Book of Abstracts

21st National Conference on Superconductivity

Materials, Strong Correlations, Topology

September 22-26, 2024
Kraków, Poland

Conference scope:

- High-temperature superconductivity and other highly correlated systems.
- Linking magnetism with superconductivity in nano- and macro-systems.
- Critical phenomena in superconductors and superfluids.
- Exotic metallic states in topological systems.
- Dynamic effects in highly correlated systems.
- Applications of conventional and exotic superconductors.

Local Organizing Committee:

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Maciej Fidrysiak
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Andrzej Kądzielawa
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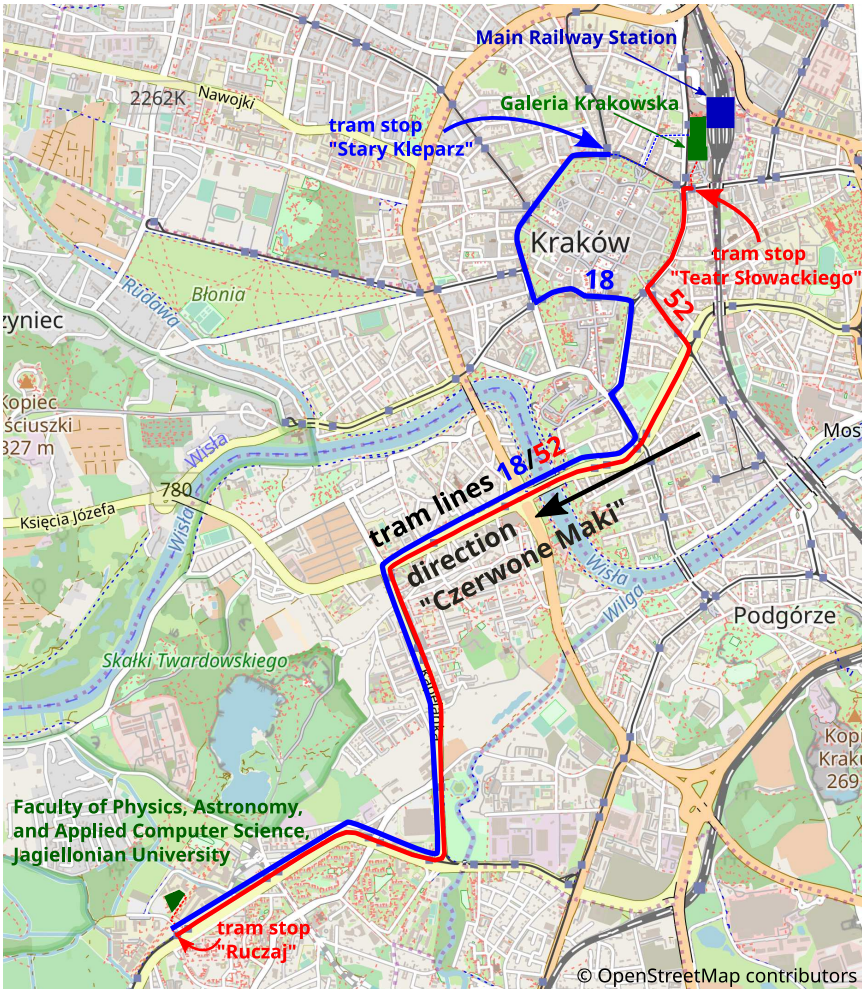
AGH UNIVERSITY OF KRAKOW

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Venue:
Faculty of Physics, Astronomy, and Applied Computer Science
Jagiellonian University
ul. prof. Stanisława Łojasiewicza 11
30-348 Kraków, Poland

Directions from/to Kraków Main Railway Station (tram lines **52** and **18**):



Directions from/to Campanile Kraków South Hotel:

Conference program

Astronomer Copernicus, or Conversations with God
Jan Matejko, 1873

Oil on canvas
Dimensions: 225 cm × 315 cm
Location: Collegium Novum, Jagiellonian University, Kraków

Sunday, September 22

16:00-18:00		**registration**	
18:00-20:00		**welcome party**	
		Chair: Organizers	
20:00-20:30	M. Cieplak	Short-range magnetic order in orbitally selective Ni-substituted $FeSe_{0.35}Te_{0.65}$ single crystals	p. 10
20:30-21:00	K. I. Wysokiński	Unconventional superconductor Sr_2RuO_4: Then and now	p. 11

Monday, September 23

		Chair: K. I. Wysokiński	
8:30-9:00	B. Wiendlocha	Superconductivity in High Entropy Alloys and the effect of disorder	p. 12
9:00-9:30	A. Durajski	20 years of research on binary hydrogen-rich superconductors. What's next?	p. 13
9:30-10:00	A. Ślebarski	Magnetic field induced reentrance of superconductivity in the cage type $Y_5Rh_6Sn_{18}$	p. 14
10:00-10:30		**coffee/tea**	
		Chair: R. Puźniak	
10:30-11:00	T. Cichorek	Vortex penetration into the putative chiral superconductor 4Hb-TaS_2 by local magnetization measurements	p. 15
11:00-11:30	P. Starowicz	Electronic structure of the Ce_3PdIn_{11} heavy fermion system with two inequivalent Ce positions	p. 16
11:30-11:50	R. Kurleto	Flat bands at the Fermi level in unconventional superconductor YFe_2Ge_2	p. 17
11:50-12:10	N. Sedlmayr	Quantized thermal Hall conductance and the topological phase diagram of a superconducting bismuth bilayer	p. 18
12:10-12:30	A. Stokłosa	Structure and concentration of electronic defects and their mobility in $YBa_2Cu_3O_{6+x}$	p. 19

12:30-14:00		**lunch/break**	
		Chair: I. Weymann	
14:00-14:30	M. M. Maśka	Emergent "quantum" critical point for charge-density-wave ordered materials	p. 20
14:30-15:00	D. Legut	Magnetism and phase transition of UTe_2	p. 21
15:00-15:30	J. Herbrych	Evidence for the valence-bond pairing in low-dimensional two-orbital system	p. 22
15:30-16:00		**coffee/tea**	
		Chair: A. Rycerz	
16:00-16:30	M. Mierzejewski	Optical manipulation of bipolarons in a system with nonlinear electron-phonon coupling	p. 23
16:30-17:00	K. Wohlfeld	Shining a light on the cuprate puzzle: Quasiparticle versus "unparticle" physics	p. 24
17:00-17:30	G. Jung	Channeled vortex motion, experimental aspects	p. 25
17:30-18:00	R. Puźniak	Correlation between enhancement of superconducting state properties and crystallinity degradation due to chemical substitutions, applied pressure, and hydrogenation in Fe-Te-Se single crystals	p. 26
19:00-21:00		**poster session**	

Tuesday, September 24

		Chair: A. M. Oleś	
8:30-9:00	I. Weymann	Phase diagram of a double-quantum-dot-based Andreev molecule	p. 27
9:00-9:30	A. Ptok	Real materials containing kagome lattice: lattice dynamics perspective	p. 28
9:30-10:00	K. Kolincio	Chiral spin fluctuations: the role of lattice geometry	p. 29
10:00-10:30		**coffee/tea**	

		Chair: K. Wohlfeld	
10:30-11:00	M. Konczykowski	Interplay of superconductivity with magnetic and charge orders tuned by disorder	p. 30
11:00-11:30	J. Jaroszynski	REBCO CC angular critical current up to 45 T using torque magnetometry	p. 31
11:30-11:50	M. Zegrodnik	Unconventional superconductivity and topology in moiré transition metal dichalcogenide bilayers	p. 32
11:50-12:10	M. Fidrysiak	Topological superconductivity in twisted bilayer cuprates: A microscopic perspective	p. 33
12:10-12:30	R. Radwański	Quantum entanglement in $NaTiO_2$ – the consequence of spin-orbit interactions	p. 34
12:30-14:00		**lunch/break**	
14:00-21:00		**excursion/free time**	

Wednesday, September 25

		Chair: W. Sadowski	
8:30-9:00	D. Kaczorowski	Unconventional superconductivity in heavy-fermion Ce-based compounds	p. 35
9:00-9:20	T. Klimczuk	Superconductivity in a ternary $Mg_4Pd_7As_6$ compound	p. 36
9:20-9:40	J. Juraszek	Low-Field Nodeless Superconducting State in the Presence of Local Magnetism in $CeRh_2As_2$ from Local Magnetization	p. 37
9:40-10:00	M. Marganska	Selective screening of the Coulomb interaction and the resulting superconductivity in monolayer $NbSe_2$	p. 38
10:00-10:30		**coffee/tea**	
		Chair: D. Rybicki	
10:30-10:50	K. Podgórska	Study of magnetic properties of EuSnP single crystals	p. 39
10:50-11:10	W. Brzezicki	Surface chiral metal and warped time-reversal symmetry	p. 40
11:10-11:30	M. Winiarski	Can analysis of chemical bonding help us find new intermetallic superconductors?	p. 41

11:30-11:50	S. Sekh	Electronic and magnetic properties of infinite-layer nickelates	p. 42
11:50-12:10	D. Gajda	The influence of Sm_2O_3 admixtures on morphology, transport critical current density and dominant pinning mechanism of MgB_2 materials investigated by using the transmission electron microscope	p. 43
12:10-12:30	S. Malick	Large magnetoresistance and first-order phase transition in antiferromagnetic single-crystalline $EuAg_4Sb_2$	p. 44
12:30-14:00		**lunch/break**	
		Chair: A. Pikul	
14:00-14:30	M. Rams	On "Computational supremacy in quantum simulation" of a quench dynamics in transverse-field Ising spin glasses.	p. 45
14:30-15:00	T. Domański	Are pairs of Majorana modes distantly cross-correlated?	p. 46
15:00-15:30	M. Birowska	The role of the electron correlations effects on electronic and magnetic properties of 2D antiferromagnetic crystals.	p. 47
15:30-16:00		**coffee/tea**	
		Chair: M. Cieplak	
16:00-16:20	I. Wrona	Superconducting properties of *p*-block-based ternary hydrides XC_2H_8 at low pressures	p. 48
16:20-16:40	S. Głodzik	Higher order spin interactions mediated by the substrate	p. 49
16:40-17:00	A. Wadge	Surface state manipulation and topological Lifshitz transitions in NbP	p. 50
17:00-17:20	A. Kądzielawa	Anharmonicity, electron-lattice coupling, and superconductivity in hydrogen-rich systems	p. 51
17:20-17:50	K. Rogacki	Controlling the anisotropic properties of MgB_2 by charge doping and band scattering	p. 52
18:00-19:00		**free time**	
19:00-22:00		**conference dinner**	

Thursday, September 26

		Chair: M. M. Maśka	
8:30-8:50	M. Dziurawiec	High harmonic generation for phase detection and ultra-fast tracking in condensed matter systems	p. 53
8:50-9:10	P. Wójcik	Unconventional superconductivity in a two dimensional electron gas at the LAO/STO interface.	p. 54
9:10-9:30	I. Biało	Strain-tuned magnetic frustration in La_2NiO_4	p. 55
9:30-9:50	A. Kobiałka	Topological superconductivity in Fibonacci quasicrystals	p. 56
9:50-10:10	P. Saha	Exploring magnetic and topological phenomena in moiré $MoTe_2/WSe_2$ heterobilayer	p. 57
10:10-10:30		**coffee/tea**	
		Chair: Z. Kąkol	
10:30-11:00	J. Zakrzewski	Surprising transport in interacting 1D chain	p. 58
11:00-11:30	M. Nowak	Topological superconductivity in planar Josephson junctions	p. 59
11:30-11:50	A. S. Aramthottil	Phenomenology of many-body localization in bond-disordered spin chains	p. 60
11:50-12:10	A. Kłosiński	Antiferromagnetic phase in infinite-layer superconducting nickelates, a Hartree-Fock perspective	p. 61
12:10-12:30	J. Spałek	Conference summary	
12:30-14:00		**lunch/break**	
14:30-16:30		**excursion to Solaris**	

Posters

Abstracts:
Oral presentations

Lady with an Ermine
Leonardo da Vinci, c. 1489-1491

Oil on walnut panel
Dimensions: 54 cm × 39 cm
Location: Czartoryski Museum, Kraków

Short-range magnetic order in orbitally selective Ni-substituted $FeSe_{0.35}Te_{0.65}$ single crystals

Marta Cieplak[1]

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Multi-orbital character of iron-based superconductors (IBS) results in various electronic phases evident in phase diagrams, including nematically or magnetically ordered phases. The role of magnetic or nematic fluctuations in superconducting (SC) pairing in IBS is a subject of intense discussions. Recent studies of FeSe isoelectronically substituted either by S or Te into Se-site have revealed one (in case of S) or two (in case of Te) SC domes, overlapping in some regions with nematic phase, suggesting a possible link between SC pairing and nematic fluctuations [1]. Another proposal in case of heavy Te-doping suggests an important role of the d_{xy} orbital, which approaches Fermi level with increasing Te content, possibly providing additional pairing channel via magnetic fluctuations [2].

In this talk, after introductory remarks on the above issues, I will present the results of our study of magnetic properties of $FeSe_{0.35}Te_{0.65}$ single crystals doped by Ni into Fe site [3]. The crystals of this composition are located close to maximum T_c in heavily Te-doped SC dome. Transport properties combined with ARPES [4] indicate that substitution of Ni dopes crystals with electrons, what eliminates some of the hole pockets from Fermi level, leaving only one, originating from the d_{xy} orbital. Anomalies in magnetization are observed, clearly linked to the localization of d_{xy} orbital on increasing temperature. Analysis of these anomalies suggests the presence of short-range magnetic orderings, both antiferromagnetic, and ferromagnetic. This implies an importance of magnetic fluctuations in the studied system, confirming a possible link to pairing in heavily doped SC dome.

The work done in collaboration with I. Zajcewa, A. Lynnyk, K. M. Kosyl, 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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Unconventional superconductor Sr_2RuO_4: Then and now

Karol Izydor Wysokiński[1]

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Superconductivity in Sr_2RuO_4 has been discovered in 1994. Already the early experiments indicated that despite the relative simplicity of its normal state, the material is a very unconventional superconductor. Over the first 25 years, its order parameter was thought to be of spin-triplet odd parity character. Moreover, many experiments, like μSR and Kerr effect measure the spontaneous time-reversal symmetry breaking below the superconducting transition temperature. New experimental developments in the last five years seem to point out that the order parameter is chiral but of a spin-singlet character. However, its precise symmetry remains a mystery. Some of the older as well as newer experimental results will be discussed in the context of the phenomenological model and novel mechanism of the Kerr effect.

Superconductivity in High Entropy Alloys and the effect of disorder

Kinga Jasiewicz[1], Sylwia Gutowska[2], Janusz Toboła[1], Bartłomiej Wiendlocha[1]

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[2] *University of Vienna*

Superconductivity in high entropy alloys (HEAs) has a decade-long history, originating with the discovery of superconductivity in a bcc-type $Ta_{0.34}Nb_{0.33}Hf_{0.08}Zr_{0.14}Ti_{0.11}$ alloy in 2014. Since then, numerous superconducting HEAs have been synthesized. However, the influence of the key ingredient of HEAs - atomic disorder - on the superconducting properties of these materials remains to be fully understood. What makes this subject even more interesting, we can distinguish several different types of disorder, namely: (a) atomic potential (chemical) disorder; (b) mass and force-constant disorder; (c) structural disorder (local distortions from the ideal high-symmetry crystal structure). Each of these forms of disorder may impact the materials' properties at different levels, including influence on the electronic and phonon structures and their scattering; influence on the electron-phonon interaction; and finally influence of all above on the formation of the superconducting phase. In this work theoretical calculations of the electronic structure and the electron-phonon interaction are conducted for several HEAs to address this issue. Surprisingly, in the fully disordered Ta-Nb-Hf-Zr-Ti alloy, the effect of chemical disorder on the electronic structure is the weakest among the studied materials. Structural and mass disorders influence electrons, phonons and the electron-phonon coupling parameter λ, but their impact on the superconducting phase seems to be weak. Conversely, despite the partial ordering in the $(ScZrNb)_{1-x}(RhPd)_x$ system, atomic potential disorder strongly scatters electrons, with their mean-free path comparable to the inter-atomic distance, placing superconductivity on the edge of the Mott-Ioffe-Regel limit.

20 years of research on binary hydrogen-rich superconductors. What's next?

Artur Durajski[1], Izabela Wrona[1]

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Recent research on compressed binary hydrides has unveiled the potential for achieving superconductivity at room temperature [1-6]. However, the current decision-making procedures for selecting constituent elements that may exhibit high critical temperatures (T_c) are far from optimal. Consequently, much experimental and numerical effort is expended on exploring unpromising compounds. By conducting an in-depth study of a database containing over 580 binary hydride superconductors, we observed intriguing relationships between T_c and certain physicochemical properties of the examined compounds. Among the studied parameters, the ratio of the molecular weight of the heavier atoms to the total mass of all hydrogen atoms in the hydride's chemical formula (M_X/M_H) was found to be the most valuable indicator for screening new promising superconductor candidates. The highest T_c values are associated with the lowest M_X/M_H ratios. Statistical analysis indicates a 28% chance of finding $T_c > 200$ K within the $0 < M_X/M_H < 15$ range. These findings are expected to improve resource efficiency by enhancing the selection process for future superconductor candidates. Additionally, they will likely accelerate ongoing experimental and numerical research, leading to new and exciting discoveries in a much shorter timeframe [7].

Acknowledgements

A. D. acknowledges financial support from the National Science Centre (Poland) under Project No. 2022/47/B/ST3/00622.

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Magnetic field induced reentrance of superconductivity in the cage type $Y_5Rh_6Sn_{18}$

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For the conventional BCS superconductors disorder generally reduces the critical temperature T_c of the superconducting state. This topic has received renewed attention because of several new reports of the observation of an enhancement of T_c in strongly correlated superconductors (e.g., $PrOs_4Sb_{12}$, $CeIrIn_5$, $CePt_3Si$), where atomic disorder acting as a perturbation within the critical regime, can be decisive and could change the nature of the quantum macrostate. Our studies focused on skutterudite-related superconductors ($R_3M_4Sn_{13}$, where R=La, Ca, and M is a 3*d* metal [1-4]; $R_5Rh_6Sn_{18}$, where R=La, Y, Sc [5-7]) which have documented an increase of T_c caused by disorder. By varying the degree of disorder (vacancies, doping), we have attempted to understand the role of atomic defects and fluctuations in composition on the superconductivity of these materials. We have proposed a phenomenological model that explains the relationships $T_c^* > T_c$ (T_c^* represents the transition to the locally-disordered superconducting phase, while T_c describes a bulk effect) due to greater lattice stiffening of the T_c^*-phase. Depending on the degree of disorder, we prove the correctness of the Werthamer–Helfand–Hohenberg theory or the percolation model, both of which are considered within the dirty limit of the BCS superconductor. $Y_5Rh_6Sn_{18}$ deserves special attention in our research, it shows a two-band superconductivity [8, 9] and the appearance of the peak effect [10, 11], when disorder increases with doping. We discuss the following issues: (i) The meaning of disorder; disorder generated by vacancies, doping, or "static" disorder. (ii) Band structure of Remeika superconducting materials (XPS, ab initio calculations, the impact of the pseudogap on the electric transport properties. (iii) Enhanced superconductivity in the presence of atomic disorder; Percolation model (Toy model) is proposed for describing the abnormal behavior in Werthamer-Helfand-Hohenberg dependencies $H_{c2} - T_c$. (iv) Magnetic field induced reentrance of superconductivity in the cage-type superconductor $Y_5Rh_6Sn_{18}$, peak effect, theoretical modelling [10, 11]. (v) Spin fluctuations in superconducting $Y_5Rh_6Sn_{18}$ when is doped with Co and/or Pd [11].

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Vortex penetration into the putative chiral superconductor 4Hb-TaS_2 by local magnetization measurements

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Heterostructures formed by alternating magnetic and superconducting layers are predicted systems for the realization of different topological quantum phases. Among them, chiral superconductors are of particular interest for both fundamental science and topologically protected quantum computation. The emergence of this one of the most elusive types of unconventional superconductivity is actively discussed for the van der Waals heterostructure 4Hb-TaS_2 formed by alternating magnetic and superconducting layers. This material exhibits a sign of spontaneous time-reversal symmetry breaking at a critical temperature $T_c \approx 2.7$ K [1] and several peculiar properties of the vortex state, including topological edge modes [2] and the magnetic memory effect [3] studied by scanning tunneling microscopy. However, the symmetry of an order parameter in 4Hb-TaS_2 remains an open question.

We focus on the influence of the Bean-Livingston surface barrier on a first vortex entry into the layered superconductor 4Hb-TaS_2. Our local magnetization measurements for several crystals of different thickness and with different degrees of non-magnetic disorder revealed a large increase of the penetration field upon cooling which excludes a conventional enhancement due to the surface barrier [4]. These results can be explained by the effect of Andreev bound states on the Bean-Livingston barrier, providing macroscopic evidence for a sign-changing gap function in 4Hb-TaS_2.

This work was supported by the Polish National Science Centre NCN (Project OPUS23 No. 2022/45/B/ST3/04117).

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Electronic structure of the Ce_3PdIn_{11} heavy fermion system with two inequivalent Ce positions

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Ce_3PdIn_{11} is a heavy fermion superconductor with two inequivalent lattice positions of Ce. Its electronic structure was investigated by means of angle-resolved photoemission spectroscopy (ARPES) and Korringa-Kohn-Rostoker (KKR) calculations within the single-particle Green function approach. ARPES spectra have been collected at 6K with photon energy of 122 eV, which corresponds to Ce 4d-4f resonant transition and assures increased spectral weight of Ce 4f electrons.

The obtained Fermi surface of Ce_3PdIn_{11} has a complex structure with some branches having similar shapes to those found previously in related heavy fermion superconductors: Ce_2PdIn_8, Ce_2RhIn_8, Ce_2IrIn_8 and $CeCoIn_5$. Heavy fermion bands with increased 4f electron contribution are observed near the Fermi energy (E_F). They exhibit hybridization effects between conduction band and Ce 4f electrons such as anomalies in the dispersion and enhanced effective mass. The calculations of the band structure resolved the contributions of Ce atoms from 2g and 1a lattice sites. The energy splitting of 50 meV found in the spectra related to $f^1_{7/2}$ final state is attributed to crystal field effect. The observed dependence of peak width near E_F indicates a Fermi liquid state in the investigated compound.

Flat bands at the Fermi level in unconventional superconductor YFe_2Ge_2

Rafał Kurleto[1,2], Swagata Acharya[3], Cheng-Hsun Wu[2], Dushyant Narayan[2], Bryan Berggren[2], Peipei Hao[2], Amanda Shackelford[2], Hope Whitelock[2], Zachary Sierzega[2], Makoto Hashimoto[4], Donghui Lu[4], Chris Jozwiak[5], Peyton Cline[3], Dimitar Pashov[6], Jiasheng Chen[7], Mark van Schilfgaarde[3], F. Malte Grosche[7], Daniel Dessau[2]

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We report heavy electron behavior in unconventional superconductor YFe_2Ge_2 ($T_C = 1.2$ K). We directly observe very heavy bands ($m_{\text{eff}} \sim 25m_e$) within $\sim$ 10 meV of the Fermi level EF using angle-resolved photoelectron spectroscopy (ARPES). The flat bands reside at the X points of the Brillouin zone and are composed principally of d_{xz} and d_{yz} orbitals. We utilize many-body perturbative theory, GW, to calculate the electronic structure of this material, obtaining excellent agreement with the ARPES data with relatively minor band renormalizations and band shifting required. We obtain further agreement at the Dynamical Mean Field Theory (DMFT) level, highlighting the emergence of the many-body physics at low energies (near EF) and temperatures.

Quantized thermal Hall conductance and the topological phase diagram of a superconducting bismuth bilayer

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Two-dimensional topological superconductors with chiral edge modes are predicted to possess a quantized thermal Hall effect proportional to the Chern number, exactly half that for chiral topological insulators. However, not much work has been done in identifying the quantized heat conductance in the literature, even for some of the standard models of topological superconductivity. Here we introduce a model based on a proximity induced superconducting bismuth bilayer and directly calculate the thermal Hall conductance of this lattice model. This model serves as a demonstration of the state of the art possible in such a calculation, as well as introducing an interesting paradigmatic topological superconductor with a rich phase diagram. We demonstrate the quantized thermal Hall plateaus in several different topological phases and compare this to numerical calculations of the Chern number, as well as analytical calculations of the Chern number's parity invariant. We demonstrate that it is possible to get a reasonable topological phase diagram from the quantized thermal Hall calculations. The technique used can be applied to a wide range of models directly in real space.

Structure and concentration of electronic defects and their mobility in $YBa_2Cu_3O_{6+x}$

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The paper presents an attempt to interpret concentrations of electronic and ionic defects and their transport properties in $YBa_2Cu_3O_{6+x}$ when assuming that dominating defects are electron holes and interstitial oxygen ions. Using the results of the studies of the deviation from the stoichiometry in $YBa_2Cu_3O_{6+x}$ in temperatures 623-1273 K, obtained by several authors, diagrams of concentrations of point defects were determined in the range of oxygen pressures where this compound exists.

Using the concentration of electronic defects in $YBa_2Cu_3O_{6+x}$ resulting from diagrams of defects' concentrations, an interpretation of the results of the studies on electrical conductivity was performed. It was found that the effective concentration of charge carriers, which is proportional to electrical conductivity of $YBa_2Cu_3O_{6+x}$, is significantly higher than the concentration of holes and it strongly increases when the oxygen pressure increases. The obtained results indicate that, in a constant temperature, the mobility of holes in $YBa_2Cu_3O_{6+x}$ depends on the square of the concentration of interstitial ions.

Using the effective concentration of charge carriers in $YBa_2Cu_3O_{6+x}$, determined using the values of electrical conductivity, the concentration of holes and electrons and fitting the kinetic constants A_h and A_e, the dependence of thermoelectric power on oxygen pressure was determined, with a good match to the experimental results.

Emergent "quantum" critical point for charge-density-wave ordered materials

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There are two broad classes of phase transitions known in critical phenomena: thermal phase transitions, which typically go from an ordered phase to a disordered phase (driven by thermal fluctuations) and quantum phase transitions, which typically go from an ordered phase to a quantum coherent phase at zero temperature (driven by quantum fluctuations). Here, we introduce a new class of transitions that lie in between these two, which we call an emergent quantum phase transition. This system has no quantum phase transition at $T = 0$, but it has a transition (here a metal-to-insulator transition) that is present for all nonzero T including the limit as $T \to 0$. At nonzero temperatures, the system displays similar behavior to that of a quantum-critical system, with scaling behavior seen in the resistivity, but the emergent quantum critical point does not arise from a thermal critical point being suppressed to $T = 0$. We illustrate this phenomena with an exact solution of the emergent metal-insulator transition of the charge-density-wave phase in an electronic system that also has both thermal order-disorder transitions and a Mott-like metal-insulator transition. We discuss the origin of this phase through thermally activated defect states, and how one can identify this behavior in experimental systems.

Magnetism and phase transition of UTe_2

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For the magnetic properties of UTe_2 the correlated band theory implemented as a combination of the relativistic density functional theory with exact diagonalization [DFT+U(ED)] of the Anderson impurity term with Coulomb repulsion U in the 5f shell needs to be applied. This allows us to determine the orbital to spin ration as well as number of the uranium valence states in close correspondence with recent experiment (XANES, XMCD). The uranium atom 5f-shell ground state with 33% of f^2 and 58% of f^3 configurations is determined [1]. In contrast to the above, for the bonding in UTe_2 it is satisfactory to be modelled by DFT+U methodology. We theoretically determined the lattice contribution to the specific heat of UTe_2 over the measured temperatures ranging from 30 to 400 K as well as the the orthorhombic-to-tetragonal phase transition pressure of 3.8 GPa at room temperature in very good agreement with the recent experimental studies. Last, but not least we determined the Raman spectra that were compared with recent Raman scattering experiments as well.

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Evidence for the valence-bond pairing in low-dimensional two-orbital system

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Resonating valence bond states as the formation mechanism of Cooper pairs, eventually leading to high-temperature superconductivity, remain a controversial topic. Although valence bond-like states find relevance in the description of quantum spin liquids and can be found in the spectrum of some specific spin models, in the realm of many-body fermionic Hamiltonians, the evidence for such states as ground states wave functions remains elusive, challenging the valence-bond pairing mechanism. Here, we present evidence of a valence bond solid-like (VBS) state with pairing tendencies in the ground state, particularly at finite doping. We achieved this for the generic two-orbital Hubbard model in low dimension, where the VBS can be associated with the presence of the topological order. Utilizing density-matrix renormalization group calculations, the study reveals key properties akin to those observed in superconductors' phase diagrams, such as pairing restricted to the regime of small but nonzero doping, presence of coherent pairs and charge-density-wave formation, all induced by the VBS ground state.

Optical manipulation of bipolarons in a system with nonlinear electron-phonon coupling

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We investigate full quantum mechanical evolution of two electrons nonlinearly coupled to quantum phonons and simulate the dynamical response of the system subject to a short spatially uniform optical pulse that couples to dipole-active vibrational modes [1]. Nonlinear electron-phonon coupling can either soften or stiffen the phonon frequency in the presence of electron density. In the former case, an external optical pulse tuned just below the phonon frequency generates attraction between electrons and leads to a long-lived bound state even after the optical pulse is switched off. It originates from a dynamical modification of the self-trapping potential that induces a metastable state. By increasing the pulse frequency, the attractive electron-electron interaction changes to repulsive. Two sequential optical pulses with different frequencies can switch between attractive and repulsive interaction. Finally, we show that the pulse-induced binding of electrons is shown to be efficient also for weakly dispersive optical phonons, in the presence anharmonic phonon spectrum and in two dimensions.

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Shining a light on the cuprate puzzle: Quasiparticle versus "unparticle" physics

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One of the fundamental questions in correlated electron systems is whether its low-energy physics can be described in terms of electronic quasiparticles – or these decay and we are left with the "unparticle" physics [1]. A paradigmatic example of such a situation can be found in the lightly doped cuprates, i.e. antiferromagnets with added mobile holes. These, depending on the system dimension, either support well-defined electronic quasiparticles (spin polarons) or fractionalisation into spinons and holons takes place [2].

In this talk, I will first give an alternative understanding of the difference between the spin polaron and the spinon-holon fractionalisation [3]. Next, I will discuss which of these two descriptions seems more appropriate to the lightly doped cuprates. To this end, I will present an overview of our recent studies of the angular-resolved photoemission (ARPES) spectra of the undoped cuprates, all showing a prominent stability of the fermionic quasiparticles irrespectively of whether they are of a quasi-1D or quasi-2D variety [4].

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Channeled vortex motion, experimental aspects

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Josephson effects with pure sine current-phase relationship persist only in weak links having dimensions of the order of the superconducting coherence length. Voltage states observed in experimentally achievable high-T_c bridges are not related to the Josephson effects but to the dissipation caused by the motion of Abrikosov vortices. The coherent motion of vortices leads to the appearance of quasi-Josephson effects. At low applied magnetic fields and currents, interactions between vortices are relatively weak and their motion is generally not coherent. To enforce the coherent motion, one has to restrict the vortex motion to spatially restricted channels of easy vortex flow. In current biased superconducting thin films, vortices penetrate the film through weak spots in the edge surface barriers and move along the paths curling between the existing natural pinning sites in the film bulk. The shape and location of such channels are determined by the surface barriers and the distribution of pinning sites in the specimen bulk. The uncontrolled and random nature of such spontaneous channels prevents observations of coherent effects in a wide range of experimental parameters. To obtain more controlled vortex motion, one has to create well-defined channels of easy vortex motion. Such channels can be fabricated by enhancing pinning outside the channel area or by lowering it inside the channel banks. Alternatively, channels can be manufactured by locally depressing superconductivity in the channel area. There are several methods for fabricating channels with suppressed superconductivity. Irradiation by accelerated ions or particles is a well-known technique for modifying the structural and electrical properties of superconducting thin films. A disadvantage of high-energy methods is the need for dedicated accelerator equipment and relatively high costs. In this talk, we discuss experimental aspects of the fabrication of vortex channels in high-T_c films using simple equipment easily available in many laboratories. Namely, irradiation with laser beam (laser writing) and low energy electron beam(electron writing) of a commercial scanning microscope.

Correlation between enhancement of superconducting state properties and crystallinity degradation due to chemical substitutions, applied pressure, and hydrogenation in Fe-Te-Se single crystals

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It was demonstrated that the almost ideal single crystal of $FeTe_{0.65}Se_{0.35}$ exhibits a greater width of superconducting transition in comparison with that of non-uniform sample of the same compound [1]. Resistivity results confirmed that the inhomogeneous spatial distribution of ions and presence of small hexagonal-like phase in chalcogenides with nanoscale phase separation seem to enhance the superconductivity in this system [2]. 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 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 confirmed that enhancement of superconductivity under pressure correlates with appearance of mosaicity [3]. It was shown that thermal diffusion of hydrogen into the crystals causes significant structural changes, leads to degeneration of crystal quality, and significantly alters superconducting properties, especially enhances the critical current density [4]. The critical current density studied in magnetic field up to 70 kOe increased 4–30 times as a consequence of hydrogenation at 200 °C for 10 h. Thermal diffusion of hydrogen into the crystals causes significant structural changes, leads to degeneration of crystal quality, and significantly alters superconducting properties. After hydrogenation, a strong correlation was noticed between the structural changes and changes in the parameters characterizing the superconducting state.

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Phase diagram of a double-quantum-dot-based Andreev molecule

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During this talk, I will present accurate results on the complete phase diagram of a double quantum dot system attached to a common superconducting contact, which comprises the so-called Andreev molecule. Such hybrid nanostructure has recently drawn a considerable attention. This is because it constitutes the basic building block of the so-called minimal Kitaev chain, i.e. Kitaev chain constructed in a bottom-up fashion in a fully controllable manner, the implementation of which shall open new avenues for exploring the physics of Majorana quasiparticles. Using the numerical renormalization group method, we map out the phase diagram of Andreev molecule, which features singlet, doublet, and a relatively uncommon triplet ground states, with the latter being a distinct signature of strong lead-mediated interactions between the quantum dots. Moreover, we benchmark the applicability of widely-used simplified effective models, such as atomic limit or zero bandwidth model, revealing their severe limitations. In particular, we show that most of effective models fails in reproducing the triplet ground state and make several false predictions. These findings provide crucial insights for interpreting experimental observations and designing superconducting devices based on quantum-dot architectures.

If the time allows, I will also review our recent results on critical behavior of hybrid quantum impurity systems, spatial extension of correlated states in such nanostructures, as well as on the concept of quartet superconductivity.

Real materials containing kagome lattice: lattice dynamics perspective

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The ideal two-dimensional kagome lattice has attracted significant attention due to its characteristic electronic band structure features. Unlike the honeycomb lattice, which exhibits Dirac and saddle points, the kagome lattice also hosts an ideal flat band. This unique lattice structure corresponds to rich physics, especially in the context of electronic properties. In several compounds containing the kagome sublattice, the realization of charge density waves (CDW) at low temperatures has been reported.

First, AV_3Sb_5 (A = K, Rb, Cs) compounds are rare examples where CDW coexists with superconductivity. The CDW is realized through atom displacement within the V-kagome sublattice [1]. Second, FeGe exemplifies a case where CDW is induced by correlation-driven phonon softening, resulting in a significant modification of the Ge atom [2]. In both cases, new system symmetries can be identified through phonon spectra analyses.

Lattice dynamics can also lead to intriguing findings. For CoSn-like compounds (P6/mmm symmetry), where both kagome and honeycomb lattices are present, we have discovered chiral phonons [3]. Additionally, in some cases, imaginary soft modes are observed, leading to new symmetries. In our study, we predicted the crystal structure of RhPb with P-62m symmetry (containing a distorted kagome lattice), which was confirmed experimentally [4].

In summary, studies of lattice dynamics can be a valuable tool to confirm [5] or negate [6] the realization of structures containing kagome-like sublattices.

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Chiral spin fluctuations: the role of lattice geometry

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The scalar spin chirality, characterizing a non-coplanar spin configuration is defined as a mixed product of three neighboring spins $\chi = S_i \cdot (S_j \times S_k)$. Via the coupling with quantum-mechanical electrons, this quantity translates the microscopic details of magnetic structure to the language of measurable off-diagonal transport responses such as Hall and Nernst effects. Apart from static spin textures such as skyrmions, finite χ can also be produced by temporary configuration of thermally fluctuating spins [1]. We demonstrate that the geometry of the underlying lattice plays the crucial role in promoting chiral spin fluctuations, and identify the arrays of at least two different polygons as the most promising class [2].

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Interplay of superconductivity with magnetic and charge orders tuned by disorder

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Composition-temperature phase diagram of iron based superconductors, heavy fermions, cuprates, ... consists of spin (SDW) or charge order (CDW) transition line intersecting superconducting dome. Those orders inhibit superconductivity (SC), but in the same time their fluctuations provide "glue" for pairing. Elucidation of this puzzle attracts big research effort. Among the deployed methods, introduction of nonmagnetic point disorder produced by energetic particle irradiation, provides additional control parameter, touchstone for possible interpretations. Disorder acts via carrier scattering and affects SC gap structure, CDW & SDW phases limits, fundamental parameters such as quantum critical points and upper critical field in multiband superconductors. In my presentation, I will review experiments tracking evolution of the superconducting gap structure under effect of disorder, interplay of itinerant magnetism with SC phase, peculiarities of SC emerging from CDW phase background (mimicking Higgs bosons), possible emergence of novel phases due to supressions by disorder of SDW ground state or non-Fermi liquid.

This work was realized in collaboration with Romain Grasset at Ecole Polytechnique and teams lead by Ruslan Prozorov, Makariy Tanatar (Ames Laboratory, USA) and Takasada Shibauchi (Tokyo University, Japan).

REBCO CC angular critical current up to 45 T using torque magnetometry

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REBCO CC tapes represent a transformative technology with profound implications for various industries, particularly in magnet technology for nuclear fusion reactors, a potential cornerstone for sustainable energy generation. However, REBCO CC tapes face challenges, especially when it comes to characterizing their performance at low T and high B, where exceptionally high I_c makes transport tests difficult. While characterization at $T \gtrsim 50$ K is easy, it does not necessarily extrapolate to lower T due to different pinning mechanisms.

A simple torque magnetometer [1] allows for the assessment of $I_c(B, T, \theta)$ across the full angular range, at T up to 50 K, and B up to 45 T. The magnetometer uses large samples, allowing the contributions of reversible magnetization from vortices to be neglected. This technique also facilitates the study of screening currents, AC losses, and flux jumps—all of which are relevant to magnet construction. The $I_c(B, T, \theta)$ values derived from torque measurements agree well with transport data. We found that $I_c(B, T) \propto \exp(-B/B_0) \exp(-T/T_1)^s$ near the $B \parallel$ ab plane, while beyond it, $I_c(B, T) \propto B^{-\alpha} \exp(-T/T_0)$. At $B = 30$ T and $T = 4.2$ K, I_c varies from about 400 to 1400 A, with the FWHM of the ab plane I_c peak spanning from 7 to 32 degrees. This rich diversity of REBCO tapes allows for the selection of appropriate conductors for different parts of the magnet.

A. M. Constantinescu, A. Xu, A. Francis, and D. Larbalestier contributed to this study. The NHMFL is supported by the NSF and the State of Florida.

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Unconventional superconductivity and topology in moiré transition metal dichalcogenide bilayers

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It has been reported in recent years that the moiré transition metal dichalcogenide (TMD) bilayers host rich physics including: interaction driven metal-insulator transition, different forms of charge ordering, unconventional superconductivity as well as quantum anomalous Hall behavior. Here, I review our recent theoretical results [1-3] concerning moiré TMDs and confront them with the available experimental data. In particular, as I show our approach based on the effective single-band model leads to a qualitative agreement with the recent measurements for the twisted WSe_2 homobilayer [4, 5]. Moreover, according to our analysis the paired state is of highly exotic type with the order parameter characterized by a mixed $d+id$ (singlet) and p-ip (triplet) symmetry. The obtained superconducting state has non-trivial topology with a non-zero value of the Chern number which could be tuned by the experimentally controllable parameters. Additionally, we analyze the formation of the Mott insulating state as well as the magnetically ordered states in moiré TMDs. Our results show that these systems are promising candidates for highly tunable materials that can serve as a testing ground for understanding the interplay between strong electronic correlations, topology and various types of symmetry broken states. This research was partly supported by National Science Centre, Poland (NCN) according to decision 2021/42/E/ST3/00128.

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Topological superconductivity in twisted bilayer cuprates: A microscopic perspective

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Application of a twist to stacked layers of a two-dimensional material may alter system electronic properties in a decisive manner, with interlayer twist angle serving as a new parameter to tune the phase diagram of the pristine system. Following progress in fabrication of thin films and monolayers derived from high-temperature cuprate superconductors, it has been recently proposed [1] that twisting copper-oxide layers may result in formation of topological superconducting states.

Incorporating the effects of strong-electronic correlations, we investigate a microscopic model of twisted bilayer cuprates, both as a function of interlayer twist angle and electronic density [2]. Extended t-J-U Hamiltonian is employed and analyzed within the framework of statistically-consistent Gutzwiller approach [3]. The obtained phase diagram encompasses gapless d-wave superconductivity, as well as gapped $d + \mathrm{e}^{i\varphi}d$ superconducting state that breaks spontaneously time-reversal symmetry and is topologically nontrivial. The $d + \mathrm{e}^{i\varphi}d$ phase occupies a butterfly-shaped region in the doping vs. twist-angle phase diagram and exhibits a reentrant behavior on its underdoped side. Relation to recent experiments will be briefly discussed.

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Quantum entanglement in $NaTiO_2$ – the consequence of spin-orbit interactions

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$NaTiO_2$ is one of the oxides exhibiting strange magnetic behaviour – it does not exhibit the long-range magnetic order showing, however, a pronounce drop of the magnetic susceptibility at 250 K. Due to this lack of the long-range magnetic order $NaTiO_2$ has been suspicious as having the Quantum Spin Liquid (QSL) ground state associated with its overall triangular lattice enabling geometrical frustration within the triangles of the Ti magnetic spins [1]. According to the developed Quantum Atomistic Solid State Theory (QUASST) [2] the ground state of the Ti^{3+} ($3d^1$) ion in $NaTiO_2$ in the exactly octahedral crystal field of oxygen ions, in the presence of the intra-ionic relativistic spin-orbit interactions, is the spin-orbital quartet (two Kramers doublets), often described by the effective $J = 3/2$, and a higher doublet (all originating from the 3-orbital t_{2g} "band"). In our calculations the trigonal off-octahedral distortion, originating from the $R\bar{3}m$ (SG166) crystal lattice, causes the splitting of the lowest quartet into two Kramers doublets. The total splitting of the t_{2g} "band" in the paramagnetic state contains within 80 meV. Spin-dependent interactions cause further splittings of three Kramers doublets.The most important result is that the Ti^{3+}-ion ground state is characterized by very small magnetic moment, of 0.04 μ_B only. The s-o interactions, even so small as 20 meV, allow to reveal the large orbital moment, of 1.04 μ_B, which almost fully compensates the spin moment of $S = 1/2$. For the possible realization of such exotic situation, leading to an exotic very weakly magnetic state of $3d^1$ oxides down to quite low temperatures, we pointed out already years ago [3] and recently for TiF_3 [4]. QUASST is the project for experimental and theoretical search of the discrete CEF+s-o low energy, below say 25 meV, electronic structure. Underlying the atomistic starting point of QUASST it is worth to put a question "how looks like the Ti atom in $NaTiO_2$ in other theoretical approaches" [5].

Our atomistic QUAAST approach underlying the importance of local distortions and the intra-ionic spin-orbit interactions for the physically adequate theoretical description of the magnetism and low-energy electronic structure, close to E_F, of 3d/4d/5d oxides one could shortly said that local lattice distortions and the intra-ionic spin-orbit interactions are strongly entangled producing the magnetism and the electronic structure. Thus, there are needs for further theoretical and experimental studies of transition-metal oxides, at the atomic and in the meV energy scale.

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Unconventional superconductivity in heavy-fermion Ce-based compounds

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Although it has been almost half a century since the discovery of this phenomenon, superconductivity in heavy-fermion systems remains incompletely understood and inadequately described theoretically. The reason is the richness of observed features, unconventional mechanisms of Cooper pairing and untrivial symmetry of wave functions that describe the superconducting condensate. In addition, new experimental findings in this field often lead to the identification of novel effects, which complicates efforts to create a coherent and universal theory of the heavy-fermion superconductivity.

In my lecture, first I will recall our team's success more than a decade ago in discovering heavy-fermion superconductivity in the previously unknown Kondo lattice Ce_2PdIn_8, which emerges in the close vicinity of the magnetic field-induced quantum magnetic phase transition. I will also briefly present our results on the related compounds Ce_3PdIn_{11} and Ce_3PtIn_{11}, casting some doubt on the actual nature of the coexistence of the heavy-fermion superconductivity and long-range antiferromagnetic ordering, which was postulated for them in the literature. Finally, I will discuss the results of our most recent studies on the unconventional superconductivity in the dense Kondo system $CeRh_2As_2$, which is currently generating an extremely heated debate due to the hypothetical interplay of the superconductivity with the quadrupole density wave, but primarily due to the observed magnetic field induced phase transition within the superconducting state, interpreted as a change in the pairing symmetry from spin-singlet to spin-triplet.

Superconductivity in a ternary $Mg_4Pd_7As_6$ compound

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The synthesis and characterization of a new compound $Mg_4Pd_7As_6$, which was found to be a superconductor with $T_c = 5.45$ K. Powder X-ray diffraction confirms the $U_4Re_7Si_6$ structure (space group Im-3m, no. 229) with the lattice parameter $a = 8.2572(1)$ Å. Magnetization, specific heat, and electrical resistivity measurements indicate that it is a moderate-coupling ($\lambda = 0.72$) type-II superconductor. The electronic and phonon structures are calculated, highlighting the importance of antibonding Pd-As interactions in determining the properties of this material. The calculated electron-phonon coupling parameter $\lambda = 0.76$ agrees very well with the experimental finding, which confirms the conventional pairing mechanism in $Mg_4Pd_7As_6$.

$Mg_4Pd_7As_6$ is the first reported superconductor in the $U_4Re_7Si_6$ structure type system.

Low-Field Nodeless Superconducting State in the Presence of Local Magnetism in $CeRh_2As_2$ from Local Magnetization

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The tetragonal heavy-fermion superconductor $CeRh_2As_2$ with a critical temperature $T_c \approx 0.34$ K is believed to be the first and so far only example of a material that exhibits a field-induced transition between spin-singlet even-parity and spin-triplet odd-parity superconducting states [1]. Specifically, this material undergoes the putative field-driven transition when a magnetic field of ≈ 4T is applied along the c axis. In low fields, the spin-singlet state is surrounded by another ordered phase of an unknown origin with zero-field $T_0 \approx 0.5$ K. Here, we report the local magnetization results for high-quality single crystals of $CeRh_2As_2$ [2] using micro-Hall probe magnetometry down to $\approx 0.02T_c$. We show a rather moderate anisotropy of the lower critical field the temperature dependence of which for both crystallographic directions saturates below about 0.2 T_c, indicating fully gapped superconductivity in the spin-singlet state. In addition, we observe a small but clear increase in the a-axis magnetization from around T_0 which amounts to about 0.2 Oe in the $T = 0$ limit. Within the accuracy of our micro-Hall probe magnetometer, a spontaneous magnetic field is absent along the c-axis. Our results place important constraints on the spin-singlet order parameter in $CeRh_2As_2$ and provide evidence that a magnetic dipole with an in-plane moment is the local ground state of $CeRh_2As_2$ when the system is at ambient conditions.

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Selective screening of the Coulomb interaction and the resulting superconductivity in monolayer $NbSe_2$

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The Fermi surface in NbSe2 is split into three pockets, around the Γ, K and K' points. The presence of different pockets divides the Coulomb scattering processes into subsets with different scattering ranges. The competing repulsion events at different ranges can result in the formation of Cooper pairs, provided that the short-range repulsion is stronger than the long-range one. We solve the set of self-consistent gap equations down to zero temperature and find that depending on which of the interaction types is dominant, the material can support superconducting gaps with different symmetries, both in the s and in the f pairing channel [1]. We analyze the dI/dV characteristics of recently performed STM experiments on NbSe2 [2] and find that while they are consistent with both one and two gaps, the agreement is better when two gaps are considered.

In order to gauge the strength of the interaction at different ranges we have calculated the screened Coulomb potential in this material, using the tight-binding model and the RPA approximation. Our results show that while the gaps at K/K' points can form in the absence of the Γ pocket, once it is included it can be a powerful player, even to the point of changing the symmetry of the gaps in the K/K' valleys.

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Study of magnetic properties of EuSnP single crystals

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EuSnP is an antiferromagnetic material in which the europium magnetic moments order at $T_N = 21$ K, although it is likely not a simple antiferromagnet [1-3]. For the study, single crystals of this compound grown from Sn flux were used. X-ray diffraction (XRD) results indicate that EuSnP crystallizes in the P4/nmm space group and EDX analysis confirms the high quality of the crystals. To gain more insight into the ordering of europium's magnetic moments, heat capacity, AC susceptibility, magnetization and Mössbauer spectroscopy (on ^{151}Eu) measurements were performed. Measurements were carried out as a function of temperature and applied magnetic field. During the presentation, the results of our study will be presented and discussed.

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Surface chiral metal and warped time-reversal symmetry

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A theory of dichroism and spin-dichroism is being developed for an archetypal quantum material Sr_2RuO_4 to describe the observed peculiarities in the circularly polarized, spin-selective, angular-resolved photoelectron spectroscopy [1]. A symmetry-broken flux phase with alternating chiral spin-orbital currents is postulated as a possible explanation. This phase is modeled using special form of a three-band t2g tight-binding model used earlier for ruthenium oxides [2,3] and it reveals a special form of a time-reversal symmetry with a non-trivial dependence on quasimomentum: warped time-reversal. This symmetry seems to play crucial role in establishing perfectly antisymmetric spin-integrated dichroic signal while keeping spin-resolved signal completely non-symmetric.

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Can analysis of chemical bonding help us find new intermetallic superconductors?

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A correlation between the occurrence of superconductivity and the presence of antibonding states at the Fermi level was recently found in several groups of materials (see eg. [1-3]). The phenomenon can be qualitatively understood as an unusual form of bonding optimization – relieving the electronic "stress" due to occupied antibonding states via an electronic structure “distortion”. Such a concept was previously proposed to rationalize the occurrence of itinerant ferromagnetism in intermetallic compounds [4].

I will present the results of chemical bonding analysis employing the molecular orbital theory and DFT-based bonding descriptors (eg. crystal orbital Hamilton population function – COHP) on several superconducting systems, including: Heusler phases, endohedral cluster compounds, and Laves phases [5, 6, 7]. I would also like to discuss the link between chemical bonding and the “magic electron count” behavior observed in many intermetallic systems.

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Electronic and magnetic properties of infinite-layer nickelates

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The discovery of unconventional superconductivity in thin film nickelates marks a significant milestone in the field of high-T_c superconductivity. Similar to cuprates, infinite-layer nickelates feature planar NiO_2 layers containing $3d$ electrons from nickel, making them compelling subjects for study. Superconductivity has been confirmed exclusively in 20% hole-doped thin films [1, 2], indicating that both doping and interface play crucial roles in understanding this phenomenon. Therefore, we conducted a comprehensive DFT+U study on bulk $NdNiO_2$ and $NdNiO_2/SrTiO_3$ thin films to uncover their electronic and magnetic properties. We investigate how Sr doping influences the electronic and magnetic structures, with particular emphasis on the impact of $4f$ electrons from Nd. For thin films, we analyze both capped and uncapped multilayers, and utilize layer-projected density of states to elucidate the role of interfaces. Our findings reveal significant differences between thin film and bulk material, suggesting a complex interplay of interface effects, hole doping, and correlation physics in nickelate compounds.

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The influence of Sm_2O_3 admixtures on morphology, transport critical current density and dominant pinning mechanism of MgB_2 materials investigated by using the transmission electron microscope

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The results shows influence of Sm_2O_3 admixtures on the morphology, crystal structure, transport critical current density at the temperature range from 15 K to 30 K, dominant pinning mechanism at 20 K and 30 K, critical temperature, irreversible magnetic field, upper magnetic field. The superconducting MgB_2 material was made by using the powder-in-tube (PIT) method. The transmission electron microscope (TEM) images were made for the longitudinal section of MgB_2 material. The transport measurements and TEM photos point out that the Sm_2O_3 doping significantly changes the morphology of the MgB_2 material, accelerates the formation of the MgB_2 phase and does not form rectangular MgB_2 crystallites. Moreover, the Sm_2O_3 admixture does not leave pure Mg and forms Sm_2O_3 areas of 10 nm and 20 nm. This indicates that the Sm_2O_3 addition allows to obtain point pinning centers. Additionally, analysis of the results indicates that the Sm_2O_3 doping significantly increases the transport critical current density, does not increase the irreversible magnetic field and slightly increases the upper magnetic field. In addition, the analyzes showed for the first time the influence of the Sm_2O_3 doping on the formation of the MgB_2 superconducting phase. The TEM images pointed out that rectangular MgB_2 crystallites are formed in undoped MgB_2 material, which have not been previously reported. Our research showed that the rate of formation of the superconducting MgB_2 phase depends on the density of the unreacted Mg + 2B material.

Large magnetoresistance and first-order phase transition in antiferromagnetic single-crystalline $EuAg_4Sb_2$

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We present the single crystal growth and results of a thorough investigation of the physical properties of a potential topological material, $EuAg_4Sb_2$, using magnetization, heat capacity, and electrical resistivity measurements. High-quality single crystals were grown using the flux method. Temperature-dependent magnetization measurements along different crystallographic orientations confirm two antiferromagnetic phase transitions around $T_{N1} = 10.5$ K and $T_{N2} = 7.5$ K. Isothermal magnetization data exhibit several metamagnetic transitions below T_{N1}. Antiferromagnetic phase transitions in $EuAg_4Sb_2$ are further confirmed by two sharp peaks in the temperature-dependent heat capacity and resistivity data, which shift to the lower temperature in the presence of an external magnetic field. Our systematic heat capacity measurements utilizing a long-pulse and single-slope analysis technique allow us to detect a first-order phase transition in $EuAg_4Sb_2$ at 7.5 K. The magnetoresistance exhibits a broad hump due to the field-induced metamagnetic transition. Remarkably, the magnetoresistance keeps increasing without showing any tendency to saturate as the applied magnetic field increases, and it reaches $\sim$20000% at 1.6 K and 60 T. At high magnetic fields, several magnetic quantum oscillations are observed, indicating a complex Fermi surface. The H-T phase diagram constructed using magnetization, heat capacity, and magnetotransport data indicates complex magnetic behavior in $EuAg_4Sb_2$.

On "Computational supremacy in quantum simulation" of a quench dynamics in transverse-field Ising spin glasses.

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Quantum computers hold the promise of solving certain problems that lie beyond the reach of conventional computers. Establishing this capability, especially for impactful and meaningful problems, remains a central challenge. One such problem is the simulation of nonequilibrium dynamics of a magnetic spin system quenched through a quantum phase transition. In this respect, a recent article [1] reports on an extensive benchmark of D-Wave quantum annealing processor comparing its performance with several leading classical approximation methods, including tensor networks and neural networks. It delineates parameter regions (system size, Ising couplings geometry, quench times) where none of the above classical methods achieve the same accuracy as the quantum annealer within a reasonable timeframe. I'll focus on the limitations of tensor networks, in particular, projected entangled-pairs states ansatz, for performing such simulations.

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Are pairs of Majorana modes distantly cross-correlated?

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Topological superconductors in low dimensional systems are the plaform for realization of Majorana quasiparticles, due to the bulk-boundary correspondence. These zero-energy modes do always emerge in pairs (at boundaries or local defects) and can be viewed as fractions of electrons, obeying non-Abelian statistics. It is not clear, however, to what extent (if at all) such pairs of the zero-energy quasiparticles are mutually crosscorrelated. To explore this issue we consider a hybrid structure with two quantum impurities interconnected through the topological superconducting nanowire. Under static conditions we don't find any evidence for their interdependence. In contrast, signatures of their nonlocal cross-correlations seem to persist over nanosecond scale in nonequilibrium situations [1]. We discuss possible means for their detection, using the currently available spectroscopic techniques.

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The role of the electron correlations effects on electronic and magnetic properties of 2D antiferromagnetic crystals.

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The intricate interplay among correlated electrons, the crystal lattice, and magnetic phenomena can result in rich physical effects [1]. In 2D materials containing open d- or f- shells, the additional quantum confinement resulting from reduced dimensionality suppresses the screening effects, potentially enhancing electron correlations. The recent emergence of magnetic 2D materials introduces a novel magnetic functionality to the existing portfolio of 2D materials [2]. The magnetic properties of these materials are highly sensitive to external factors such as pressure, stacking configurations, and external fields.

In this work, we focuses on the transition metal phosphorous trichalcogenides semiconductors (MPX_3 , M=Mn, Ni, Fe, Co, X=S, Se) – as a prototype antiferromagnetic (AFM) semiconducting materials exhibiting honeycomb lattice [3]. We investigate the role of electron correlations on the magnetic interactions and impact of the magnetic interactions on various properties [4]. The effective model hamiltonians, based on the ab intio result within DFT+U approach [5, 6] qualitatively reproduce the ratios and signs of all experimentally observed magnetic couplings [5]. Our results reveal an effective tuning of magnetic interactions and anisotropies upon nonmagnetic substitution [6]. Finally, we demonstrate electronic and magnetic phase diagrams for different parameter spaces considered in monolayers and explain the role of electron correlations in this class of materials.

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Superconducting properties of p-block-based ternary hydrides XC_2H_8 at low pressures

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The search for high-temperature superconducting hydrides has entered a new phase, departing from examining binary hydrides and shifting the attention toward ternary compounds characterized by potentially better superconducting properties. Therefore, we have analysed the $Fm\overline{3}m$ space group, which has been identified as responsible for the highest critical temperatures in binary hydrides [1], adding a third element to the system. We have shown that carbon is a promising dopant to stabilize the structure simultaneously reducing the pressure [2]. Furthermore, we predicted a novel family of superconducting ternary hydrides under moderate compression, XC_2H_8 (where X = Ga, In, Tl, Sn, Pb, Sb, Bi, Te, Po). We have demonstrated that superconductors containing elements from the 13^{th} group of the periodic table achieve stability at the lowest pressures (12 GPa) while the highest critical temperature of 73 K (100 GPa) was obtained for the SbC_2H_8.

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Higher order spin interactions mediated by the substrate

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Itinerant electrons are known to be capable of mediating an effective interaction between local moments over large distances. Such a coupling between two impurities is the well established Ruderman-Kittel-Kasuya-Yosida interaction, which due to its oscillatory nature influences the magnetic ordering of impurities depending on their concentration. A question arises if a larger collection of local moments can also interact via the underlying lattice's electrons. A perturbative treatment of the problem reveals that it is the case, and the effective interaction resembles the ring (or cyclic) exchange, known as a higher order effect in the Hubbard model.

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Surface state manipulation and topological Lifshitz transitions in NbP

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Proximity-induced superconductivity has emerged as a fertile ground for manifesting Majorana zero-bias states in topological materials [1]. This advancement underscores the necessity of manipulating and controlling surface states [2]. In our study, we utilized angle-resolved photoemission spectroscopy (ARPES), a surface-sensitive technique, on a single crystal of NbP (topological Weyl semimetal) to explore these phenomena. We identified cleaved surfaces with P- and Nb-terminations, each displaying distinct features in constant energy contours [3]. By depositing Nb and Pb on the cleaved (001) surface of NbP, we successfully created Pb/NbP and Nb/NbP interfaces and investigated their electronic structures. Our results show that 0.5 ML of Pb and 0.8 ML of Nb deposited on P-terminated NbP induce significant modifications in the Fermi surface, attributed to a topological quantum Lifshitz transition (TQLT). This transition is evidenced by transforming the Fermi surface from a bow-tie shape (trivial surface states) to a lemniscate (∞) shape. Additionally, the deposition of 1.9 ML of Pb on Nb-terminated NbP results in Fermi surface modification showing ordinary Lifshitz transition [4]. These findings provide valuable insights into the electronic structure modifications of NbP surfaces, enhancing our understanding of topological and superconducting states in these materials.

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Anharmonicity, electron-lattice coupling, and superconductivity in hydrogen-rich systems

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The advancements in high-pressure physics have unveiled a new class of superconducting materials, particularly hydrogen-rich compounds such as silane, hydrogen sulfide, and hydrogen lanthanide. These materials exhibit remarkable superconducting transition temperatures under extreme pressures. We investigate electron-correlation-driven conductivity, which is closely associated with the formation of high-symmetry hydrogen molecular and atomic planes. This study also encompasses a series of quantum phase transitions, both structural and electronic in nature.

To analyze these phenomena, we employ a combination of quantum chemical methods and density functional theory (DFT) calculations. These tools allow for an in-depth examination of the electronic structure, lattice dynamics, and the interactions governing the behavior of these complex systems. Additionally, we incorporate the effects of anharmonicity in the lattice vibrations, which play a critical role in accurately describing the phonon spectra and, consequently, the superconducting properties of these materials. Finally, by applying the McMillan formula, we predict the superconducting transition temperatures as functions of effective pressure, including both external and chemical contributions

Controlling the anisotropic properties of MgB_2 by charge doping and band scattering

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We will present selected normal and superconducting properties of MgB_2, which is increasingly used in technology, including magnetic resonance imaging devices. We will focus on several important characteristics of this compound, such as electrical resistance, thermopower and upper critical field, to determine the effect of well-defined doping (electron, hole, isovalent, and electron-hole simultanously) on these properties and thus better understand the nature of superconductivity in this compound and find a way to increase its critical parameters. We will present the results of experimental studies performed on single crystals (hence we will be able to determine their anisotropy) doped with Al, Li, C and Mn and simultaneously Al-Li and C-Li. The results were developed within simple models, which allowed the determination of important parameters characterizing inter- and intraband scattering and electron-phonon coupling in this compound.

High harmonic generation for phase detection and ultra-fast tracking in condensed matter systems

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The interaction between a strong laser field and matter results in a nonlinear optical process that gives rise to the generation of high harmonics of the incident frequency, which has emerged as a transformative technique for studying electronic systems, a contribution recognized with the 2023 Nobel Prize in Physics. Recently, there has been a growing interest in the use of high harmonic generation (HHG) to probe various properties of solid state systems. Spectroscopy based on HHG can serve as a tool of ultrafast imaging to detect signatures of quantum phase transitions in high-temperature superconductors, distinguish between trivial and nontrivial topology, and probe dynamical and structural properties of electrons. Here, we present theoretical results for high-harmonic spectroscopy for various condensed matter platforms. In particular, we show that it provides information about localization, delocalization and phenomena resulting from the interplay between them. Moreover, through a time-resolved emission of high harmonics, we capture the nature and dynamics of various optical excitations in a strongly correlated electronic system. Finally, we explore the possibilities of detecting different nontrivial topological phases through their nonlinear response.

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Unconventional superconductivity in a two dimensional electron gas at the LAO/STO interface.

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In recent years, oxide interfaces have attracted growing interest as a natural platform for studying the interplay among superconductivity, magnetism, spin-orbit interactions, and ferroelectricity [1]. The occurrence of all these phenomena within a single material, as observed in the $LaAlO_3/SrTiO_3$ (LAO/STO) interface, provides access to a variety of extraordinary superconducting phases, including p-wave or topological superconductivity, as well as the coexistence of magnetism and the superconducting state.

Although it is now well established that LAO/STO exhibits gate-tunable superconductivity with a dome-like shape of the critical temperature (T_c) as a function of electron concentration, similar to that observed in cuprates or Fe-based superconductors, the physical mechanism behind this behavior is still unclear and is the subject of ongoing debate. During the presentation, we will provide a brief overview of existing theoretical concepts explaining this phenomenon and present our model [2-4], in which the characteristic shape of T_c is explained as resulting from the interplay between the topology of the Fermi surface and the specific extended s-wave symmetry of the superconducting gap. Finally, we also analyze the critical in-plane magnetic field exhibiting a four-fold anisotropy due to the C4 symmetry of the Fermi surface. Our results will be discussed in the context of recent experiments.

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Strain-tuned magnetic frustration in La_2NiO_4

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Magnetic frustration is a route that can lead to the emergence of novel ground states [1], including spin liquids [2]. Such frustration can be introduced through either lattice geometry or incompatible exchange interactions. In this study [3], we devise a design principle for tuning antiferromagnetic (AF) exchange interactions on the square lattice. By studying the magnon excitations in La_2NiO_4 films using resonant inelastic x-ray scattering (RIXS) we show that, in contrast to the cuprates [4], the magnon dispersion peaks at the AF zone boundary. This indicates the presence of AF nearest neighbor (NN) and AF next-nearest neighbor (NNN) spin interaction. Using first principles simulations and an effective spin model, we demonstrate that the AF-NNN coupling is a consequence of the two-orbital nature of La_2NiO_4. By exploring La_2NiO_4 films grown on a different substrate, we illustrate that compressive epitaxial strain enhances this coupling and, as a result, increases the level of incompatibility between exchange interactions within a model square-lattice system.

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Topological superconductivity in Fibonacci quasicrystals

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We investigate the properties of a Fibonacci quasicrystal (QC) arrangement of a one-dimensional topological superconductor, such as a magnetic atom chain deposited on a superconducting surface. We uncover a general mutually exclusive competition between the QC properties and the topological superconducting phase with Majorana bound states (MBS): there are no MBS inside the QC gaps and the MBS never behaves as QC subgap states, and likewise, no critical, or winding, QC subgap states exist inside the topological superconducting gaps.

Surprisingly, despite this competition, we find that the QC is still highly beneficial for realizing topological superconductivity with MBS. It both leads to additional large nontrivial regions with MBS in parameter space, that are topologically trivial in crystalline systems, and increases the topological gap protecting the MBS. We also find that shorter approximants of the Fibonacci QC display the largest benefits.

As a consequence, our results promote QCs, and especially their short approximants, as an appealing platform for improved experimental possibilities to realize MBS as well as generally highlights the fundamental interplay between different topologies.

Exploring magnetic and topological phenomena in moiré $MoTe_2/WSe_2$ heterobilayer

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It has been reported in recent years, that the moiré $MoTe_2/WSe_2$ heterobilayer shows quantum anomalous Hall behavior indicating that it is an example of a two-dimensional topological insulator [1]. Interestingly, the fact that this phenomena is observed only at half-filling suggests that the interactions play a significant role. Here, we use an extended Hubbard model outlined in Ref. [2] to examine the interplay between topology and strong Coulomb interaction in the mentioned system. The applied theoretical approach resembles that of Kane and Mele [3] but supplemented with the interaction terms. By using both the mean-field approximation and the Gutzwiller approach we analyze the interplay between topology and interactions. In particular, we demonstrate the emergence of a topologically non-trivial canted AFM phase at half-filling in accord with the available experimental data. Additionally, at 2/3 filling we report the appearance of the Charge-Density-Wave state in the upper layer of the heterostructure, which is due to the significant value of the intersite Coulomb repulsion. This research was partly supported by National Science Centre, Poland (NCN) according to decision 2021/42/E/ST3/00128.

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Surprising transport in interacting 1D chain

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I will show that in a periodically driven, many-body titled lattice, there are sets of spatially fractured resonances. The confluence of these fractured resonances dramatically enhances transport. At one confluence, the interaction strength is finite and the essential resonance arises due to the interplay of interaction with the counter-rotating terms of the periodic drive. I will discuss the origin and structure of the fractured resonances, as well as the scaling of the conductance with system parameters. These results furnish a new example of the richness of open, driven, many-body systems. For details see arXiv:2308.12346.

Topological superconductivity in planar Josephson junctions

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Semiconductor-superconductor hybrids are a promising platform for realization of topological superconductivity that host exotic quasiparticle excitations like Majorana bound states. Recently, research efforts lean towards the exploitation of planar Josephson junctions realized on proximitized two-dimensional electron gases. In such structures the phase difference between the superconductors constitutes a convenient knob that allows the system to be tuned to the topological regime [1]. In these systems the Majorana bound states can be probed experimentally via tunneling spectroscopy, which, as we show, reveal the evolution of Andreev bound states in an external magnetic field [2]. We show that the topological transition is imprinted in the change of non-local conductance sign, but unfortunately this can be obscured in realistic systems, where the phase bias is realized by flux biasing a superconductor loop embedding the Josephson junction [3]. We demonstrate how this problem can be overcome by amplification of the spin splitting by elongation of the junction [4].

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Phenomenology of many-body localization in bond-disordered spin chains

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The phenomenon of many-body localization (MBL) is an intriguing area of study, as it challenges the principles of statistical mechanics by avoiding thermalization. Although the status of MBL as a dynamical phase of matter is to be addressed, this does not diminish the importance of the regime of (nearly) arrested dynamics at strong disorder strengths. Typical studies on MBL consider the presence of on-site disorder; the phenomenological properties in the MBL regime can then be described within the framework of local integrals of motions (LIOMs) identified as dressed single-site operators. This talk will focus on a bond-disordered Hamiltonian, a model relevant for experiments in Rydberg atom platforms, which shows nonparadigmatic features in the MBL regime that are not captured within a standard LIOM description. Instead, a simple renormalization group-based scheme will be used to elucidate the eigenstate properties and reveal appropriate probes for experiments. It will also illustrate how to extend this scheme to more generic Hamiltonians.

The talk is based on: arXiv:2405.10062

Antiferromagnetic phase in infinite-layer superconducting nickelates, a Hartree-Fock perspective

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We investigate infinite-layer, superconducting nickelates by performing unrestricted Hartree-Fock calculations for a two-layer system – an interacting Nickel layer coupled to a non-interacting Neodymium layer. We consider different electronic fillings n, as well as different Nickel-Neodymium charge transfer energies ϵ. Our results show that the ground state of the undoped system with a realistic value of ϵ lies right at the phase bondary between ferromagnetic (FM) and antiferromagnetic (AFM) phases. As the total filling n increases beyond the undoped case ($n = 1$), the AFM phase becomes the ground state. Similarly, increasing ϵ also pushes the system towards an AFM ground state. We explain these results by analyzing the 'self-doping' effect, that is the escape of charge from the Nickel to the Neodymium plane, captured by our calculations.

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Abstracts:
Poster presentations

Prussian Homage
Jan Matejko, 1879–1882

Oil on canvas
Dimensions: 388 cm × 785 cm
Location: Sukiennice Museum, Kraków

Unconventional superconductivity in moiré transition metal dichalcogenide heterobilayer

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In recent years, it has been established experimentally that the moiré transition metal dichalcogenide (TMD) bilayers host rich physics including: interaction driven metal-insulator transition, different forms of charge ordering, unconventional superconductivity as well as quantum anomalous Hall behavior. Here, we study the general features of the unconventional superconducting state for the case of effective single- band model as applied to the WS_2-WSe_2 heterobilayer. Our analysis indicate the stability of the paired state which is of mixed singlet-triplet type, however, the spin-triplet contribution plays the major role. Our calculations do not find any prominent changes of the superconducting symmetry due to the longer-range interaction and hopping terms. We find that the inclusion of the intersite Coulomb repulsion term suppresses the superconducting pairing, however the paired state still survives for realistic values of the interaction integral, V. Our theoretical analysis indicate the WS_2-WSe_2 heterobilayer as a promising candidate for the appearance of the unconventional superconducting state.

Vortex dynamics in disordered niobium thin films

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Vortex matter in type-II superconductors is one of the most intriguing research topics in superconducting physics. Both the VG phase transition and flux lines creep phenomenon have been widely studied in the past, mostly in high temperature superconductors where thermal fluctuations play a crucial role. Evaluation of these subjects is also very interesting in case of ultrathin conventional SC films which can be useful in many applications. In our work, we study the evolution of vortex matter in ultrathin, polycrystalline niobium films with film thickness ranging between 7.4 and 44 nm, using resistance and current-voltage characteristics measurements. We analyze creep behavior using recent strong pinning theory what provides detailed insight into vortex physics. Our findings reveal the existence of two distinct regimes of vortex pinning. One regime, which is due to spatial variations of the mean free path, occurs in thickest film, and the other regime, due to spatial variations of the superconducting transition temperature, arises in thinner films. According to strong pinning analysis, the temperature dependence of the activation barrier energy (a major parameter for describing thermal creep of the vortex system) does not strictly follow existing theoretical predictions, what calls for more theoretical studies of the subject.

Electronic structure of PrBi, a candidate for a strongly correlated Dirac semimetal

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PrBi is a simple monopnictide, which crystallizes in a rock salt structure. It was theoretically predicted that PrBi is a strongly correlated Dirac semimetal with symmetry protected Dirac nodes [1]. It is expected that a non-Fermi liquid state is realized in this compound [1] and in contrast to a concept of Landau quasiparticles the imaginary part of self-energy is predicted to depend on square root of energy. In addition to the intriguing theoretical predictions, it was found experimentally that PrBi has a very large [2] and anisotropic [3] magnetoresistance. We present angle-resolved photoemission studies of PrBi crystals cleaved along (100) plane. Band structure and Fermi surface is mapped systematically for photon energies between 12 eV and 100 eV. It appears that the observed band structure has an important contribution of quasi two-dimensional features. Prominent hole pockets around the Γ point are well visible. Dirac cones at $\bar{M}$ and nodal lines along $\bar{\Gamma}$ - $\bar{M}$ are clearly recognized. The spectra are also analyzed to verify the predicted absence of Landau quasiparticles.

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Superconducting properties of 2DEG at the (111) $LaAlO_3/SrTiO_3$ interface

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The two-dimensional electron gas (2DEG) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface not only exhibits a characteristic dome-like shape of the critical temperature as a function of electron concentration but also sparks a discussion about the coexistence of superconductivity and magnetic ordering in these heterostructures. The superconducting properties of LAO/STO have recently been widely studied for materials grown along the [001] crystallographic direction, but much fewer experimental and theoretical works have been dedicated to the [111] direction.

In this work, we present a theoretical study of the superconducting properties of 2DEG in LAO/STO grown along the [111] crystallographic direction. We find that honeycomb lattice leads to non-trivial superconducting gap symmetries, including non-negligible contribution of exotic triplet *p-wave* symmetry. Moreover, we find that due to the intrinsic electric field at the interface, next-to-nearest-neighbor pairing plays a crucial role in superconducting properties, generating superconducting gaps larger compared to those generated by nearest-neighbor pairing.

To provide a direct comparison with the experimental results, we also analyze the critical temperatures as a function of the electron concentration.

Many-body localization crossover is sharper in quasiperiodic spin chains

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Due to a phenomenon of many-body localization (MBL), the strong disorder may significantly slow down or even completely hinder the thermalization of quantum many-body systems. A sufficiently deep quasiperiodic potential may also inhibit thermalization. In this work, we numerically demonstrate direct differences in the behavior of standard ergodicity breaking indicators at the MBL crossover in random and quasiperiodic systems. Our key finding is the exponential increase in the sharpness of the MBL crossover with system size for quasiperiodic systems, a trend that is only linear in disordered systems. The strong tendency towards a non-analytic behavior in quasiperiodic systems is consistent with the existence of dynamical regimes with sharply defined boundaries or an MBL phase transition. It highlights the importance of quasiperiodic systems for our understanding of many-body dynamics.

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^+ molecules/ions with the help of our original **E**xact **D**iagonalization **AB I**nitio (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 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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Theoretical studies of interplay between unconventional superconductivity and altermagnetism

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Altermagnetism [1, 2] is new type of magnetism, comprising features of ferromagnetism and antiferromagnetism. Just like ferromagnets, altermagnets presents spin-split electron structure and broken time-reversal symmetry. Despite this, total net magnetization of altermagnetic compounds is zero, what is characteristic for antiferromagnetic materials. However, opposite spin sublattices are connected by rotational, not translational or invariant symmetries. The most recognized example of altermagnet is RuO_2. Wide studies of this compound, both experimental and theoretical, provided evidence for creation of two Fermi surfaces with different spin orientation ("spin up" and "spin down"), with *d*-wave symmetry. Here, we discuss possible coexistence of unconventional superconductivity and altermagnetism within an effective single band model supplemented with intersite Cooper pairing term. Our approach allows for studying various pairing and altermagnetic symmetries. As we discuss, interplay between the two phenomena might lead to the appearance of non-zero momentum Cooper pairing in the absence of external electric and magnetic field, i.e. Fulde-Ferrell-Larkin-Ovchinnikov phase (FFLO) [3, 4].

Research partly supported by program "Excellence initiative – research university" for the AGH University of Krakow.

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Evolution of the supercoducting state in $Zr_{2-x}Hf_xCo$ solid solutions

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In single-gap, BCS-type intermetallic superconductors, the critical temperature usually decreases with the applied pressure. Surprisingly, the critical temperature of Zr_2Co almost doubles under the pressure of 8 GPa [1].

In this study, we report the synthesis and physical properties of $Zr_{2-x}Hf_xCo$ solid solutions for $0 < x \leqslant 0.625$, probed with magnetic susceptibility, transport, and heat capacity techniques and supplemented with electronic structure calculations. We confirm that Hf substitution shrinks the crystal lattice of Zr_2Co, acting as a "positive" chemical pressure. With increasing x, there is a monotonic decrease in the critical temperature, which changes from 5.1 K (x = 0) to 3.0 K (x = 0.625). A similar effect is observed for the Sommerfeld coefficient γ, which changes from 20.1 mJ mol^{-1} K^{-2} (x = 0) to 16.9 mJ mol^{-1} K^{-2} (x = 0.625). This result is in contrast to the increase in γ inferred from the electronic structure calculations. We discuss these discrepancies in the context of experimental evidence for multigap/anisotropic superconductivity [1, 2] as well as a possible influence of spin fluctuations on the superconducting state of Zr_2Co [3].

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Study of lattice dynamics and electron-phonon interaction in SnTe:In and PbTe:Tl

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Resonantly doped SnTe and PbTe are well known for their exceptional thermoelectric performance, thus they have been extensively researched for decades. However, some of their properties are still not well understood. Upon doping $Sn_{1-x}In_xTe$ and $Pb_{1-x}Tl_xTe$, these compounds become superconductors with critical temperatures of few Kelvins, despite having very low carrier concentration. With so few carriers to form Cooper pairs, unconventional superconductivity of non electron-phonon origin is often proposed.

In this work, we explore electronic structure and lattice dynamics to check whether isotropic electron-phonon interaction is enough to explain superconductivity. Disordered systems were treated both with supercell approach using Quantum Espresso, VASP and Phonopy [1-3], and Korringa-Kohn-Rostoker Method with Coherent Potential Approxation [4]. Structure relaxation lowers average phonon frequencies and enhances electron-phonon interaction around dopant atoms and neighbouring Te. Obtained electron-phonon coupling constant $\lambda \approx 0.22$ in $Sn_{31}In_1Te_{32}$ does not rule out phonon mediated pairing. Accounting for rombohedral distortion resulted in slightly higher value of λ.

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Strongly correlated fermions obeying exclusion and superexclusion principles

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In this work we investigate influence of the exclusion and superexclusion [1, 2, 3] principles (the latter postulated by storngly correlated fermions as exclusion of doubly occupied states in **k**-space) on the basic statistical mechanical properties of the corresponding particles of spin 1/2. In particular, by incorporating the Zeeman field into the model we examine the changes in the spin-dependent energy levels and occupancies as a function of both temperature and the field.

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Detection of relativistic fermions in topological semimetals TaAs and NbP by magnetostriction measurements

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Detection of Dirac or Weyl fermions in topological semimetals via transport and thermodynamic properties remains often elusive, since in these materials conventional charge carriers exist as well. Using the prototype Weyl semimetals TaAs and NbP as examples and performing measurements at low temperatures, we show that the magnetostriction, i.e., the field-induced length change that in a diamagnetic material results from the interaction between the electron and elastic degrees of freedom, can be an effective probe of the massless quasiparticles. For TaAs and in moderate magnetic fields up to $B = 16$ T, which are too weak to confine large groups of massive quasiparticles at their zeroth Landau levels, the magnetostriction contains a linear-in-field term that identifies the presence of relativistic fermions. Specifically, a firm evidence for Weyl fermions was found along the [001] dilatometric direction with the highest fundamental frequency for relativistic fermions of $F_W \approx 7.2$ T [1]. In NbP, however, the situation is reversed: $F_W \approx 39.6$ T is much higher than the quantum limit of about 8.5 T for the trivial charge carriers. Applying pulsed magnetic fields up to $B = 50$ T and along the [001] direction, we were able to observe an entirely linear-in-field increase in accordance with the theoretical predictions [1]. Our combined experimental and theoretical study shows how dilatometry can be used to unveil Weyl fermions in candidate topological semimetals.

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First-principles investigations of structural, electronic, optical, and thermoelectric properties of ternary chalcopyrite semiconductor

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The copper-indium-telluride chalcopyrite semiconductor has garnered significant attention due to its suitable bandgap for solar cells and high-temperature thermoelectric applications. In this study, we investigate the structural, electronic, optical, and thermoelectric properties of using state-of-the-art density functional theory (DFT) with the modified Becke-Johnson (mBJ) semi-local exchange functional. Our band structure calculations reveals that this compound exhibit a p-type semiconductors character with a direct band gap at the Γ point. The calculated band gap is in good agreement with the experimental data. Density of state analysis shows that this compound is primarily influenced by Cu d-states at the upper valence band and their hybridization with Te p-states bellow the first valence band. Furthermore, we validate our results by calculating optical properties, including the dielectric function, absorption coefficient, the real part of optical conductivity, optical reflectivity, and the refractive index. The refractive index finding shows reasonable agreement with the experimental data. These findings indicate that compound exhibits high absorption in the visible light range. Additionally, the Boltzmann transport theory was employed to analyze the thermoelectric properties. The calculation of Seebeck coefficient confirms the p-type nature of this compound. We found that the compound possesses a high electrical conductivity, and Seebeck coefficient with low thermal conductivity. According to our results, the figure of merit ZT can reach 1.66 at and for doping concentration of . This structure, with its suitable bandgap, is capable of absorbing a significant amount of light, making it a prospective choice for solar cells as well as for high-temperature thermoelectric applications.

Experimental evidence of the crystal field states in SmB_6

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The physical properties of Samarium hexaboride (SmB_6) are still under investigation. Particular attention is drawn to the lack of clear evidence of magnetic ordering up to low temperatures and the behaviour of the temperature dependence of specific heat. The difficulty in describing these properties stems from the fact that SmB_6 does not exist in a clearly defined oxidation state. In the case of SmB_6, rejecting the strong multiplet description of the Sm^{2+} ion sheds some light.

In an attempt to explain the non-trivial large contribution to the heat capacity, it was possible to raise the importance of the spin-orbital interaction with respect to the Sm^{2+} ion, which, in combination with the extended basis function, is responsible for this large specific heat [1].

The IR peak positions of the fundamental structural bands were detected and identified. This experiment confirms the highly complicated structure of the Sm^{2+} ion's energy states in SmB_6.

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Robust nonergodic behavior in the quantum sun model

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Ergodicity breaking in paradigmatic Many-body localized models, like the Heisenberg XXZ chain, is much debated as possibly a transient phenomenon, not present in the thermodynamic limit of the model. Here, we present an interesting toy model that exhibits robust signatures of ergodicity breaking, the quantum sun model. Based on state-of-the-art numerical calculations of spectral gap ratios, entanglement entropy of eigenstates and its dynamics, only a very minor finite size effect is seen, suggesting robustness of the transition. Moreover, the model exhibits the many-body mobility edge, meaning energy dependence of the critical point. Variant of the model with particle number conservation is also discussed.

Superconductivity in the high entropy alloy $(NbTa)_{0.67}(MoWTh)_{0.33}$

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High entropy alloys (HEAs) are solid solutions of five or more elements in non-negligible proportions. They crystallize in simple structures and are characterized by high configurational entropy during solidification. HEAs are known for their exceptional mechanical properties, thermal stability, and corrosion resistance, so they are considered materials with high potential for applications such as high-durability mechanical devices, magnets, or superconductors. Currently, the study of HEA with uranium or thorium is mainly focused on the development of advanced high-strength materials. However, a superconducting state has also been discovered in one of the alloys, namely $(TaNb)_{0.31}(TiUHf)_{0.69}$.

Here we present the crystal structure and physical properties of a high-entropy alloy $(NbTa)_{0.67}(MoWTh)_{0.33}$, which exhibits BCS superconductivity with a critical temperature of approximately 5.6-7.5 K. Additionally, we present the results of a numerical study of the electron structure of the alloy using the DFT formalism.

Analysis of physico-chemical and superconducting properties of Y-123 foams produced by top-seed infiltration-growth (TSIG)

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A polyurethane foams of different densities, elasticities and skeleton types (T - upholstery foams, CL - flame retardant foam, high-elastic foam) and melamine were used to produce Y-123 superconducting foams by the top-seed infiltration-growth (TSIG) method [1]. During the TSIG process, the precursor foams were infiltrated with the green phase (Y-211) and thermally transformed into Y-123 superconductors using single crystal Nd-123 seeds oriented in the [100] direction [2-4]. XRD studies showed that the growth tendency of the Y-123 structure retains the crystallographic direction of the Nd-123 seed regardless of the initial orientation of the polyurethane skeleton fiber [5]. Scanning electron microscopy (SEM) and micro-computed tomography (µCT) studies have shown that the highest porosity for superconducting foam structures occurs for foams with density and elasticity: T-25/38, HR-30/38 [5]. On the other hand, superconducting foams with extreme mechanical parameters (T-18/30 or T-40/50) do not show high pore heterogeneity and size diversity [5]. Raman and X-ray absorption spectroscopy (XAS) spectra confirmed the superconducting phase (orthorhombic Y-123) through a characteristic vibration mode around 500 cm^{-1} and the dominance of the ZRS (Zhang-Rice singlets) contribution over the UHB (upper Hubbard band). High density and stiffness foams (T-40/50) favor the evolution of the Y-123 phase, while low stiffness foam structures (T-18/30) poorly transform Y-211 to Y-123 [5]. Furthermore, the studies show that the foam structures maintain a critical temperature (T_c) above 90 K, which is characteristic of Y-123. In general, T_c is not significantly affected by the preparation methodology (T-25/38(1)-(4) samples), mechanical parameters or their structure (porosity). However, the above-mentioned features affect the nature of superconductivity through the assimilation of Y-211 by the foam structures and the conversion efficiency of Y-211 to Y-123 in the TSIG process.

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Electronic structures of Dirac semimetals $LaCuSb_2$ and $LaAgSb_2$

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Dirac semimetals $LaCuSb_2$ and $LaAgSb_2$ have garnered significant research interest due to their unique electronic properties, characterized by Dirac-like linear band dispersions and the existence of Dirac fermions [1]. Electronic structure of both materials is investigated using Angle-Resolved Photoemission Spectroscopy (ARPES) and Density Functional Theory (DFT) calculations. $LaCuSb_2$ is a superconductor exhibiting nodal lines and linear bands indicative of Dirac fermions, which contribute to its complex electronic structure [2]. In contrast, $LaAgSb_2$ displays charge density wave (CDW) order with two distinct transition temperatures and linear magnetoresistance. Despite the shared Dirac-like characteristics, the two compounds exhibit distinct electronic structures and different physical properties [3]. $LaAgSb_2$ manifests pronounced CDW phases, while $LaCuSb_2$ lacks CDW formation despite stronger Fermi surface nesting, underscoring fundamental differences in their electronic behaviors. This comparative analysis provides insights into the differences between these two semimetals, contributing to our understanding of the complex interactions governing their electronic properties and the topological phenomena in Dirac semimetals.

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Thermoelectric effects of a quantum dot hybrid coupled to ferromagnetic metal and topological insulator

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Thermoelectric properties of hybrid systems based on a single-level quantum dot coupled to ferromagnetic metallic lead and attached to the surface states of a three-dimensional (3D) topological insulator are theoretically investigated. On the surface of a 3D topological insulator, massless helical Dirac fermions emerge. These helical Dirac fermions reveal interesting properties that have become a focus of many studies [1-4]. In a helical metal, spins are coupled to momenta so that magnetic properties are expected to be highly nontrivial opposite to the ones emerged in a metallic ferromagnet. However, combining both materials with quantum dot may result in interesting spin-dependent effects revealed in transport and thermoelectric properties. Therefore, we calculate the thermoelectric coefficients, including electric conductance, Seebeck coefficient (thermopower), heat conductance, and the figure of merit, by means of nonequilibrium Green's function technique and analyse the results in terms of the emergence of new effects. The calculations are made within the Hubbard I approximation in respect to the dot's Coulomb interactions. Morover, due to spin-dependent coupling of the quantum dot to the leads a spin degeneracy of the dot's level occurs influencing the transport properties of the system. We take this effect perturbatively to obtain spin-dependent renormalization of the dot's level. Magnetic field can further increase the dot's level spin splitting or compensate it depending on its direction. Thus, external magnetic field is also included in the model.

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Majorana bound states in superconducting ladder

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Majorana bound states can appear on the ends of a one dimensional chain due to the interplay between s-wave superconductivity, spin-orbit coupling and external magnetic field. Recent experimental progress has given unprecedented control over atoms and made it possible to build a chain via atom-by-atom engineering. The magnetic order of these atoms can also be controlled in the process creating an anti ferromagnetic order as observed in $BaFe_2Se_3$. In this talk we will present our recent work, where we studied one such case where two chains are placed side by side forming a ladder like in $BaFe_2Se_3$. Employing the tight binding model and symmetry arguments we categorize our system to be of BDI topological class assuming the periodic boundary conditions. We show various aspects of the topological phase from the evaluated winding number. We demonstrate the band inversion as the topological phase of the Ladder changes. To exemplify the presence of Majorana bound states, we study the ladder with finite size within the tight binding framework in real space. Evaluating the local density of states for the zero modes, we show the existence of Majorana fermions.

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Percolative superconductivity in highly underdoped $La_{2-x}Sr_xCuO_4$ thin films

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The superconductor-insulator transition (SIT) in 2D systems has been the focus of many experimental and theoretical works. Recently, special attention has been paid to "anomalous metal regime" (called also "failed superconductor"), which appears in close vicinity of the SIT [1]. This feature is usually observed in strongly inhomogeneous systems, such as granular superconducting films or Josephson junction arrays, which may be understood as a set of superconducting islands immersed in the metallic matrix. Thin films of high temperature superconductor $La_{2-x}Sr_xCuO_4$ (LSCO) are among materials, which are investigated in this context. In thin films large substrate-induced strain contributes to inhomogeneity of various properties, including, among others, charge inhomogeneity, which may lead to the appearance of "anomalous metal regime" [2, 3]. Here we consider the impact of structural and electronic inhomogeneity on the emergence of percolative superconductivity in thin, underdoped LSCO films with low density of carriers. We use the effective medium theory (EMT) to describe temperature dependencies of resistance for films with strontium content x between 0.045 and 0.13. The EMT is often used as a valuable guide to investigate the effects of mesoscopic inhomogeneity. The method assumes that a sample is broken up into large macroscopic "puddles," each with a given conductivity, with randomly distributed critical temperatures, and this system is represented as random resistor network [4]. We find that while the fitting using the EMT reproduces well the transition to the superconducting state, it is not suitable for the description of "anomalous metal regime".

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