QUEST - QUantum matErials for Sustainable Technologies

Report of Contributions

https://indico.elettra.eu/e/QUEST24

Contribution ID: **5** Type: **Invited Oral**

Indenene –a triangular lattice goes topological

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 □m 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.

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Presenter: MOSER, Simon (Deutsch)

Contribution ID: **6** Type: **Invited Oral**

Charge and Lattice Dynamics in Hybrid Materials Probed by Time Resolved Soft X-Ray Spectroscopies at ELETTRA Synchrotron.

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.

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Contribution ID: **7** Type: **Invited Oral**

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

With its direct correspondence to the electronic structure, angle-resolved photoemission spectroscopy (ARPES) is a ubiquitous tool for the study of quantum materials. When ex-tended 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 dy-namical 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 ex-citonic 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).

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Contribution ID: **11** Type: **Invited Oral**

KISS exfoliation of quantum materials for surface science studies

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

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Contribution ID: **13** Type: **Invited Oral**

Graphene on Magnetic Substrates

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.

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Contribution ID: **14** Type: **Invited Oral**

The rich physics of bilayer kagome metals

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, RV6Sn6 (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, ScV6Sn6 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 AV3Sb5 (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.

References:
[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).

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Contribution ID: **15** Type: **Invited Oral**

2D twistronics

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 2D materials 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.

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Presenter: WILSON, Neil (University of Warwick)

Contribution ID: **16** Type: **Invited Oral**

Metallic and insulating domains in the CDW system 1T-TaSe2

We study the electronic structure of bulk 1T-TaSe2 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-TaSe2 are dictated by the stacking arrangement while correlation effects play a secondary role.

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Contribution ID: **19** Type: **Invited Oral**

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

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)

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Contribution ID: **20** Type: **Invited Oral**

Effects of Uniaxial Strain on the Electronic Structure of 2H-NbSe2

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.

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Contribution ID: **21** Type: **Invited Oral**

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

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 Mn1+xSb2-xTe4 (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 73K. 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 EF. 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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Contribution ID: **22** Type: **Invited Oral**

Signatures of surface spin-orbital chiral metal

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 Sr2RuO4, and find out that the signal collected is compatible with that of a surface spin-spin orbital chiral metal.

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Contribution ID: **23** Type: **Invited Oral**

Kramers-Weyl fermions in chiral crystals

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 CdAs2 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

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Contribution ID: **26** Type: **Invited Oral**

Strong Inter-valley Electron-Phonon Coupling in Magic-Angle Twisted Bilayer Graphene

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.

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