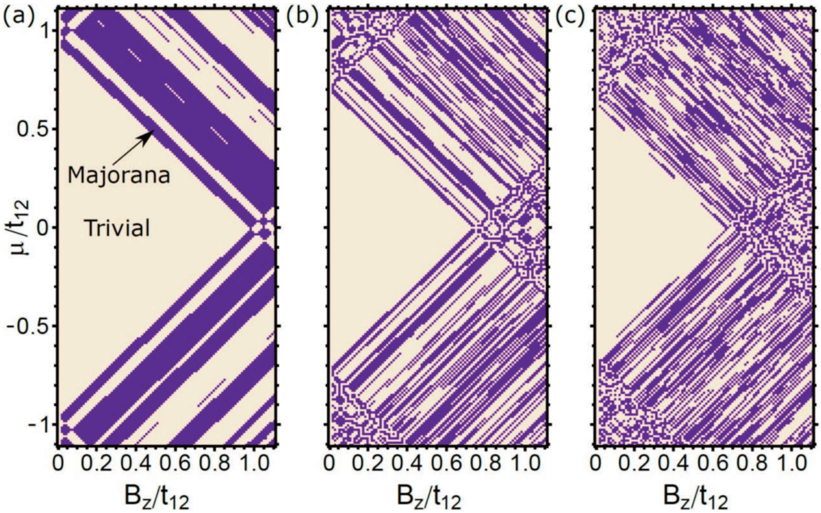

Figure 1: Topological phase diagrams for SnTe nanowires in presence of induced superconductivity. The thicknesses of the nanowires are (a) 8, (b) 10 and (c) 18 atoms.

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Robustness of Majorana-fermion states in one-dimensional structures

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Key words: Majorana fermions; topological superconductors; Rashba spin-orbit coupling; oxide interfaces

We investigate the properties of one-dimensional structures that may be tailored at the $LaAlO_3/SrTiO_3$ oxide interface by means of top gating. These structures are modeled via a single-band model with Rashba-type spin-orbit coupling, superconductivity and a magnetic field in the direction parallel to the one-dimensional chain. We discuss the conditions for the occurrence of a topological superconducting phase and the related formation of Majorana fermions at the chain endpoints, highlighting a close similarity between this model and the Kitaev model, which also reflects in a similar condition the formation of a topological phase. Solving the model in real space, we also study the spatial extension of the wave function of the Majorana fermions and how this increases with approaching the limit condition for the topological state. Using a scattering matrix formalism, we investigate the stability of the Majorana fermions in the presence of disorder and discuss the evolution of the topological phase with increasing disorder.

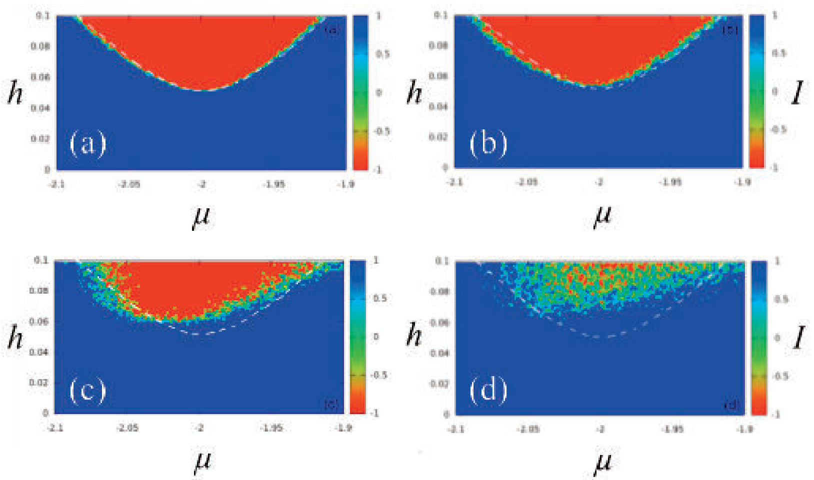

Figure 1: Sign of the topological invariant I, as a function of the chemical potential, μ, and of the Zeeman field, h, in a disordered chain with nearest neighbour hopping $t = 1$, Rashba spin-orbit coupling $\alpha = 0.1t$, superconducting gap $\Delta = 0.05t$, for a number of sites $N = 400$ and for different values the dimensionless disordered strength s. The topological region of the phase diagram appears in red. Panel (**a**): $s = 0.1$; Panel (**b**): $s = 0.2$; Panel (**c**): $s = 0.4$; Panel (**d**): $s = 0.6$. The white dotted curve represents the line separating the topological and non-topological phases in the absence of disorder (adapted from Ref. 1).

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Natural Superlattice Design of Quantum Materials

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Connecting theoretical models for exotic quantum states to real materials is a key goal in quantum materials synthesis. Two-dimensional model systems have been proposed to host a wide variety of exotic phases- historically a number of techniques have been used to realize these including thin film growth and mechanical exfoliation. We describe here our recent progress in experimentally realizing 2D model systems using bulk crystal synthesis including unusual superconducting and topological states. We discuss their structures and the new phenomena that they supported. We comment on the perspective for realizing further 2D model systems in complex material structures and their connections to other methods for realizing 2D systems.

Chasing the interplay between magnetism and topological states in the optical response of Na-doped $CaMnBi_2$

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Materials based on quasi two-dimensional bismuth layers $AMnBi_2$ (A = alkaline as well as rare earth atom) were recently designed and provide an arena for the investigation of low-energy quasiparticle excitations in topological materials, related to the rather elusive Dirac and Weyl fermions, and for the study of the interplay between anisotropic Dirac fermions, magnetism and structural changes. Our data on the optical reflectivity cover a vast spectral range extending from the far infrared up to the ultraviolet and were collected at different temperatures. We convey our most recent optical measurements of $Ca_{1-x}Na_xMnBi_2$ [1,2]. Besides observing a vestigial linear frequency dependent behaviour of the optical conductivity, which is reminiscent of electronic interband transitions involving Dirac bands [3], the asset of our work consists in experimentally revealing an incipient Fermi surface gapping, which strengthens with Na doping and turns out to pair with the anomaly in the dc transport properties, ascribed to the onset of a spin-canting within the antiferromagnetic order. The occurrence of a spin-canting is directly revealed by our own magneto-torque experiments. With the support of devoted first-principles band structure calculations, we conjecture that this latter (spin-canting) transition induces a substantial reconstruction of the electronic band structure. Our findings may generally underline the proneness towards FS instabilities in topological materials.

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Topology and Geometry in Superconductors

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Key words: superconductivity, topological matter, superconducting spintronics

Topological phenomena in superconductors reveal themselves as mid-gap Andreev bound states localized near interfaces or near topological defects. These can arise at edges of unconventional superconductors, near superconducting vortices [1], in superconductors exhibiting spin-orbit split energy bands [2], or in hybrid structures with spin-active materials [3-5]. If the number of mid-gap Andreev bound states is odd, then a topologically protected Majorana bound state exists. Thus, spin-polarized superconducting materials are promising not only for applications, but also as a playground for topological and geometric phenomena. The interplay between spin and superconducting order allows for geometric phases to be utilized in superconducting spintronics devices. The building blocks of such devices are spin-polarized Cooper pairs, which combine particle-hole and spin degrees of freedom, allowing for a high degree of flexibility and control.

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Nuclear magnetic resonance of three dimensional topological insulators

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Key words: Three dimensional topological insulators, nuclear magnetic resonance, band inversion

With their discovery in the late 2000ers, three dimensional topological insulators were rapidly experimentally confirmed with surface sensitive methods, especially ARPES, as suggested by Fu and Kane. A bulk probe like nuclear magnetic resonance (NMR) appears to be rather insensitive to the material's non-trivial band topology. However, in recent years, several NMR studies revealed a number of unexpected electronic phenomena in the model system Bi2Se3 and related compounds. For example, we were involved in proving special couplings among distant magnetic moments (1), as well as the characterization of an unusual rotation of the atomic scale charge symmetry by a magnetic field (2,3,4), which is poorly understood. We also showed that the inversion of the bulk energy band structure which distinguishes Bi_2Se_3 from a trivial insulator can simply be measured with NMR (2). We will discuss these effects in more detail including their measurements with NMR of quadrupolar nuclei in single crystal topological insulators.

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Time-reversal symmetry-breaking charge order in the kagome superconductor KV3Sb5

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The kagome lattice, which is composed of a network of corner-sharing triangles, is a structural motif in quantum physics first recognized more than seventy years ago. It has been gradually realized that materials which host such special lattice structures can exhibit quantum diversity, ranging from spin-liquid phases, topological matter [1,2], superconductivity [3], to intertwined orders. Recently, charge sensitive probes have suggested that the kagome superconductors AV_3Sb_5 (A = K, Rb, Cs) exhibit unconventional chiral charge order, which is analogous to the long-sought-after quantum order in the Haldane model or Varma model. However, direct evidence for the time-reversal symmetry-breaking of the charge order remains elusive. Here we utilize muon spin relaxation to probe the kagome charge order and superconductivity in KV_3Sb_5 [4]. We observe a striking enhancement of the internal field width sensed by the muon ensemble, which takes place just below the charge ordering temperature and persists into the superconducting state. Remarkably, the muon spin relaxation rate below the charge ordering temperature is substantially enhanced by applying an external magnetic field. We further show the multigap nature of superconductivity in KV_3Sb_5 and that the T_c/λ_{ab}^{-2} ratio is comparable to those of unconventional high-temperature superconductors. Our results point to time-reversal symmetry breaking charge order intertwining with unconventional superconductivity in the correlated kagome lattice.

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Complex phase diagram of the extended Falicov-Kimball model: possible hint for hidden order and topological phases

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Key words: extended Falicov-Kimball model, phase diagram, charge-order, exact results, intersite interactions, dynamical mean field theory

The Falicov-Kimball model is a simplified version of the Hubbard model, where only electrons with, e.g., spin down, are itinerant and the other are localized [1-3]. We discuss results for the extended Falicov-Kimball, which includes both on-site U and intersite V density-density interactions between particles occupying neighboring sites [4-7]. The model is studied at half-filling on the Bethe lattice in the large-dimension limit within the dynamical mean field theory formalism, which is an exact approach for this model [3-6]. In this approach, we found rigorous analytical expressions for the temperature-dependent density of states for interacting particles [4,5]. We identified the stability regions of eight different phases with long-range order, where the charge order coexists with the antiferromagnetic order (five of them are insulator phases and three of them are metallic phases) as well as three different disordered phases. In addition, we analyzed their thermodynamic properties [5-7]. These results were compared with those found using the standard Hartree-Fock broken symmetry approximation [6,7]. For small values of the interactions parameters, an anomalous temperature dependence of the order parameter can be observed, which is characterized by a strong reduction of its value at a temperature close to half of the critical temperature [6]. The detailed analysis of density of states of interacting particles reveals the inversion of subbands in the main energy gap [5], what can be a possible hint for the hidden order parameter or some topological effects.

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The role of Lewis base-alkali metal adducts in tuning of superconducting properties of intercalated iron monochalcogenides

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Key words: intercalated iron based superconductor, molecular intercalation, crystal structure, electron doping, layered iron selenides

Non-stoichiometric iron monoselenides, due to their specific layered structure and relatively weak bonding between Fe-Se sheets, are capable of accepting many types of inorganic and organic molecules (i.e. alkali metal ions, hydroxides, molecular alkali metal adducts with ammonia or amines, long-chain tetraalkylammonium cations) in their van der Waals gaps. This makes it possible to modify both the magnetic and electrical properties of the intercalated materials by appropriate selection of the electron-donating organic molecules, controlling the level of electron doping and the type / shape and orientation of organic molecules. In recent years, significant progress has been made in the field of intercalation chemistry, expanding the gallery of intercalated iron superconductors with novel inorganic-organic phases showing superconducting transition temperatures close to 50K. However, the role played by organic molecules in increasing the critical temperature of these materials is not entirely clear, especially in terms of their interactions with the chalcogenide matrix and the necessity of additional electron doping resulting from complexation of lighter alkali metals. For these reasons the research in this area is still ongoing involving utilization of organic molecules with a more complex architecture and different donating ability. The study attempts to systematize the existing knowledge in this field by finding relationships between the chemical structure of organic donors, their arrangement between the layers of the inorganic host, the necessity of electron doping achieved by complexing of selected alkali metals with organic donors and the influence of these factors on the superconducting properties of intercalated phases.

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Rashba Physics and topological order in FeSe: Determination of Fermi surface of FeSe monolayer by Landau level spectroscopy

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We described and discovered Rashba Physics and topological order in FeSe ~ Skyrmion Orbital Order. WE made a direct observation of Landau quantization by scanning tunneling spectroscopy for FeSe monolayer grown on graphene/SiC(0001) substrate. Using Landau level spectroscopy and quasiparticle interference (QPI), we found parabolic hole band and an elongated ellipse Fermi surface with a long and short axis ratio of 1.5 around Gamma point. We found also a non-parabolic electron band at X point, exhibiting unique Landau quantization behavior as En ~(nB)^{4/3}. With the method of symmetry invariants and Landau quantization, the shape of electron band around X point is determined. WE have also developed a model describing the Rashba Physics in FeSe.

From excitons to topological excitons and their fingerprints on the electronic bandstructure

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Here I will discuss some recent work where, by using the ultrafast angle resolved photoemission spectroscopy exciton formation in semiconductors and in the presence of topology are discussed.
Coulomb-bound electrons and holes forming excitonic quasi-particles and induced by coherent light-matter interactions in semiconductors, have attracted significant interest given their critical roles in both fundamental science and applications. Whether these excitonic state can be driven in the presence of topological invariants, what properties of the topological state persists and what are their fingerprints in the material's band structure are all open questions. Here I will discuss some recent work where, by using the ultrafast angle resolved photoemission spectroscopy we study and reveal under which conditions exciton state can be driven in a topological insulators and we discuss the differences with respect to semiconductor excitons and their fingerprints on the electronic structure.

Controllable topological superconductivity in superconductor/ferromagnet heterostructures

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Key words: Majorana zero modes, topological superconductivity, ferromagnets

Over the last two decades numerous scientific groups have focused on the pursuit of fault-tolerant quantum computation. Although elaborate algorithms have been developed so far for quantum error correction, topological superconductivity and Majorana zero modes offer a promising alternative tackling the quantum state-decoherence problem at the hardware level. Majorana zero modes emerge at the defects of topological p-wave superconductors. However, p-wave superconductivity is scarce in nature and therefore several proposals have been put forward to engineer Majorana zero modes using conventional superconductors. Our group proposes a novel platform for topological superconductivity and Majorana zero modes comprising conventional superconductor/ferromagnet heterostructures [1]. The heterostructures consist of ferromagnetic nanowires in between conventional superconductors which are in proximity with magnetic insulators. Instead of spin-orbit coupling which is a crucial factor in the vast majority of relevant proposals, our mechanism relies on the interplay of applied supercurrents and weak exchange fields emerging from the magnetic insulators in proximity with the conventional superconductors. We demonstrate that the coexistence of the supercurrent, the exchange field and conventional superconductivity induces triplet p-wave correlations which mediate in the ferromagnet, realizing an effectively spinless topological superconductor. We assert that the proposed superconductor/ferromagnet heterostructures exhibit enhanced controllability since topological superconductivity can be tuned apart from gate voltages applied on the superconductor or the ferromagnet also by the direction of the applied supercurrents and the orientation of the magnetization of the magnetic insulators.

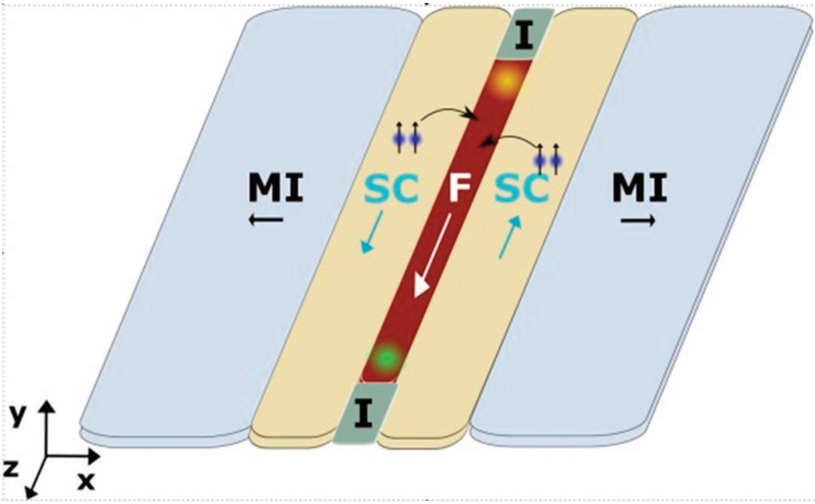

Figure 1: Ferromagnetic nanowire (F) in between conventional superconductor (SC) in proximity with magnetic insulators (MI). Black and white arrows indicate the magnetization of the MI and F respectively while blue arrows indicate the supercurrents. Equal spin pairing correlation (blue dots) are induced in the SC due to the coexistence of the supercurrents with the exchange field of the MI and mediate into the F wire realising intraband or effectively spinless superconductivity. Majorana zero energy modes (green and yellow dots) emerge at the boundaries of the wire.

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Unconventional superconductivity of Sr_2RuO_4 beyond the traditional framework

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After more than 25 years since its discovery, studies of the unconventional superconductivity of Sr_2RuO_4 have been reactivated in the last couple of years. As the main trigger, it was revealed that previous NMR results had a technical problem of overheating the sample. Now the reduction of the spin susceptibility below Tc consistent with the spin-singlet pairing has been confirmed. As another new development, uniaxial pressure can drive its multi-band Fermi surfaces across a Lifshitz transition, and increases its T_c from 1.5 K to 3.5 K. Correspondingly, muon spin resonance indicates a splitting between the enhanced T_c and the onset of the time-reversal-symmetry breaking at T_{TRSB} that remains at about 1.5 K. In combination with other results such as the unusual jump in a shear elastic constant in ultrasound experiments, one promising pairing symmetry is Eg with the chiral d-wave "d + *id* " order parameter. However, such a state is controversial since it implies a gap structure that does not allow pairing of electrons within the plane despite the quasi-2-dimensional nature. In order to settle this issue, some promising theories propose the inter-orbital pairing. The spin-triplet, inter-orbital singlet pairing may explain most of the observations including the pseudo-spin singlet, even parity behavior. We discuss how we may examine such a possibility experimentally. Superconductivity of Sr_2RuO_4 may help to establish such a pairing state beyond the traditional "unconventional" pairing.

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Current-induced phenomena in Ca_2RuO_4: The challenge of overcoming Joule heating

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Key words: non-equilibrium, current-induced, Mott insulators

The capability to control the properties of quantum materials by external parameters is a crucial milestone of condensed matter physics. In this perspective, the flow of direct current is an appealing control parameter, allowing to trigger exotic electronic and magnetic states while being compatible with modern integrated electronics.
The strongly correlated Mott insulator Ca_2RuO_4 offers a unique playground for exploring non-equilibrium steady states triggered by direct current, where phenomena such as modulation of the Mott gap [1] or inter-phase Peltier effects [2] have been recently reported. When conducting measurements with current, however, the effects of the unavoidable Joule heating need to be carefully addressed. On the one hand, direct current heating can be used to trigger the metal–insulator transition of Ca_2RuO_4 and control regions of phase coexistence [3–5]. On the other hand, localised heating of materials used for building sample holders can lead to effects of extrinsic nature, such as unexpectedly strong diamagnetic-like signals [6]. It is hence necessary to formulate a robust measurement protocol to perform measurements with applied electrical current, with the aim of limiting the Joule heating and accurately assess the sample temperature.
In this talk, I will present recent advances in studying the properties of Ca_2RuO_4 bulk single crystals under the flow of electric current, focusing on its electronic and magnetic properties. I will discuss the chal-

lenges involved in dealing with large currents, describe a simple model that allows to account for the main contributions of Joule heating, in view of unravelling current-induced phenomena intrinsic to this strongly correlated material.

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Multicomponent superconductivity at the unconventional Lifshitz transition in a three-dimensional heterostructure with tunable Rashba spin-orbit coupling

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Key words: superconductivity, Fano-Faschbach resonance, topological matter, Lifshitz transition, Rashba spin-orbit coupling.

In this work we consider a three-dimensional (3D) superlattice of metallic layers of thickness L separated by a spacer of width W and periodicity d. The presence of a confinement potential along the direction orthogonal to the layers is reflected in an electronic multiband structure which, as known, leads to multigap superconductivity and modulation of the critical temperature.
Parallelly, interfacing different materials in the direction of confinement breaks the spatial inversion symmetry allowing a Rashba spin-orbit coupling (RSOC). The electrons in-plane are, thus, subjected to an effective magnetic field which orients the spin in a direction orthogonal to the momentum. This is reflected in a spin-splitting of the subbands that characterize the superlattice.
The main purpose of this work is to study the combined effect of multigaps superconductivity and RSOC and to see how, by appropriately varying the intensity of the Rashba coupling, the structural characteri-

stics of the system and the parameters that define the superconducting phase, it is possible to obtain an amplification of the critical temperature.

As we will see, the interplay of the RSOC and superlattice structure leads to an extended van Hove singularity in the density of states (DOS) at the Brillouin zone edge with an unconventional Lifshitz transition for one of the two helicity states of the spinorbit split electron spectrum. This is reflected in an amplification of the gaps and critical temperature where the DOS shows a maximum. The evaluation of the superconducting gap and the critical temperature is done by including in the Bogoliubov-de Gennes equation the quantum configuration interaction between the gaps.

This is taken into account by considering an electron-phonon interaction dependent both on the band indices and on the wavevectors along the confinement direction.

Therefore, unlike the Bardeen–Cooper–Schrieffer (BCS) theory, the superconducting coupling is not constant but has a matrix structure. The possibility to suitably vary each term of this matrix allows to study the effect on the superconducting phase of the coexistence of different condensates in different coupling regimes.

It is found that the presence of the RSOC amplifies both the gap and the critical temperature when the Fermi energy crosses the band edge of the higher energy subband. However, there is a limit to the variation of the Rashba coupling constant, as we will see, this quantity is inversely proportional to superlattice modulation parameter: increasing the first is equivalent to decreasing the second, this reduces the separation between adjacent subbands and generates overlapping and interference effects.

Having fixed a maximum coupling constant and, therefore, a minimum periodicity, we see how by suitably varying the thickness of the layers it is possible to increase both the electron-phonon coupling constant and the cut-off energy. This allows to reconstruct the *superconducting dome* typical of materials at high critical temperatures and to obtain critical temperatures close to room temperature.

Our results suggest, on the one hand, a method to effectively vary the effect of the RSOC via the tuning of the superlattice modulation parameter, on the other hand, they provide precise indications on the values of the parameters involved in view of possible practical realizations in a way potentially relevant for spintronics functionalities in several existing experimental platforms and materials.

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Euclidean Q-balls of fluctuating SDW/CDW in the 'nested' Hubbard model of high-Tc superconductors as the origin of pseudogap and superconducting behaviors

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Euclidean Q-ball type solutions carrying Cooper/local-pair condensates inside finite volume with classically oscillating in Matsubara time spin-/charge densities (SDW/CDW) are found in the 'nested' repulsive Hubbard model of high-Tc superconductors [1]. An exchange between fermions with coherently oscillating SDW/CDW inside the Q-balls provides 'pairing glue', that couples fermions into Cooper/local-pairs. Euclidean Q-ball solutions arise below some temperature T* due to global invariance of the effective theory under the phase rotation of the SDW/CDW fluctuations amplitudes, that conserves a 'Noether charge' Q along the Matsubara time axis. At T* the classical SDW/CDW fluctuations arise via 1st order phase transition, while superconducting condensate density inside Q-balls is zero at T* and possesses a steep maximum at T<T*, causing a similar maximum in specific heat of the Q-balls 'gas'. Below T* the volume of the Q-balls is inversely proportional to the square of SDW/CDW fluctuation amplitude. The fermionic spectral gap inside Euclidean Q-balls arises in the vicinity of the 'nested' regions of the bare Fermi surface and scales with the square root of the superconducting density. All the described solutions are found analytically from the Eliashberg like equations for the two cases of 'nesting' wave vectors: a CDW wave vector Q_{CDW}, connecting regions near the Fermi surface with equal signs of the superconducting order parameter, or for a SDW wave vector Q_{SDW}, connecting regions with the opposite signs of the d-wave superconducting order parameter. Possible relation of the presented theory with thermodynamic time-crystals and different properties of superconductors is discussed.

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Transport and optical study of nodal-line and Dirac semimetals in high magnetic fields

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Key words: nodal-line semimetals, Dirac semimetals, transport and optical spectroscopy, high magnetic field

After the discovery of topological insulators, it was realized that at the border between ordinary and topological insulator, a state of matter with a stabile touching of a valence and conduction band could exist. These materials are known as 3D Dirac or Weyl semimetals and Dirac nodal-line semimetals. We shall present magneto-transport and optical spectroscopy on several of those materials (such as ZrSiS or TlBiSSe), which have been synthesized in our laboratory. In particular, we present how magneto-optic spectroscopy is a method of choice for detecting the non-trivial topology. The method is more powerful than the quantum oscillations detected by de Haas-van Alphen or Shubnikov-de Haas effect, although the both methods detect the Landau levels. Finally, we plan to present several of our results in magnetic susceptibility and optical conductivity, which we believe are the direct consequence of the nodal-line and Dirac physics.

First Principle Studies of Topological Phase in Chains of 3d Transition Metals

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Key words: 3d transition metal chain, magnetic order, band structure, magnetic order

Recent experiments have shown the signatures of Majorana bound states at the ends of magnetic chains deposited on a superconducting substrate [1]. Here, we employ first principles calculations to directly investigate the topological properties of *3d* transition metal nanochains (i.e., Mn, Cr, Fe and Co) for isolated and surface---deposited wires. Our results stand in opposition to bulk calculations which have been previously used. From the obtained band structure, we found the exact tight binding model in the Wannier orbital basis with realistic parameters [2]. For these models, we calculate topological invariant of Z_2 phase, from which we conclude that the non-trivial topological phase can exist only in Mn and Co isolated (free-standing) chains. Additionally, we discuss phases with non-collinear order of magnetic moments as possible source of the non-trivial topological phase. We show that this type of magnetic order is unstable in the case of the Fe and Co wires and cannot be the source of the non-trivial topological phase. Finally, we discuss the influence of the substrate on the band structure and magnetic properties of the nanochain's atoms. We show that the coupling of the chain to substrate leads to suppression of the magnetic moment value and to strong modification of the band structures. This

work investigates the Fano resonances die to interplay of localized and delocalized states in complex topology of hyperbolic space.
The non-collinear magnetic order is unstable in the case of the Fe and Co chains. This result may be expected taking strong ferromagnetic instabilities in the bulk Fe and Co [3]. These transition metals demonstrate that the existence of Majorana zero modes in the magnetic chains cannot be considered to be a consequence of the non-collinear magnetic order in the chain. Instead, we suggest that the Majorana modes may occur when the number of electrons per atom is *even* as in Mn or Co, while they are absent for an *odd* electron number. Moreover, the existence of strong magnetic moments in *3d* transition metals cannot be correctly captured within the one band model. On the contrary, this phenomenon is associated not only with Hund's exchange in partly filled *3d* orbital states [3] but also with larger number of bands crossing the Fermi level.

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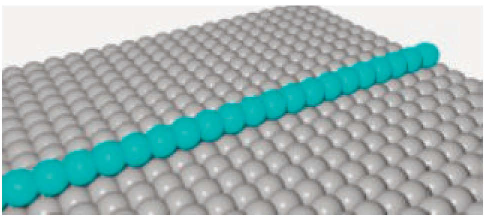

Figure 1: Schematic representation of the monoatomic chain of 3d transition metal ions.

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Band superconductivity in a periodic constricted nanoribbon structures

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Key words: Bogoliubov – de Gennes equations, superconductor nanostructures, superlattice, gap energy

Our work [1] investigates how superconductivity in a quasi-1D superlattice is affected by the interplay between the quasi-momentum and the phase difference along the lattice. Contrary to systems where the longitudinal and transversal degrees of freedom are separable, see e.g. [2,3], we investigate constriction of a 2D-shape, see Figure 1, which results in strong mixing.

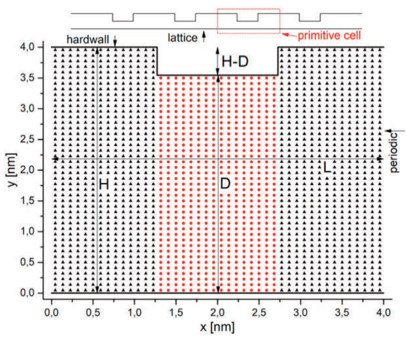

Figure 1: Top: Nanoribbon schematics. Bottom: Geometrical definition of the unit cell of the periodic nanoribbon, which is 4 nm by 4 nm and it is discretised with a mesh of nx = ny = 44 points. Triangles show mesh points of the nanoribbon area, circles show mesh points of the constriction area. D(H) is the width in the constricted (unconstricted) region and L is the length of the unit cell.

Periodic geometrically constricted 2D $NbSe_2$ nanowire is investigated with the Anderson approximation of Bogoliubov – de Gennes equations [4].
The superconducting order parameter is related to the single particle DOS around the Fermi level, but the introduction of an inter-cell phase difference changes this relation from average-like (accounting for the miniband-proximity effect) to strictly local. A miniband-crossing-related "shape resonance" [5-10] is identified as a function of the periodic constriction.
The phase difference leads to modulation or suppression of the superconducting gap, compare [11,12], which is shown to typically be strictly coupled with the vanishing of the order parameter. However, an exception to the general rule is discussed, where significant $\Delta(\mathbf{r})$ exists with a closed gap as a consequence of the mixing of different transverse symmetries.
We show that redefinition of the properties of the system via manipulation of its geometry or the electron concentration is possible.
Finally, the ongoing further development work on the model is briefly sketched. It considers taking into account, more realistically, the existence of multiple σ band pairs and π bands in a few-monolayer MgB_2-like material, as well as the inter miniband extension of the Anderson approximation.

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Charge order and Strange metals in cuprate superconductors

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Charge orders and charge fluctuations have been ubiquitously observed in the phase diagram of Cuprate superconductors. We will review the experimental status of these various observations, differentiating the under-doped region and the optimally-doped and over-doped ones. Various theories have been advanced to explain the presence of these orders and their implication for our understanding of the pseudo-gap, from the idea of "vestigial order" to the one of "fluctuating Pair Density Wave (PDW)". We will discuss these theoretical approaches in direct comparison with experiments. We will then introduce a proposal of "fractionalization of a PDW" in order to explain the pseudo-gap state. We will show that this idea produces a strong phenomenology, especially ARPES experiments, and giving a clue for the puzzling transport properties recently reported in the optimally doped and over-doped regions. We will then focus on the strange metal phase of those compounds and make a proposal for electric transport in this phase.

Interplay between superconducting fluctuations, pairing resonances, and topology of the Fermi surface in complex and nanostructured superconductors

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Key words: Electronic Topological Transitions, Lifshitz transitions, shape resonances, multigap superconductivity, BCS-BEC crossover, pseudogap, screening.

The superconductivity in iron-based, magnesium diborides, and other high-Tc superconducting materials, including indications of high-Tc superconductivity in the organic potassium doped paraterphenyl, has a strong multi-band, multi-gap, and resonant character. Recent experiments support a BCS-BEC crossover induced by strong-coupling and proximity of the chemical potential to the band edge of one of the bands, with evidences for Lifshitz transitions associated with changes in the Fermi surface topology [1,2,3].

Here we study the BCS-BEC crossover, superconducting fluctuations, and complex pseudogap phenomena in a two-band / two-gap superconductor, considering tunable interactions, including mean-field and fluctuations effects. When the gap is of the order of the local chemical potential, superconductivity is in the crossover regime of the BCS-BEC crossover and the Fermi surface of the small band is completely smeared by the gap opening. In this situation, small and large Cooper pairs coexist in the condensate, which is the optimal condition for very high-Tc superconductivity, thanks to the screening of superconducting fluctuations generated by the deep band, showing in addition unexpected consequences on the pseudogap phenomenon above the critical temperature [4].

We discuss different physical systems in which the multigap and multiband BCS-BEC crossover can be realized, pointing toward very high-Tc superconductivity. As an example we consider here superconducting stripes in which shape resonances and multigap physics at the band edge play a cooperative role in enhancing superconductivity in the crossover regime of pairing [4,5,6,7]. A key prediction of the above discussed physics is recalled and discussed in comparison with experiments: the isotope effect of the superconducting critical temperature in the vicinity of a Lifshitz transition, which has a unique dependence on the energy distance between the chemical potential and the Lifshitz transition point [6].

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Band Structure Engineering in 3D Topological Insulators

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We will present our recent combined experimental and theoretical results on band structure engineering in 3D topological insulator (3D TI) bilayers and superlattices. These results show how new topologies emerge in complex structures, as compared to the routine Fermi level control by alloying, and provide a starting point in search for novel topological phases. In topological pn-junction we have demonstrated Fermi level control by the relative thicknesses of the layers [1], while in superlattices that combine Bi2Te3 quintuple layers and Bi-bilayers we have predicted dual topological properties, and experimentally demonstrated the existence of non-trivial topological crystalline insulator (TCI) crossings away from the surface Brillouin zone center [2].

In addition to this, we will discuss recent progress in setting up a high-resolution spin-polarized laser-ARPES system at PGI-6 in Juelich, Germany, and the first results on topological insulator spin texture [3].

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Controlling strong correlations of HTSs with Van der Waals heterostructure

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Key words: Low-dimensional superconductivity, nanoscale superconductivity, high temperature superconductivity, quantum devices.

The Van der Waals (VdW) heterostructures formed by mechanically stacking layers of 2-Dimensional (2D) materials possess unique properties and new functionalities, not seen in standard materials, that make them irreplaceable platform for emergent electronics. Hindering the progress in utilizing VdW uniqueness is the fact that many of their features, especially the novel topological quantum states and related phenomena are restricted to low temperatures. This poses a challenge to create VdW heterostructures that maintain their capacity to harbor topological quantum matter physics at elevated temperatures. Employing High Temperature Superconductors (HTSCs) based 2D films for manufacturing VdW heterostructures offers the most advantageous route to increase the temperature range in which the topological states and phenomena associated with VdW devices can be studied and used. Nanofabrication and processing of these systems in a conventional clean-room facility will fail since it requires even higher standards than processing of organic semiconductors. Therefore, this methodology poses a number of formidable challenges not only in device fabrication, but also in terms of signal-to-noise ratio in spectroscopic experiments, which is essential for a true control over the properties of HTSCs VdW heterostructures. In this talk, I'll review therefore the recent progress in this field and I´ll show our contribution to this research. I'll also give an outlook of this research towards applications for quantum information.

Artificial separation of trivial and topological superconducting domains

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Key words: nanoflake, edge mode, topological phase, phase separation

Interplay between superconductivity, spin-orbit coupling, and magnetic field can lead to realization of the topological phase shift [1]. Existence of this topological phase allows for emergence of the bound states, which the most famous example are Majorana bound states that emerge at the boundary of one dimensional nanostructure [2,3]. However, the similar topological bound state can also exist in the two-dimensional system [4]. Moreover, recent experimental works suggest a possibility of realization of the topological superconducting domain in magnetic nanostructure coupled with bulk superconductor [5,6]. In such a case, boundary between trivial and topological phases is "marked" by nearly-zero in-gap bound state. In this seminar, I will discuss and shown how using artificial nanoflake structure can envision a similar situation - topological domain surrounded by the nearly-zero energy bound state [7].

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Correlation between enhancement of superconducting state properties and crystallinity degradation under pressure in Fe-Te-Se single crystals

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Key words: superconductors, Fe–Te–Se system, single-crystal x-ray diffraction studies, thermodynamic properties, hydrostatic pressure

We have already shown that the inhomogeneous spatial distribution of ions with nanoscale phase separation enhances the superconductivity in superconducting Fe Te Se chalcogenides [1]. The almost ideal single crystal of $FeTe_{0.65}Se_{0.35}$ exhibits a greater width of superconducting transition and a considerably smaller value of the critical current density in comparison with non-uniform sample of the same compound. Resistivity results confirm that the inhomogeneous spatial distribution of ions and presence of small hexagonal-like phase in chalcogenides with nanoscale phase separation seems to enhance the superconductivity in this system [2]. Here, detailed investigations of Ni substituted $Fe_{0.994}Ni_{0.007}Te_{0.66}Se_{0.34}$ and unsubstituted $Fe_{0.99}Te_{0.66}Se_{0.34}$ crystals performed at ambient and under hydrostatic pressure are presented. Under ambient pressure the weakening of superconducting state properties was observed in $Fe_{0.994}Ni_{0.007}Te_{0.66}Se_{0.34}$ crystal, with disorder introduced by Ni substitution, as compared with those in $Fe_{0.99}Te_{0.66}Se_{0.34}$. For $Fe_{0.994}Ni_{0.007}Te_{0.66}Se_{0.34}$, the x-ray diffraction studies have revealed a degradation of crystal quality under applied elevated pressure. Superconducting state properties of single phase $Fe_{0.99}Te_{0.66}Se_{0.34}$ crystal, such as the upper and lower critical fields, were found to be poorer, at both ambient and hydrostatic pressure, than those observed for $FeTe_{0.5}Se_{0.5}$ crystals exhibiting pronounced nanoscale phase separation. Comprehensive studies of impact of pressure on crystal structure and on superconducting state properties confirm that enhancement of superconductivity under pressure correlates with appearance of mosaicity [3].

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Coupling between the magnetic and charge degrees of freedom in a Weyl ferromagnet

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Fe_3Sn_2 is a ferromagnet with a very high Curie temperature ~650 K that undergoes spin reorientation around 120 K. We discovered based on DFT calculations that besides its fascinating magnetic properties, it hosts Weyl nodes at or very close to the Fermi level that are switchable based on the magnetization direction.
The presence of magnetic order introduces a high degree of complexity and how the topological features are related to the magnetic order is a fundamentally important problem not yet fully explored. Here, I will discuss how the presence of magnetic order affects the magnetotransport properties and is manifested in the spin reorientation, anisotropic magnetoresistance, planar Hall effect, and electronic band structure in this system.

Superconductivity in the pressurized Weyl-semimetals and three-dimensional topological insulators

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Key words: superconductivity, Weyl-semimetals, topological insulators, high pressure

It has been established that the superconductivity in a material is dictated by its degrees of freedom of electronic charge, orbital, spin and crystallographic structure, which can be manipulated by the control parameters such as pressure, magnetic field and chemical composition. Pressure is a 'clean' way to tune basic electronic and structural properties without changing the basic chemistry, and can help to understand the corresponding physics. In this talk, we will present some interesting phenomena obtained by our recent high-pressure studies, including superconductivity emerging from Weyl semimetal WTe_2 [1] $TaIrTe_4$ [2], independence of topological surface state and bulk conductace in three-dimensional topological insulators [3] and universal superconducting behaviours in pressurized tetradymite topological insulators [4].

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STM on topological materials

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SmB_6 has been proposed a topological Kondo insulator with nontrivial surface states inside a bulk hybridization gap. While the hybridization between localized 4*f* and conduction band states at low temperatures is experimentally well established, an experimental confirmation of the topological nature of the surface states turned out challenging. Using Scanning Tunneling Microscopy and Spectroscopy (STM/S), we find that introducing magnetic impurities in samples $(Sm_{1-x}R_x)B_6$ with R = Gd represses the surface states on a much larger length scale compared to non-magnetic impurities *R* = Y [1,2]. This is interpreted in terms of breaking time reversal symmetry and is confirmed by spin-polarized STM. The influence of Sm vacancies on the surface states and surface manipulation by focused ion beam (FIB) will also be discussed.
Related to the concept of topological insulators are Dirac semimetals in which lines of Dirac nodes are protected by symmetry. One example is HfSiS belonging to a non-symmorphic space group. Utilizing STS in applied magnetic fields [3], Rashba-split surface states are characterized by measuring Landau quantization above 7 T and standing waves at step edges, both revealing a quasilinear dispersive band structure.
Another material of topical interest is the magnetic Kagome lattice Weyl semimetal Co3Sn2S2 in which time-reversal symmetry breaking causes fascinating physics [4]. The measured local density of states reveals a semimetallic gap of ~300 mV, verified as the gap in the spin-minority band using spin-resolved tunneling spectra [5].

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Construction of Fractal Order and Phase Transition with Rydberg Atoms

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We propose the construction of a many-body phase of matter with fractal structure using arrays of Rydberg atoms. The degenerate low energy excited states of this phase form a self-similar fractal structure. This phase is analogous to the so-called “type-II fracton topological states”. The main challenge in realizing fracton-like models in standard condensed matter platforms is the creation of multi-spin interactions, since realistic systems are typically dominated by two-body interactions. In this work, we demonstrate that the Van der Waals interaction and experimental tunability of Rydberg-based platforms enable the simulation of exotic phases of matter with fractal structures, and the study of a quantum phase transition involving a fractal ordered phase.

Correlations, topology, and unconventional superconductivity in magic angle twisted bilayer graphene

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We have explored magic angle twisted bilayer graphene’s (MATBG) electronic properties using variety of spectroscopic methods with the scanning tunneling microscope (STM). Beside unraveling signatures of strong correlations [1] driving a cascade of transitions [2] in its electronic properties, we have shown that such correlations also drive formation of topological Chern insulators stabilized with weak magnetic fields [3]. Most recently, we have focused our attention on the nature of superconducting state that forms near half filling of MATBG’s valance flat band. Our experiments show signature of nodal superconductivity with tunneling gap to transition ratio that far exceeds the BCS limit. Moreover, we find superconductivity emerges from a pseudogap phase, which might be indication of either preformed pairs or the formation of some ordered state that makes superconductivity possible. Remarkably, we find in samples with perfect alignment with the hexagonal BN substrate, both the pesudogap phase and superconductivity are suppressed [4].

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