QUEST - QUantum matErials for Sustainable Technologies

Monday, December 2, 2024 - Tuesday, December 3, 2024

Adriatico Guesthouse, ICTP, Trieste, Italy

Book of Abstracts

Contents

Monday, December 2, 9:00; Session 1, Part 1

Topological or not? An ARPES answer on the candidate high-TC FM TI $Mn_{1+x}Sb_{2-x}Te_4$

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The combination of nontrivial band topology & magnetism results in a wide variety of exotic electronic phases that -if realised at high temperatures- could revolutionise fields like spintronics or low-power consumption electronics. The new, second-generation ferrimagnetic compound $Mn_{1+x}Sb_{2-x}Te_4$ (0.1 ≤ x ≤ 1, abbreviated here as MST) promises to host the quantum anomalous Hall effect (QAHE) and other topological phases at higher temperatures than any of its predecessors, wth TCurie's up to 73 K. Their long-range magnetic order is confirmed and thus the big question is "**are they topologically non-trivial?**". MST crystals are significantly p-type doped, meaning the Dirac point of the putative TSS's is well above E_F. Nevertheless, I will aim to persuade you that our temperature-dependent ARPES data (recorded at MAX-IV and CLS) clearly argue that the answer is "yes".

Research carried out in collaboration with:
Sergio Barquero Pierantoni (UvA), Anna Isaeva (UvA and TU Dortmund), Katya Kochetkova (IFW Dresden & UvA), Saumya Mukherjee (UvA, now SPECS), M. Farhan Tanzim (UvA), Irene Aguilera (UvA), Marie Tardieux (UvA), Falk Pabst (UvA), Floris Kooij (UU), J. Oziecki (MAX-IV), Craig Polley (MAX-IV), Sergey Gorovokov (CLS) and Marta Zonno (CLS, now SOLEIL) and Steef Smit (UBC)

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Monday, December 2, 9:30; Session 1, Part 1

Graphene on magnetic substrates

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One of the limitations in exploiting the spin injection and transport properties of graphene is its strong electronic interaction with magnetic contacts. The π-states form complex and non-linear hybrid states when graphene is interfaced with 3d magnetic materials, such as Fe, Co, and Ni. Using density functional theory calculations and angle- and spin-resolved photoemission spectroscopy, I show that the graphene/Eu/Ni(111) system presents a largely doped and nearly freestanding dispersion of the ππ* states, along with a lifting of spin degeneracy (Phys. Rev. Lett. 2024, 132, 266401). The interaction with the Eu states leads to the opening of a large gap in the Dirac cones, which significantly differs for the two spin channels, and to the presence of a spin-polarized van Hove singularity at the Fermi level. The results obtained for this specific system will be discussed in the context of the current literature and used to outline potential developments.

Monday, December 2, 10:00; Session 1, Part 1

Indenene - a triangular lattice goes topological

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Large gap atomic quantum spin Hall insulators (QSHIs) grown epitaxially on SiC(0001) are promising candidates for spintronics at room temperature. The newly discovered QSHI indenene, a triangular monolayer of indium, exhibits a 120 meV gap and substrate-matched monodomainic growth yielding high quality films on the technologically relevant μm scale. Orbital interference on the lattice triangle produces a honeycomb connectivity that is reminiscent of graphene, and a characteristic energy staggering of its orbital angular momentum (OAM) polarized Dirac states that can be experimentally probed by scanning tunneling (STS) and dichroic angle-resolved photoelectron spectroscopy (CD-ARPES). While pristine indenene is unstable in air, which destroys the system along with its topological character, indenene intercalation into epitaxial graphene offers effective protection from the oxidizing environment and fully conserves its topological character. This opens an unprecedented realm of experimental opportunities for ex-situ experiments, and brings the QSHI indenene one step closer towards actual devices.

Monday, December 2, 11:00; Session 1, Part 2

Nanoscale engineering of quantum systems at surfaces

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The increasing interest in quantum technologies calls for purpose-designed nanoscale structures at surfaces. In my talk I will focus on tailored-made molecular structures that are made for two very different purposes: firstly, self-assembled molecular layers engineered for orbital cinematography, i.e., spatial and temporal imaging of electron dynamics in molecules at their intrinsic time scales, and secondly, single-molecule devices created at the tip apices of scanning probe microscopes that can be used as quantum sensors to investigate the properties of surfaces and two-dimensional quantum materials with unprecedented sensitivity and resolution.

Monday, December 2, 11:30; Session 1, Part 2

Strong inter-valley electron-phonon coupling in magic-angle twisted bilayer graphene

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The unusual properties of superconductivity in magic-angle twisted bilayer graphene (MATBG) have sparked enormous research interest. However, despite the dedication of intensive experimental efforts and the proposal of several possible pairing mechanisms, the origin of its superconductivity remains elusive. Here, using angle-resolved photoemission spectroscopy with micrometer spatial resolution, we discover replicas of the flat bands in superconducting MATBG unaligned with its hexagonal boron nitride (hBN) substrate, which are absent in non-superconducting MATBG aligned with the hBN substrate. Crucially, the replicas are evenly spaced in energy, separated by 150 ± 15 meV, signalling the strong coupling of electrons in MATBG to a bosonic mode of this energy. By comparing our observations to simulations, the formation of replicas is attributed to the presence of strong inter-valley electron-phonon coupling to a K-point phonon mode. In total, the observation of these replica flat bands and the

corresponding phonon mode in MATBG could provide important information for understanding the origin and the unusual properties of its superconducting phase.

Monday, December 2, 12:00; Session 1, Part 2

KISS exfoliation of quantum materials for surface science studies

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Two-dimensional (2D) materials offer a versatile platform for exploring novel quantum phenomena and designing nanostructures with tailored functionalities. However, techniques such as photoemission spectroscopy, commonly used in 2D material studies, impose strict requirements for sample quality, uniformity, surface cleanliness, and size. Achieving these standards via traditional mechanical exfoliation in glove boxes is often challenging.

In this presentation, I will introduce an innovative *in situ* exfoliation method for 2D materials performed directly under ultra-high vacuum conditions [1]. This approach yields large flakes with exceptional crystallinity and surface purity. Our experiments focused on exfoliating various semiconducting and metallic transition metal dichalcogenides onto Au, Ag, and Ge substrates, demonstrating the broad applicability of this technique. The materials were characterized using angle-resolved photoemission spectroscopy, a well-established surface analysis technique.

Crucially, this method is straightforward, requiring no specialized equipment, making it ideal for studying the electronic structure of air-sensitive 2D materials. The entire sample preparation and exfoliation process occurs within an ultra-high vacuum environment, ensuring pristine sample conditions throughout.

[1] A. Grubišić-Čabo et al., In-situ exfoliation method of large-area 2D materials, Advanced Science 10, 2023; DOI: 10.1002/advs.202301243, 2023

Monday, December 2, 14:00; Session 2, Part 1

Probing condensates' coherence by time-resolved ARPES: from superconductors to excitonic insulators

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With its direct correspondence to the electronic structure, angle-resolved photoemission spectroscopy (ARPES) is a ubiquitous tool for the study of quantum materials. When extended to the temporal domain, time-resolved ARPES offers the potential to move beyond equilibrium properties, exploring both the unoccupied electronic structure as well as its dynamical response under ultrafast perturbation [1]. In this talk, I will discuss how time-resolved ARPES can probe the coherence of many-body condensates, from high-temperature superconductivity [2,3], to spin-correlation-driven pseudogap [4], and excitonic insulating behavior [5].

[1] F. Boschini, M. Zonno, A. Damascelli, Rev. Mod. Phys. 96, 015003 (2024).
[2] F. Boschini et al., Nature Materials 17, 416 (2018).
[3] M. Zonno, F. Boschini, A. Damascelli, JESRP 251, 147091 (2021).
[4] F. Boschini et al., npj Quantum Materials 5, 6 (2020).
[5] D. Golez et al., Phys. Rev. B 106, L121106 (2022).

Monday, December 2, 14:30; Session 2, Part 1

Higgs-spectroscopy of superconductors

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High field THz-pulses allow accessing the Higgs mode, the amplitude mode of the order parameter, in superconductors. Using a phase-resolved THz-high-harmonics-spectroscopy we perform a complex Higgs-spectroscopy of the order parameter dynamics, symmetry and interaction with other collective modes [1,2]. In high-Tc cuprates and $NbSe_2$ this allows investigating the interplay of charge density waves (fluctuations) and superconductivity based on a generalised Fano-interference of the driven order parameters [1,3,4]. As time-resolved technique THz-Higgs spectroscopy also allows probing transient superconducting states driven by ultrashort light pulses [5] and applying a 2D THz-third harmonics spectroscopy disentangles different sources of third harmonics generation. A novel and direct view on Higgs can be opened by non-equilibrium Raman spectroscopy in the anti-Stokes channel [6].

[1] H. Chu et al. Nat. Commun. 11, 1793 (2020)
[2] L. Schwarz et al. Nat Commun. 11, 287 (2020)
[3] H. Chu et al. Nat Commun. 14, 1343 (2023)
[4] L. Feng et al. PRB 108, L100504 (2023)
[5] M.-J. Kim et al. Sci. Adv. 10, eadi7598 (2024)
[6] T. Glier et al. arxiv:2310.08162

Monday, December 2, 15:00; Session 2, Part 1

Charge and lattice dynamics in hybrid materials probed by time resolved soft X-ray spectroscopies at Elettra synchrotron

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In the fields of optoelectronics and photochemistry, there is growing interest in studying the response to optical excitation of hybrid heterojunctions involving organic molecules. These systems are critical for developing the next generation of environmentally sustainable optoelectronic devices and catalysts. To investigate charge and lattice dynamics in hybrid heterojunctions at the sub-nanosecond timescale, we have developed a setup at the ALOISA beamline of the Elettra synchrotron which takes advantage from the chemical selectivity of X-ray absorption spectroscopy (XAS) and X-ray photoemission spectroscopy (XPS) in an optical pump/X-ray probe experiment.

In this talk, I will present our recent findings on tracking charge dynamics in perylene thin films within hybrid heterojunction systems. We will explore how film morphology affects these dynamics by comparing the behavior of perylene molecules with varying terminations at their interfaces. Finally, I will demonstrate how our setup can monitor structural transitions in several examples of 2D materials, providing deeper insights into the behavior of hybrid heterojunctions under optical excitation.

Monday, December 2, 16:00; Session 2, Part 2

Effects of uniaxial strain on the electronic structure of 2H-$NbSe_2$

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Interplay of superconductivity and density wave orders has been at the forefront of research of correlated electronic phases for a long time. The balance between these two competing orders can be tuned by means of lattice deformation, i.e. pressure or strain. 2H-$NbSe_2$ is considered to be an ideal system for studying this interplay, but the origin of charge density wave in this material is still unresolved. Here, by using angle-resolved photoemission spectroscopy, we revisit the charge density wave order and study the effects of uniaxial strain on the electronic structure of 2H-$NbSe_2$. Our results indicate previously undetected signatures of charge density waves on the Fermi surface. The application of small amount of uniaxial strain induces substantial changes in the electronic structure and lowers its symmetry. This, and the altered lattice should affect both the charge density wave phase and superconductivity and should be observable in the macroscopic properties.

Monday, December 2, 16:30; Session 2, Part 2

Metallic and insulating domains in the CDW system 1T-$TaSe_2$

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We study the electronic structure of bulk 1T-$TaSe_2$ in the charge density wave (CDW) phase at low temperature. Our spatially and angle resolved photoemission (ARPES) data show insulating areas coexisting with metallic regions characterised by a chiral Fermi surface and weakly correlated low energy quasiparticle bands. Additionally, high-resolution laser ARPES reveals strong variations in the metallic regions, with series of low-energy states, whose energy and number are consistent with the formation of quantum well states of different thicknesses. Dynamical mean field calculations show that the observed rich behaviour can be explained naturally by assuming occasional stacking faults of the charge density wave. Our results indicate that the diverse electronic phenomena reported previously in 1T-$TaSe_2$ are dictated by the stacking arrangement while correlation effects play a secondary role.

Monday, December 2, 17:00; Session 2, Part 2

On the origin of circular dichroism in ARPES spectra from graphene, WSe_2, and other quantum materials

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On the example of graphene, we will discuss various contributions to circular dichroism in angle-resolved photoemission (CD-ARPES) [1,2] which include phase shifts of the participating partial waves [3], the interatomic phase shifts [4], and the CD due to elastic scattering of an excited electron [5]. Multiple scattering calculations are performed using the EDAC cluster code [6] and the KKR-based one-step model [7]. Subsequently, we perform similar analysis for WSe_2, a material where orbital characters are relatively well-defined. Finally, a simple interatomic interference model that qualitatively explains asymmetric spin-polarized ARPES (spin-ARPES) spin texture from WTe_2 single crystal surface [4] is presented. This study aims to explore how CD-ARPES and spin-ARPES techniques can enhance the understanding of topological materials.

[1] arXiv:2309.02187 (2023)
[2] JESRP 258, 147219 (2022)
[3] JESRP 214, 29 (2017)
[4] PRL 130, 146401 (2023)
[5] JJAP 32, L1480 (1993)
[6] PRB 63, 75404 (2001)
[7] PRB 83, 121408(R) (2011)

Monday, December 2, 17:30; Session 3, Posters

Insights into the electronic band structure of TCNB-based 2D metal-organic frameworks

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The intrusion of transition metals (TMs) into two-dimensional (2D) layers of organic molecules self-assembled over metallic substrates significantly affects the properties of the resulting metal-organic frameworks (MOFs). A previous study demonstrated the impactful effect of Ni adsorption on the geometrical arrangement and electronic properties of a 1,2,4,5-tetracyanobenzene (TCNB) monolayer deposited over Ag(100).[1] In this study, Fe and Co are introduced as alternative TMs, while maintaining the same organic ligand, with the aim to engineer the electronic structures of the corresponding MOFs.[2]
After establishing the equivalent geometrical arrangement of the three MOFs, a combined experimental and theoretical approach is applied to evaluate the electronic features near the Fermi level. Experimentally, photoelectron emission microscopy (PEEM) is employed to investigate the evolution of the band structure in the three MOFs relative to a monolayer of TCNB molecules on Ag(100). The experimental data suggest that the introduction of TMs induces the formation of new hybrid states, primarily with π-character, whose energy positions and bandwidths vary strongly depending on the TM.
To further interpret the experimental data, structural models of the three MOFs are optimized using DFT calculations based on the geometrical insights. The resulting density of states and band structures manifest strong agreement with the experimental data, confirming the formation of hybrid states and a predominantly π-character interaction. Indeed, the overlap involves mainly the TM $d_{xz/yz}$ orbitals and the TCNB LUMO, all of which are out-of-plane orbitals. Additionally, the differing energy distribution of the 3d states in the three TMs explain the varying energy positions and bandwidths of the hybrid features, with the orbital overlap increasing from Ni to Fe.

[1] D. Baranowski et al., ACS Nano 18, 19618 (2024)
[2] S. Mearini et al., Adv Sci, 2404667 (2024)

Monday, December 2, 17:30; Session 3, Posters

Giant tunable out-of-plane spin polarization in a two-dimensional bilayer of topological antimonene

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We show first-principles calculations and angle- and spin- resolved photoemission spectroscopy studies of a two-dimensional bilayer of β-antimonene supported on bulk bismuth selenide. The trivial insulator β-antimonene inherits the topological surface state of the substrate as a result of the topological proximity effect. The new topological state exhibits an unusually high, almost complete out-of-plane spin polarization within the substrate gap, that we explain by a symmetry-protected band crossing of spin-polarized surface states. The spin polarization can be finely and reversibly tuned from nearly full out-of-plane to nearly full in-plane by electron doping. Our findings pave the way towards advanced spintronics applications exploiting the giant out-of-plane spin polarization of topological surface states.

Monday, December 2, 17:30; Session 3, Posters

The structural, chemical and surface electronic properties of $Bi_2Se_{3-y}S_y$ (y 0.66) and $Bi_{1.993}Cr_{0.007}Se_3$

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Bi_2Se_3 belongs to a class of compounds known as tetradymites, is a well-known thermoelectric material that has also come into focus in recent years for its topological insulating properties. A three dimensional (3D) topological insulator (TI) is a material that is an insulator in the bulk and has metallic conductivity at the surface. The surface conductivity of TI arises from spin-orbit interactions. Electronic states called topological surface states (TSSs) occur on the surface of TI, and exhibit linear dependence of energy on momentum [1]. TSSs are spin polarized and their backscattering from non-magnetic defects/impurities is prevented. The addition of magnetic impurities on the surface of TIs, should have an effect on TSSs, i.e., an opening of an energy gap. These properties make TIs attractive for a variety of nano electronic applications such as spin-transfer torque non-volatile memories and field-effect transistors [2], but also in the field of optoelectronics for helicity-dependent photocurrents and catalysis. Presently, material scientists are working on the synthesis and characterization of new TIs and revisiting previously known compounds from the topological insulating prospective. This is the general context of the studies reported here, where Bi_2Se_3 is the starting material.
For the quasi binary system Bi_2Se_3-Bi_2S_3, some publications have suggested that Bi_2Se_2S in its stoichiometric form should be a stable TI [3], but the few available experimental results are not yet conclusive on this issue [4,5]. We investigated the topological insulating nature of Bi_2Se_3-Bi_2S_3 quasi binary system for a S content in the range 0≤y≤0.66. We prepared single crystals of $Bi_2Se_{3-y}S_y$ by the Bridgman

method, studied their electronic properties by means of angle-resolved photoemission spectroscopy (ARPES) and the spin-polarized ARPES. We demonstrated that the $Bi_2Se_{3-y}S_y$ solid solution supports spin-polarized TSSs for S content in the range 0≤y≤0.66 [6].
The interest in the quasi-binary Bi_2Se_3-Cr_2Se_3 system stems from the search for conditions for the synthesis of Cr-doped Bi_2Se_3 bulk single crystals as an alternative to Cr-doped Bi_2Se_3 thin films [8–10]. The preparation of Cr doped Bi_2Se_3 single crystals was reported to be challenging due to the presence of secondary phase precipitates [7], while the growth of Cr doped Bi_2Se_3 thin films by molecular beam epitaxy has been reported, and the opening of the gap has been observed [8–10]. Starting from a supersaturated melt, through a process of crystallization and phase separation, we showed that is possible to prepare Bi_2Se_3 single-crystal with Cr dopant at a concentration exactly corresponding to the solubility limit without introducing secondary phases, allowing accurate measurement of ARPES maps and the observation of an apparent energy gap similarly to the case of Bi_2Se_3 thin films [11].

[1] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 2005, 95, 226801.
[2] W. Tian, W. Yu, J. Shi, and Y. Wang, Materials (Basel). 2017, 10, 814.
[3] H. Lin, T. Das, L. A. Wray, S. Y. Xu, M. Z. Hasan, and A. Bansil, New J. Phys. 2011, 13, 095005.
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[6] Z. R. Benher, S. Gardonio, M. Fanetti, P. Moras, A. K. Kundu, C. Bigi, and M. Valant, J. Mater. Chem. C, 2021, 9, 3058.
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[10] X. F. Kou, W. J. Jiang, M. R. Lang, F. X. Xiu et al., J. Appl. Phys., 2012, 112, 063912.
[11] S.Gardonio, Z.R. Benher, et al. J. Mater. Chem. C , 2024, 12, 13236-13241.

Monday, December 2, 17:30; Session 3, Posters

Emergence of electronic hybrid states and magnetism in 2D metal-organic frameworks

Yan Yan Grisan Qiu[1], Andreas Windischbacher[2], Claus Michael Schneider[1], Daniel Baranowski[1]; Dominik Brandstetter[2], Giovanni Zamborlini[2], Iulia Cojocariu[3], Manuel Valvidares[4], Matteo Jugovac[5], Peter Puschnig[2], Pierluigi Gargiani[4], Simone Mearini[1], Vitaliy Feyer[1]

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Significant efforts in fundamental research have been dedicated to the study of two-dimensional metal-organic frameworks (2D MOFs) due to their potential in technological applications. These materials combine the structural flexibility of molecular systems with the ordered crystalline arrangement of solids. However, in metal-supported 2D MOFs, interactions with the substrate can significantly alter this flexibility. Consequently, the reported electronic and magnetic properties of metal-supported 2D MOFs do not exclusively reflect their intrinsic characteristics. In this study, we investigate a single-layer MOF, comprised of Ni metal ions coordinated by 7,7,8,8-tetracyanoquinodimethane (TCNQ) ligands, grown on a graphene substrate. Through a combination of spectroscopic characterization and theoretical modeling, two distinct coordination environments of transition metal (TM) centers within the 2D MOF are identified. Specifically, variations in the ligand field induce different hybridization pathways between Ni 3d orbitals and the π-symmetric molecular orbitals of the TCNQ ligands. These variations result in the coexistence of two Ni redox states: a Ni(I) state, favored by a "planar"configuration and a Ni(II) state, stabilized by a "twisted"configuration. Each state exhibits a distinct spin configuration, leading to a complex magnetic response within the system. Furthermore, we extend our study to MOFs synthesized on Au(111) and Ag(100) substrates to explore how substrate interactions influence the electronic and magnetic structure. Specifically, substrate interactions contribute to an axial displacement of the Ni metal centers in the MOF, leading to further modulations of the system properties. Our findings contribute to advancing the general understanding of MOFs and offer insights into the development of functional materials, finding applications in single-atom catalysis, molecular electronics and spintronics.

Monday, December 2, 17:30; Session 3, Posters

Quench of the electronic order in VTe_2 by enhanced lattice fluctuations

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Charge-density-wave (CDW) materials, in which electrons and phonons cooperatively interact to form a new symmetry-broken state, stand as ideal candidates to study the mechanisms governing the melting of a macroscopically ordered phase. Furthermore, given their sensitivity to external stimuli, CDW materials constitute a promising platform to investigate the possibility of controlling their properties. Particularly interesting, although little explored, is the case in which the CDW phase transition is determined by the presence of a strong momentum dependent electron-phonon coupling, since it can lead to significant modifications of the properties of these compounds.
TR-ARPES experiments performed on the TMDC compound VTe_2 have revealed that the closure of the CDW gap is not driven by the amplitude modes (AMs) of the system, but is instead dominated by an incoherent process. By applying a so-called three-temperature model (3TM), we demonstrated that the quench of the CDW gap arises a consequence of the excitation of a subset of strongly-coupled phonon modes which determine a loss of the long-range CDW order. These results therefore suggest that the photoinduced phase transition is determined by non-CDW phonons that interact with the CDW order, thus highlighting the role played by the phonon-phonon interactions.

Monday, December 2, 17:30; Session 3, Posters

Static electronic analysis of the as-prepared and aged Ti_3C_2Tx MXene using x-ray photoemission and absorption spectroscopy

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MXenes, the two-dimensional class of nanomaterials consisting of transition metal carbides, nitrides, or carbonitrides, have been spotlighted in the last decade due to their exceptional properties allowing them to be applicable in different fields. In particular, the Ti_3C_2Tx MXene phase has been paid a great deal of attention from the whole scientific community due to its unique characteristics which make it possible for that phase to be intensively used in electronic and optoelectronic applications. Therefore, it is crucial for such applications to understand the stability of that phase, which gets oxidized very easily, after applying an X-ray beam. Testing the stability of the aged sample governs the possibility of engineering that phase of MXene in different durable applications to ensure their long-term performance. Accordingly, X-ray photoelectron spectroscopy (XPS), and near-edge X-ray absorption fine structure (NEXAFS) measurements with the synchrotron soft X-ray source have been implemented on Ti_3C_2Tx MXene thin film deposited on a quartz substrate for the same sample right following the preparation and a year later.

Monday, December 2, 17:30; Session 3, Posters

Correlated-electron transport in flat-band systems

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Flatband systems have attracted quite some interests due to their peculiar transport properties. The vanishing of the group velocity in the flatband makes the standard theory of transport not applicable. In recent years it has been shown that the underlying mechanism which allows transport in these system might be related to quantum geometric effects. In our work we study the transport through a model system featuring a flatband in the presence of electron-electron interactions. By using the non-equilibirum Green's function approach we show that interactions can indeed restore the transport in these systems and, unlike in normal dispersive bands, in flatbands a moderate interaction can actually favor the transport.

Monday, December 2, 17:30; Session 3, Posters

Tune MoS_2 doping by switching its support material

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Tuning the electronic properties of a 2D crystal by the interaction with its support is the key to design well-controlled nanoelectronic devices based on transition metal dichalcogenides (TMDCs). In particular, the establishing of a low resistance between a metallic contact and the TMDC has been challenging and different strategies for this have been introduced. It was suggested that a low Schottky barrier could be achieved not only by choosing contact materials with the suitable work function but also by introducing interface defects that can contribute independent of the metal contact work function[1].

Here we present a combined ARPES, STM, LEED and XPS study of MoS_2 grown on Au(111) using well established methods[2]. After intercalation of Bi, which is semimetallic, and its further treatment we observe a doping consistent with what was inferred from recent transport measurements[3]. The results shown here shed light on a potential way for tuning the effects of contacts of a 2D layer and their influence on the TMDC electronic structure.

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[2] Harsh Bana et al., 2D Mater. 5, 035012, 2018.
[3] P.C. Shen et al., Nature vol. 593, pages 211-217, 2021.

Monday, December 2, 17:30; Session 3, Posters

Ultrafast band structure dynamics in bulk VSe_2

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Complex materials encompassing different phases of matter can display new photoinduced metastable states differing from those attainable under equilibrium conditions. These states can be realized when energy is injected in the material following a non-equilibrium pathway, unbalancing the unperturbed energy landscape of the material. Guided by the fact that photoemission experiments allow for detailed insights in the electronic band structure of ordered systems, here we study bulk 1T-VSe_2 in its metallic and charge-density-wave phase by time- and angle-resolved photoelectron spectroscopy. After near-infrared optical excitation, the system shows a net increase of the density of states in the energy range of the valence bands, in the vicinity of the Fermi level, lasting for several picoseconds. We discuss possible origins as band shifts or correlation effects on the basis of a band structure analysis. Our results uncover the possibility of altering the electronic band structure of bulk 1T-VSe_2 for low excitation fluences, contributing to the understanding of light-induced electronic states.

Monday, December 2, 17:30; Session 3, Posters

Impact of coherent phonons on the linear and non linear time-resolved optical properties of tellurium and tungsten ditelluride

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The study of transient, far-from-equilibrium states in complex materials can offer profound insights into their microscopic properties, particularly when multiple observables are examined simultaneously. A central question in this field is whether atomic lattice displacements can be accurately tracked and controlled.

In this work, we investigate the ultrafast dynamics of Tellurium (Te) and Tungsten ditelluride (WTe_2) through time-resolved reflectivity (TR-R) and second-harmonic generation (TR-SHG) measurements, as a function of the pump fluence. This dual-probe approach, comprising both linear and nonlinear optical responses, provides a comprehensive framework for analyzing electronic and lattice dynamics in both crystals.

Tellurium has four zone-center optical phonons, three of which are Raman active. These include the non-degenerate A_1 mode, which is linked to symmetric intrachain dilation and compression along the chain axis, impacting bond lengths and angles. Our measurements specifically identify the A_1 mode in tellurium sample, where a marked reduction of the SHG signal after Te photoexcitation suggests a transient transition toward a more centrosymmetric phase.

We conducted TR-R and TR-SHG measurements on WTe_2, with the electric field oriented along two orthogonal in-plane axes of its orthorhombic unit cell. We identified two primary coherent phonon modes. One, having frequency of $\sim$ 0.24 THz, consists in a uniform in-plane atomic shift and is termed shear mode, while the other, at $\sim$ 2.4 THz, reflects atomic displacements depending on the specific atom.

A notable ($\sim 90°$) phase shift in the shear mode, as induced by varying the pump fluence, is observed in both the TR-R and TR-SHG signals, and along the two crystallographic directions. This finding suggests

that the phase shift of the coherent oscillation is induced by a true fluence-dependent modification of the initial phase of the atomic displacements, allowing for a precise control of the atom dynamics.

These findings provide new perspectives on the interactions between coherent phonons and the electronic and lattice properties of complex materials, emphasizing the importance of selecting appropriate experimental observables to extract quantitative information on material properties. Notably, we demonstrate that pump fluence can serve as an effective tool to significantly adjust and tune the initial oscillation phase of coherent displacements.

Monday, December 2, 17:30; Session 3, Posters

Fermi surface topology and spin-polarized surface states in $Pd_3Bi_2Se_2$

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Topological superconductors are of great interest in the study of quantum materials due to their unique properties and potential applications in the fields like quantum computation and spintronics. $Pd_3Bi_2Se_3$, a topological superconductor with a superconducting transition temperature of 0.80 K, is a promising candidate. Although it has been theoretically identified as a nontrivial topological material, direct experimental evidence is still lacking. In this work, we will present ARPES and Spin-ARPES studies on $Pd_3Bi_2Se_2$, focusing on its Fermi surface topology, surface states, and spin-polarized states at low temperatures. These insights will contribute to a deeper understanding of its electronic structure and fundamental properties, which are critical for advancing research on topological superconductors.

Monday, December 2, 17:30; Session 3, Posters

Electronic structure of catalytically active topological semimetal Ni_2Ga_3

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Recently, alloys and intermetallic compounds have gained significant attention due to their unique electronic and geometric structure, which are favourable for efficient catalytic applications. They offer promising alternatives to traditional monometallic catalysts, particularly in terms of cost, activity, stability, and selectivity. In this context, Ni-Ga bimetallic based catalysts demonstrates effective catalyse that reduces CO_2 to methanol at ambient pressure. The surface electronic structure is expected to play an important role in the material's catalytic activity.

In this study we investigated the surface electronic structure of Ni_2Ga_3, a stable and active compound in the Ni-Ga bimetallic family, utilizing angle-resolved photoemission spectroscopy (ARPES) combined with density functional theory (DFT). Trigonal structure Ni_2Ga_3 represents a topological semimetal characterized by a tilted type-II Dirac crossing within its unoccupied states which is robust, under significant spin-orbit coupling effects. Moreover, the material is hosting multiple surface states. ARPES spectra display the presence of several bands across the Brillouine zone (BZ), including dispersive bulk bands that form electron pocket-like states close to the Fermi level (E_F) corresponding to the triangular warped pockets encircling the corner of the Brillouin zone. A bunch of hole-like bands across the zone centre is crossing the E_F forming a star-like Fermi contour around the centre of the BZ. In addition,

parabolic arc-like and Dirac-like surface states are also evident in the valence band. Since, the bulk band entanglements and presence of robust surface states favours the topological materials to stand high as a potentially active and highly efficient catalysts, the presence of multiple electron-hole pockets at E_F together with surface states Fermi contours may be favouring the Ni_2Ga_3 catalytic activity.

Tuesday, December 3, 8:45; Session 4, Part 1

Elettra 2.0: new advances in synchrotron radiation research

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Elettra 2.0 represents the latest evolution of Italy's third-generation synchrotron radiation facility, which has served scientific and industrial communities since 1993. Approved by the Italian Government in 2017, the Elettra 2.0 project involves replacing the current machine with a low-emittance storage ring, marking a significant milestone in synchrotron research. With enhanced brightness and coherence, Elettra 2.0 offers exceptional possibilities for cutting-edge scientific research across diverse fields.

Over 40% of the project's budget is allocated to new beamline construction and upgrades. The diverse portfolio of beamlines will enable experiments in a wide range of photon energies, from a few tens of eV to several tens of keV. Researchers in fields such as physics, chemistry, biology, medicine, and cultural heritage will benefit from access to advanced experimental techniques. My presentation will start with an overview of the new machine's features, then discuss the capabilities of the beamlines and their potential for conducting advanced experimental research.

Tuesday, December 3, 9:15; Session 4, Part 1

Three different charge orders in kagome lattice materials

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Kagome lattice is one of the most fertile geometric motifs in condensed matter physics, where a unique interplay between topology, correlation, and frustration gives rise to a plethora of quantum phenomena. Charge ordering is an example of quantum states prevalently observed in various Kagome lattice materials, including AV_3Sb_5, ScV_6Sn_6, and FeGe, and is found to be intertwined with superconductivity, magnetism, and anomalous Hall effect in a nontrivial manner.
In this talk, I will present our comprehensive investigations of charge orders in Kagome lattice materials using a suite of scattering and spectroscopy techniques, including ARPES and time-resolved XRD. Our results point toward that despite their apparently similar phenomenology, the charge orders in AV_3Sb_5, ScV_6Sn_6, and FeGe each have a completely different nature, emerging from electronic instability, lattice instability, and magnetism-driven transition, respectively. Our investigations not only provide guidance on the classification of charge order in broader quantum materials, but also highlight the utility of combining complementary photon science techniques –photon-in-electron-out, photon-in-photon-out, static and time-resolved –for a deeper understanding of quantum phenomena in solids.

Tuesday, December 3, 9:45; Session 4, Part 1

The rich physics of bilayer kagome metals

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Long-range electronic order descending from a metallic parent state constitutes a rich playground to study the intricate interplay of structural and electronic degrees of freedom. Kagome materials appeared as the perfect stage for such explorations. Specifically, RV_6Sn_6 (R = rare earth atom) bilayer kagome metals are topological systems with Dirac-like itinerant states, van Hove singularities and correlated flat bands [1,2]. Interestingly, within this family, ScV_6Sn_6 also features a charge density wave (CDW)

phase that affects the susceptibility, the neutron scattering, and the specific heat, and whose motif differs significantly from that of the siblings AV_3Sb_5 (A = K, Rb, Cs) and FeGe. As such, in this presentation, I will give an overview about the rich physics recently unveiled in bilayer kagome metals, and will also discuss about the dynamics of that CDW phase [3]. Specifically, while there is no consensus yet on its microscopic origin, with contradicting affirmations supporting both electron- electron and electron-phonon interaction, we reveal a prominent role played by the structural degrees of freedom in the stabilization of the charge order.

[1] D. Di Sante et al, Nature Physics 19, 1135 (2023).
[2] H. Li et al, Nature Physics 20, 1103 (2024)
[3] M. Tuniz et al, Communications Materials 4, 103 (2023).

Tuesday, December 3, 10:45; Session 4, Part 2

2D twistronics

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The wide family of 2D materials (2DMs) includes metals, semiconductors, superconductors, dielectrics, ferroics and more, each displaying novel phenomena due to the qualitatively different nature of interactions in 2D. However, the real delight is in the ability to combine different 2DMs into atomically defined heterostructures by simply stacking layers, engineering interactions between them. From this a new parameter space arises, the twist angle between neighbouring layers. Changing the twist angle can be used to tune interlayer interactions. This is exemplified by 'magic-angle'twisted graphene, engineering strongly correlated behaviour through moire interactions, an effect also used to trap ordered arrays of excitons in transition metal dichalcogenide (TMDC) heterobilayers. moire effects conventionally require a moire wavelength much longer than the atomic scale. But for larger lattice mismatch, Umklapp processes can result in unexpected electronic structure changes. Here, I will present our recent studies of electronic structure measurements of twisted 2DMs, including twisted graphenes and TMDCs, illustrating the effects of these twist-angle dependent inter-layer interactions.

Tuesday, December 3, 11:15; Session 4, Part 2

Kramers-Weyl fermions in chiral crystals

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The study of chiral crystals is one of the frontiers in the field of topological materials. Weyl fermions with unique properties emerge in the absence of inversion and mirror symmetries [1]. Kramers-Weyl fermions, for example, are pinned at different high-symmetry points and surface arcs can connect them spanning over the entire Brillouin zone [2 - 4]. The physics of chiral crystals is further enriched by the spin arrangements in momentum space [5], that can go beyond those described by Rashba [6] and Dresselhaus [7].

In my talk, I will show the results of our research activity on chiral crystals. I will start by discussing the radial spin texture observed in tellurium, one of the simplest chiral crystals available [8]. I will explain how the spin texture evolves in the momentum space under the influence of the local point group symmetry. Based on symmetry constrains, we have screened materials databases for compounds that realize spin texture more complex than the basic hedgehog [9]. From this analysis we identify several interesting crystals: I will show you that in the semiconducting $CdAs_2$ Weyl fermions of different origin and with different spin texture emerge in nearly degenerate valleys, connected by helicoid states [10].

[1] P. Tang et al., Phys. Rev. Lett. 119 206402 (2017)
[2] G. Chang et al., Nat. Mater. 17 978 (2018)
[3] D.S. Sanchez et al. Nature 567 500 (2019)
[4] N.B.M. Scröter et al., Nat. Phys. 15 759 (2019)
[5] M. Hirayama et al., Phys. Rev. Lett. 114 206401 (2015)
[6] E. I. Rashba and V. I. Sheka, Fiz. Tverd. Tela: Collected Papers II 162, 62 (1959)
[7] G. Dresselhaus, Phys. Rev. 100, 580 (1955)
[8] G. Gatti et al., Phys. Rev. Lett. 125, 216402 (2020)
[9] D. Gosálbez-Martinez et al., Phys. Rev. B 108, L201114 (2023)
[10] A. Crepaldi et al., in preparation

Tuesday, December 3, 11:45; Session 4, Part 2

Signatures of surface spin-orbital chiral metal

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Surface experimental probes, such as angle-resolved photoelectron spectroscopy provide researchers access to the electronic structure of solids. Despite the advances in the field, recently, new forms of surface local magnetism completely different from standard descriptions have appeared. One example of such forms of magnetism are the one generated by the so-called loop currents, generated by the collective motion of electrons in solids.

Such currents are of paramount importance and their manifestation is tightly connected to the symmetries of a material. For example, if they involve the orbital and angular momentum, then there will be asymmetries upon mirror operator which will affect the orbital-and-angular momentum conservation. While this phenomenology can be often elucidated by muon spectroscopy in bulk systems, surface and interface effects remain elusive.

Here, I aim to give an overview of a new powerful methodology, based on the combination of circular dichroism and spin-resolved photoelectron spectroscopy, to uncover such elusive phases. I will do this starting from simple concepts and showing, at the end, my current research. In particular, I will show a new methodology able to access what is known as loop current, even if the latter manifest at the surface of a certain material. I will use as a prototype material Sr_2RuO_4, and find out that the signal collected is compatible with that of a surface spin-spin orbital chiral metal.

Tuesday, December 3, 12:15; Fonda-Fasella Award

Advancing imaging and magnetization dynamics studies at the FERMI DiProI beamline using OAM beams and THz pulses

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During the past four years, I had the opportunity to participate in and contribute to the development of new techniques that expand the capabilities of the DiProI beamline at the FERMI free-electron laser (FEL) source. In particular, I will present a few results related (i) to the properties of light beams possessing orbital angular momentum (OAM) and (ii) to the magnetic dynamics triggered by high-amplitude, quasi-single-cycle terahertz (THz) pulses.

The use of OAM light beams is rapidly becoming a powerful way for probing condensed-matter systems, even in the extreme ultraviolet range. The wavefronts of these beams are characterized by an azimuthal angular dependence of the electric field phase, associated with an OAM topological charge $\ell \neq 0$. For imaging purposes, it has been shown that OAM beams can increase image resolution compared to gaussian illumination ($\ell = 0$) [1]. We tested this feature at the DiProI beamline by conducting ptychographic experiments with a standard sample [2,3]. Our results show that ptychographic reconstructions with OAM beams exhibit higher image resolution, and the retrieved illumination functions proved to be very sensitive to optical aberrations. This study could provide the basis for new characterization and diagnostic tools [4], as the extra degree of freedom given by ℓ can be exploited for tuning light-matter interaction even during pump-probe experiments.

Indeed, although we primarily investigated the role of OAM beams as a probe, a FEL source demonstrates its full potential while performing pump-probe experiments on an ultrafast time scale. In this context, we developed a compact THz source to be mounted inside DiProI. It is based on optical rectification in a BNA organic crystal [5], which allows us to obtain quasi-single-cycle THz pulses with a spectrum centered at approx. 1 THz. These pulses serve as a pump to investigate, for instance, THz-induced nutation dynamics in ferromagnetic materials [6]. Nutation, which is related to magnetic inertia, manifests as a perturbation of the precessional motion undertaken by the magnetization during its recovery to equilibrium. As shown in refs. [6,7], the nutation resonance frequency in standard ferromagnetic materials lies in the 0.5 - 2 THz range, making this phenomenon an ideal test case for our THz source. A detailed experimental characterization of the magnetization evolution on an ultrafast time scale is not only of interest for fundamental research, but could also have a significant impact in the development of future devices, as magnetic inertia affects the energy balance associated with ultrafast magnetization switching [8].

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