International Workshop
MAP project

Quantum materials, novel phases of matter and transport phenomena

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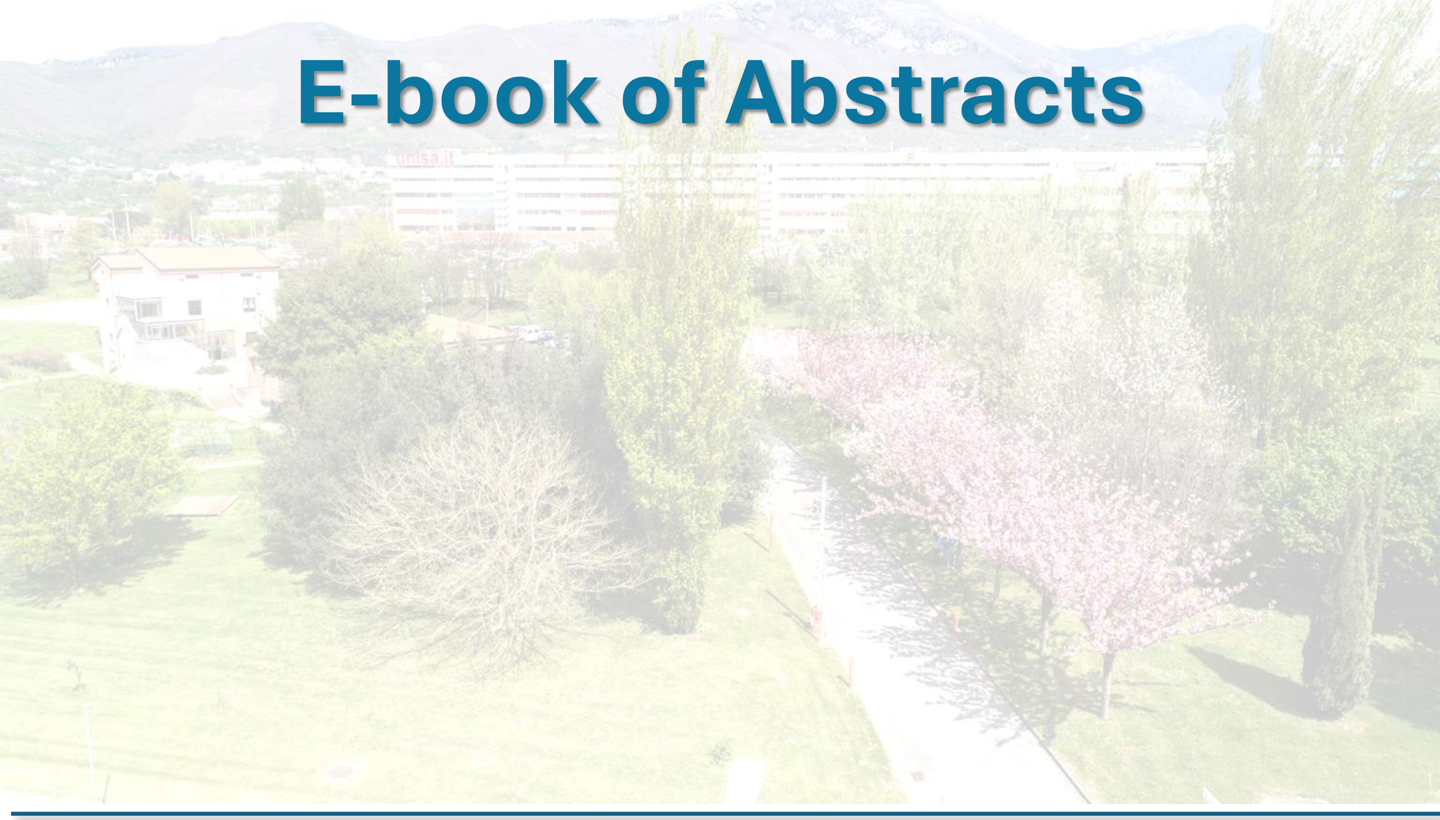
E-book of Abstracts



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University of Salerno -21 June 2024

The workshop is organized within the bilateral Italy – Korea project MAP, a partnership between CNR-SPIN and the University of Salerno from the Italian side, Korea Advanced Institute of Science and Technology (KAIST) and Seoul National University from the Korean side.

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Abstracts

Evidence for superconducting topological surface states in $PtBi_2$

Bernd Büchner
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Due to their intrinsic topology, Weyl semimetals are potential candidates for topological superconductivity, but so far have always been connected with bulk superconductivity, leaving the possibility of intrinsic superconductivity of their topological surface states, the Fermi arcs, practically without attention, even from the theory side. By means of angle-resolved photoemission spectroscopy (ARPES) and ab initio calculations, we identify topological Fermi arcs on two opposing surfaces of the non-centrosymmetric Weyl material trigonal $PtBi_2$. We show these states become superconducting at temperatures around 10 K. Remarkably, the corresponding coherence peaks appear as the strongest and sharpest excitations ever detected by photoemission from solids. Superconductivity is also found in our STM measurements showing in addition spatial inhomogeneity of the superconducting gap. In some samples superconducting gaps as large as 20 meV are revealed by STM resembling the phenomenology found in high-T_c superconductors. However bulk probes such as magnetization, transport and thermodynamics do not show superconductivity. This is consistent with the absence of gaps in bulk electronic states measured by ARPES. Our findings indicate that superconductivity in $PtBi_2$ can occur exclusively at the surface, rendering it a possible platform to host Majorana modes in intrinsically topological superconductor–normal metal–superconductor junctions.

Ultrafast carrier dynamics throughout the three-dimensional Brillouin zone of the Weyl semimetal PtB_2

Paulina Majchrzak[1], Charlotte Sanders[2], Yu Zhang[2], Andrii Kuibarov[3], Oleksandr Suvorov[3], Emma Springate[2], Saicharan Aswarthamm[3], Grigory Shipunov[3], Bernd Büchner[3], Alexander N. Yaresko[4], Sergey Borisenko[3], **Philip Hofmann** [1]
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Using time- and angle-resolved photoemission spectroscopy, we examine the unoccupied electronic structure and electron dynamics of the type-I Weyl semimetal

$PtBi_2$. Using the ability to change the probe photon energy over a wide range, we identify the predicted Weyl points in the unoccupied three-dimensional band structure and we discuss the effect of k_z broadening in the normally unoccupied states. We characterise the electron dynamics close to the Weyl point and in other parts of three-dimensional Brillouin zone using k-means, an unsupervised machine learning technique. This reveals distinct differences, in particular a faster dynamics in the parts of the Brillouin zone hosting most of the bulk Fermi surface compared to the parts close to the Weyl points. In addition to these primary results, it will be briefly discussed how to use machine learning techniques in order to identify trends in multi-dimensional data sets or to aid with data acquisition in a multi-dimensional parameter space.

2-D Terahertz Spectroscopy of Cuprate Superconductors

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Quantum materials, systems in which quantum effects lead to unique macroscopic phenomena with tremendous technological potential, comprise the forefront of condensed matter physics research. In particular, collective excitations associated with broken-symmetry phases have attracted tremendous attention as powerful windows into their microscopic physics and dynamics. However, spectroscopy of these collective excitations has been hindered by the so-called ‘terahertz gap’, which refers to difficulties in generation and detection of radiation in the terahertz frequency range, where many relevant modes of quantum materials are found.

In response to this challenge, we translate a technique known as 2-D spectroscopy, an optical analogue of multi-dimensional NMR spectroscopy, into the terahertz frequency range. We implement, for the first time to our knowledge, 2-D Terahertz Spectroscopy in a non-collinear, reflection geometry, enabling study of opaque materials and isolation of their constituent terahertz nonlinearities. We apply this technique to the Josephson plasma resonance in $La_{2-x}Sr_xCuO_4$, a layered high-temperature superconductor, to distill the underlying plasmon correlations and reveal a disordered superconducting state [1]. Measurements of the superconducting transition then reveal evidence of finite-momentum superconducting fluctuations that we directly probe with our technique [2]. I will conclude with an outlook for light-induced phase transitions.

[1] A. Liu *et al.*, arXiV:2308.14849 (2023).

[2] A. G. Salvador *et al.*, arXiV:2401.05503 (2024).

A novel platform for topological superconductivity and spin-orbitronics at oxides interfaces

Roberta Citro

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I will discuss a novel platform for topological superconductivity and spin-orbitronics based on the two dimensional gases (2DEGs) at the interface between band insulating oxides, like $LaAlO_3$ and $SrTiO_3$. Being characterized by a unique combination of unconventional spin-orbit coupling, magnetism, and 2D-superconductivity, these systems naturally possess most of the fundamental characteristics needed for the realization of a topological superconductor [1-3]. These properties can be widely tuned by electric field effect acting on the orbital splitting and occupation of the non-degenerate $3d_{xy}$ and $3d_{xz,yz}$ bands. The topological state in oxide 2DEGs and quasi-one-dimensional nanochannels could be therefore suitably controlled, leading to conceptual new methods for the realization of a topological quantum electronics based on the tuning of the orbital degrees of freedom [4,5]. Fingerprints of topological superconductivity and spin-orbitronics phenomena will also be discussed in the context of Josephson junctions' properties and Edelstein effect.

[1] C.A. Perroni, V. Cataudella, M. Salluzzo, M. Cuoco and R. Citro. *Physical Review B*, **100**, 094526 (2019).

[2] J. Settino, F. Forte, C.A. Perroni, V. Cataudella, M. Cuoco, and R. Citro. *Physical Review B* **102**, 224508 (2020).

[3] G. Singh *et al.*. *npj Quantum Materials* **7**, 2 (2022).

[4] A. Maiellaro *et al.*. Hallmarks of non-trivial topology in Josephson junctions based on oxide nanochannels. *Phys. Rev. B* **107**, L201405 (2023)

[5] A. Barthelemy, N. Bergeal, M. Bibes, A. Caviglia, R. Citro, M. Cuoco, A. Kalaboukhov, B. Kalisky, C. A. Perroni, J. Santamaria, D. Stornaiuolo and M. Salluzzo. *Eur. Phys. Lett.* **133**, 17001 (2021).

Freestanding oxide heterostructure membranes hosting a 2-dimensional electron gas

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Two-dimensional electron gases (2DEGs) at oxide interfaces, as $LaAlO_3/SrTiO_3$ (LAO/STO) and its several variants, show multiple functional properties of major physical interest, including a high low-temperature mobility, superconductivity, a large Rashba spin-orbit coupling, an exceptionally large spin-to-charge conversion efficiency and a yet controversial magnetic ground state. Such properties are tunable under external control parameters, as electric field effect. In a number of experiments briefly described in the talk, we will first show the capability of tailoring unexpected samples properties by pushing growth control of our crystalline interfaces to the highest level. We will then focus on the control of strain relaxation, selecting the conditions in which an epitaxially strained state is retained much above the expected critical thickness. In this regime, strain relaxation is highly disruptive and surprisingly causes the formation of freestanding LAO/STO membranes, which preserve the metallic and superconducting properties of macroscopic LAO/STO samples. Such membranes can be manipulated, contacted and employed as elements of microscopic circuits on a generic surface. Methods allowing to successfully predetermine the shape and position of membranes will also be shown.

Correlated and topological surface states formed at the edge of electride

Yeongkwan Kim

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Electrides, materials in which electrons play the role of anions, hold a unique potential to host different surface states at the edges of the system due to the unique electrostatic and topological properties of the atomic layer. Specifically, the surfaces of 2D electrides such as Ca_2N, Y_2C, and Gd_2C are expected to host floating electrons confined on the vacuum side over the top-terminated atomic layer, rather than beneath the surface. In addition to this unique surface state, the topological aspect of 2D electrides has been revealed, leading to corresponding topological surface states expected to be located at the topmost atomic layer.

In this talk, we report the observation of such floating electrons and topological surface states at the edge of the 2D electride Gd_2C, studied using angle-resolved photoemission spectroscopy, scanning tunneling microscopy, and first-principles calculations. Floating electrons are clearly captured with a simple parabolic band and are found to be in a liquid phase with significant electron correlation, which could transition to a non-Fermi liquid phase upon reducing the electron density. Additionally, a topological Fermi arc surface state is observed as a consequence of bulk Weyl fermions in Gd_2C. Interestingly, our slab calculation reveals that these Fermi arc states are located at the level of the topmost Gd atoms, separated from the floating electrons above the topmost Gd atoms. Our work thus highlights 2D-electrides as a new platform to explore pure correlated and topological physics and the possible interplay between them.

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.

[1] S.-H. Lee *et al.*, Emergent excitations in a geometrically frustrated magnet. *Nature* **418**, 856–858 (2002).

[2] L. Balents, Spin liquids in frustrated magnets. *Nature* **464**, 199 (2010).

[3] I. Biało *et al.*, Strain-Tuned Magnetic Frustration in a Square Lattice J_1-J_2 Material, arXiv:2306.05828 (2023).

[4] O. Ivashko *et al.*, Strain-engineering Mott-insulating La_2CuO_4. *Nat. Commun.* **10**, 786 (2019).

A tunable room-temperature nonlinear Hall effect in elemental bismuth thin films

Carmine Ortix

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The nonlinear Hall effect with time-reversal symmetry [1,2] is a quantum transport effect that provides a direct way to detect in nonmagnetic materials the Berry curvature — a quantity in which the geometry of electronic wavefunctions is encoded. This effect is also at the basis of terahertz optoelectronic applications of interest for instance for sixth generation communication networks. In various material platforms, including graphene architectures [3] and oxide heterostructures [4], the nonlinear Hall effect is however limited to low temperatures. In this talk, I will discuss our recent finding of a room-temperature nonlinear Hall effect in polycrystalline bismuth thin films [5]. In this elemental semimetal, the room-temperature nonlinear Hall effect is generated by surface states that possess a Berry curvature triple activating side-jumps and skew scatterings. Furthermore, we also show that the strength of the nonlinear Hall effect can be controlled using an extrinsic classical shape effect: the geometric nonlinear Hall effect. This effect is demonstrated in arc-shaped bismuth Hall bars and endows the nonlinear Hall effect of bismuth with the tenability encountered only in low-dimensional materials at low temperatures.

[1] I. Sodemann *et al.*, *Phys. Rev. Lett.* **115**, 216806 (2015).

[2] C. Ortix, *Advanced Quantum Technologies* **2100056** (2021).

[3] S-C. Ho, ..., C. Ortix and T-M. Chen, *Nature Electronics* **4**, 116 (2021).

[4] E. Lesne, ..., C. Ortix and A. Caviglia, *Nature Materials* **22**, 576 (2023).

[5] P. Makushko, ..., D. Makarov and C. Ortix, *Nature Electronics* **7**, 207 (2024).

Atomic-scale imaging of structure-property relationships in strontium ruthenates

Peter Wahl

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The phenomenology and radical changes seen in the properties of materials which exhibit strong electron correlations has captivated condensed matter research over the past decades. Correlations lead to novel ground states, including magnetic order, nematicity and unconventional superconductivity. To provide a microscopic model for these requires knowledge of the electronic structure in the vicinity of the Fermi energy. The strontium ruthenates provide a family of ideal model systems to explore this physics using spectroscopic techniques: they exhibit an anisotropic, quasi-two-dimensional electronic structure and occur as single-, double- and triple-layer compounds with similar crystal structure but disparate ground states ranging from unconventional superconductivity via metamagnetism to itinerant ferromagnetism. In the metamagnetic compounds, spectroscopic information about the low energy electronic structure enables detailed modelling of how their exotic properties emerge from a complex electronic structure with multiple Van Hove singularities in the vicinity of the Fermi energy. I will present spectroscopic imaging of the electronic structure of strontium ruthenates performed at temperatures down to 100 mK and in vector-magnetic fields. Notably, for several of the strontium ruthenates, the surface provides a platform to study the properties of the electronic structure under conditions not accessible in the bulk. Comparison with detailed modelling enables completely new insights into the properties of these materials.[1]

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[1] This work was done in close collaboration with C.A. Marques, L.C. Rhodes, M. Naritsuka, I. Benedičič, colleagues from the group of P. King at the University of St Andrews, and R. Fittipaldi, A. Vecchione and collaborators from CNR-SPIN.

Effect of orbital doping on magnetism in $Ca_2(Ru,Mn)O_4$

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The Mott insulator Ca_2RuO_4 is a $S = 1/2$ antiferromagnet with an orbital angular momentum $L = 1$, composed of two-dimensional layers of corner-shared distorted RuO_6 octahedra. Substituting Ru with Mn ($S = 3/2$, $L = 0$) gradually relieves this distortion while increasing the Néel temperature. To gain a microscopic insight into magnetic order and its relation to orbital degrees of freedom, we perform temperature- and polarization-resolved Raman spectroscopic studies on $Ca_2(Ru,Mn)O_4$ for various Ru/Mn ratios. We directly probe the magnetic exchange interaction via one-magnon scattering and find a systematic increase in its energy with Mn content. A resonance study carried out using different photon energies unveils additional non-Fleury-Loudon terms contributing to the magnetic Raman scattering process. These terms are closely linked to dd-transitions, and leave characteristic fingerprints on the symmetry of one-magnon excitations.

Signatures of a spin-orbital chiral metal

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The interplay of crystal symmetries and electron correlations often results into the formation of unconventional magnetism beyond the traditional forms, arising from the long-range order of magnetic dipole moments. Detection of such hidden orders is a key challenge in condensed matter physics. Here, we present a theory for symmetry-broken chiral ground states and a methodology based on circularly polarized spin-selective angular-resolved photoelectron spectroscopy to probe them. We exploit the archetypal quantum material Sr_2RuO_4 and consider the nature of spectroscopic signatures which may be reconciled with the formation of spin-orbital chiral currents at the material surface [1].

[1] F. Mazzola, W. Brzezicki, M.T. Mercaldo, *et al.*, Signatures of a surface spin–orbital chiral metal. *Nature* **626**, 752–758 (2024).

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