Mo-01

Superconducting Arcs

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Topological superconductivity is essential to generate Majorana fermions needed for quantum computing. Bulk topological superconductors remain elusive and two most promising approaches exploiting the proximity-induced superconductivity seem hard to realize. Weyl semimetals with Fermi surface arcs at the surface belong to potential canidates too, but search for Majorana fermions has always been connected with the superconductivity in the bulk, leaving the possibility of intrinsic superconductivity of the arcs themselves practically without attention, even from the theory side. Here, using angle-resolved photoemission spectroscopy and ab-initio calculations, we unambiguously identify topological Fermi arcs on two opposing surfaces of non-centrosymmetric Weyl material $PtBi_2$ and show that these states become superconducting at different temperatures around 10K. Remarkably, the corresponding coherence peaks appear as the strongest and sharpest excitations ever detected by photoemission from solids (Fig. 1), suggesting significant technological relevance. Topological superconductivity in $PtBi_2$ appears to occur exclusively at the surface, which not only makes it an ideal host of Majorana fermions, but also may reveal a unique quantum phase - an intrinsic topological SNS Josephson junction [1].

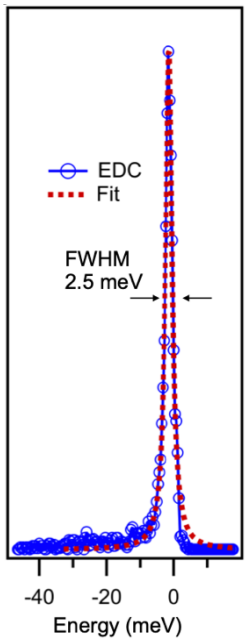

Fig. 1*: Energy distribution curve corresponding to the topological surface state (arc) in $PtBi_2$.*

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Mo-02

Recent progresses on Iron-Majorana platform

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In this talk I will report our recent progresses of Majorana zero mode in Fe-based superconductors (FeSCs). Following our original findings of superconducting topological surface state and Majorana zero mode (MZM) of Fe-based superconductor Fe(Te, Se), we have observed a half-integer level shift of vortex bound states and quantized Majorana conductance in this material, which are hallmarks of MZMs. In addition, we have also found that most of Fe-based superconductors, including monolayer Fe(Te,Se)/STO, have similar topological electronic structures. We have also found that pressure can be used as a good tuning method to control MZMs in FeSCs. The combination of intrinsic topological nature of vortex and large energy spacing among the discreet bound states, all of which can be tuned by pressure, offers compelling evidence for the Majorana nature of vortex zero-modes discovered in FeSCs, thus creating the new and promising Iron-Majorana platform.

Mo-03

Three Dimensional Flat Bands in Pyrochlore Metal $CaNi_2$

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The investigation of complex atomic geometries in materials has attracted significant attention due to their ability to exhibit exotic electronic states. One of the most prominent example is the electronic flat band arising from the suppressed electron kinetic energy in such systems. So far, the experimental realization of electronic flat bands has been limited to (quasi) two-dimensional (2D) crystalline materials such as twisted bilayer graphene [1] and the kagome lattice [2,3]. Consequently, a question that naturally arises is whether the flat band can exist in the three-dimensional (3D) system while remaining dispersionless along all momentum directions k_x, k_y, and k_z. To answer these questions, we conducted angle-resolved photoemission spectroscopy (ARPES) experiments on the C15 Laves phase $CaNi_2$, which consists of a Ca diamond network and a Ni pyrochlore network. We observe a partially flat band and a 3D flat band below the Fermi level. Moreover, we find that the energy of the flat bands and their dispersion can be modulated through chemical substitution, specifically by replacing Ni with Rh, ultimately resulting in the flat band aligning with the Fermi level. Interestingly, the emergence of superconductivity is observed in $CaRh_2$, where the flat band is located at the Fermi level. Although direct experimental evidence demonstrating flat-band induced superconductivity is still elusive, our results offer a promising material platform for investigating novel emergent phenomena originating from the divergent density of states associated with 3D flat bands in complex lattice systems.

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Mo-04

Electronic properties of new topological quantum materials

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Abstract

Topological materials are characterized by the presence of nontrivial quantum electronic states, where often the electron spin is locked to its momentum. This opens up the possibility for developing new devices in which information is processed or stored by means of spin rather than charge.

The field of topological quantum materials traditionally follows a different paradigm from other areas of Condensed Matter Physics. It is mostly driven by theory and Density Functional Theory calculations in contrast to fields such as superconductivity for example, where new materials are typically discovered by experimentalists. New topological materials and phenomena are usually first discovered in-silico an then confirmed experimentally. Such was the case for topological insulators, crystalline topological insulators and Weyl semimetals.

In this talk we will discuss notable exemptions to this rule and several recent discoveries that were driven by experiment. I will present data from Angle Resolved Photoemission that details fascinating electronic properties of these materials and link these results to some old outstanding problems in more traditional condensed matter physics. Perhaps the most interesting amongst them is discovery of spin textured Fermi arcs that appear in AFM state of some rare-earth monopnictides and undergo novel splitting that is different from previously reported Rashba and Zeeman splitting.

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Mo-05

Observation of Topological Surface States in Superconducting PdSeTe Single Crystal

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Topological semimetals with topologically non-trivial band structure have been the focus of recent theoretical and experimental studies [1-3]. Dirac semimetals (DSMs), Weyl semimetals (WSMs), and topological nodal-line semimetals are the three main sub-categories of topological semimetals, which can be characterized according to the form and degeneracy of the band crossings near the Fermi level [4]. The layered transition metal chalcogenides are particularly significant for their various intriguing physical properties, such as superconductivity and charge density wave (CDW) with application potentials [5].

In this study, we have successfully synthesized high-quality single crystals of PdSeTe by a two-step melting method and investigated the electronic band structure as well as the superconducting properties. We performed angle-resolved photoemission spectroscopy (ARPES) of PdSeTe on the beamline HiSOR BL-1, Hiroshima University, Japan. We have done the density functional theory (DFT) calculations and found that PdSeTe hosts four-fold degenerate Dirac crossings at the A point, originating from the non-symmorphic symmetry. These band crossings form a Dirac line node along the $\Gamma - A$ direction, which is located almost near the Fermi level and shows almost no energy dispersion. Therefore, Dirac fermions in PdSeTe can be studied using transport measurements. In order to verify the surface contribution in the ARPES results, we have done $h\nu$-dependent measurements and directly confirmed the presence of surface states in PdSeTe. The observed surface-derived states match well with the DFT calculation for the slab model.

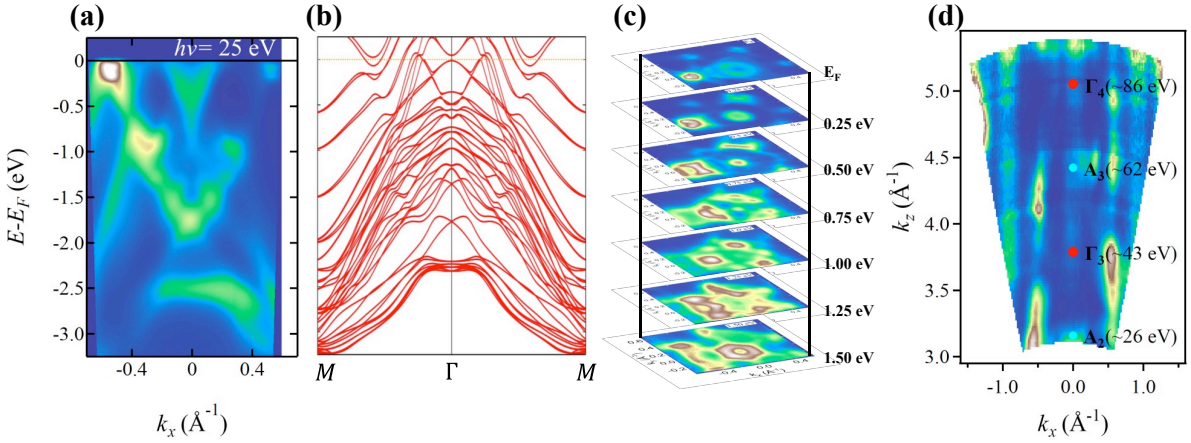

Fig. 1: *(a) and (b) represent the measured ARPES spectrum along* $\bar{M}-\bar{\Gamma}-\bar{M}$ *direction with 25eV photon energy at 20K and simulated bands for slab (5 atomic layers) respectively. (c) The Fermi surface and constant-energy contours of the ARPES spectra at different binding energies. (d) The shows the experimental* k_z*-dispersion along* $\Gamma-A$ *deduced from the* $h\nu$*-dependent data measured along the* $\bar{M}-\bar{\Gamma}-\bar{M}$ *direction.*

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Mo-06

Nonequilibrium DMFT approach to RIXS and Raman scattering

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Resonant inelastic X-ray scattering (RIXS) and Raman scattering are photon-in / photon-out techniques which provide information on low-energy excitations of solids. In recent years, these techniques have also been used as probes in pump-probe experiments. The theoretical calculation of RIXS and Raman amplitudes is challenging, because the standard diagrammatic treatment involves the measurement of four-point correlation functions. I will present an alternative approach, based on nonequilibrium dynamical mean field theory (DMFT), which reduces the problem to a two-point measurement [1,2,3]. The idea is to explicitly simulate the incoming light pulse, and to measure the outgoing photon flux. Since this formalism is implemented on the real-time axis, it can easily treat nonequilibrium situations, such as pump excited solids. It is in particular well suited for the study of local excitations.

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Mo-07

Electron-Magnon Scattering in Elementary Ferromagnets

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I report on the combination of two powerful self-energy techniques: the well-known GW method and a self-energy recently developed by us that describes renormalization effects caused by the scattering of electrons with magnons and Stoner excitations. This GT self-energy [1], which is fully k-dependent and contains infinitely many spin-flip ladder diagrams T [2], was shown to have a profound impact on the electronic band structure of Fe, Co, and Ni [3, 4]. In the presentation, I present the refinement of the method by combining GT with the GW self-energy. The resulting GWT spectral functions [5] exhibit strong lifetime effects and emergent dispersion anomalies. They are in an overall better agreement with experimental spectra than those obtained with GW or GT alone, even showing partial improvements over local-spin-density approximation dynamical mean-field theory [3]. According to our analysis, this method provides a basis for applying the GWT technique to a wider class of magnetic materials. By comparing spin- and momentum-resolved photoemission spectroscopy measurements to these many-body calculations we found a surprising kink in the electronic band dispersion of a ferromagnetic material at much deeper binding energies than ever expected (Eb = 1.5 eV).

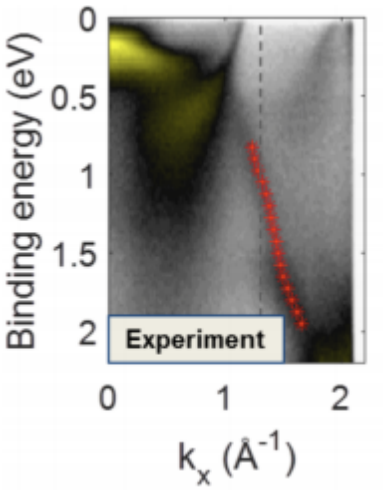

Fig. 1: Kink far below the Fermi level observed by the photoemission experiment [3] and reproduced by the *GT* theory [1].

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Mo-08

Spin-state excitation induced insulator-metal transition in $FeSb_2$

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The iron antimonide $FeSb_2$ is a well-known correlated narrow-gap semiconductor, which has been investigated for decades because of its puzzling properties. $FeSb_2$ undergoes metal-insulator transition (MIT), accompanied by the crossover from paramagnetism to diamagnetism. Extensive efforts have been taken to reveal the underlying physical mechanism of the MIT in $FeSb_2$, but a census has yet to be reached. The macroscopic transport and magnetic measurements can be explained by totally different theoretical proposals, and microscopic evidence is of the essence to distinguish the physical origin. In this talk, I will present our recent progress on synchrotron-based X-ray spectroscopic study and the corresponding simulations on $FeSb_2$. Our results demonstrate that $FeSb_2$ is with a ground state of mixed spin state. Furthermore, the spin states drifted toward the high spin state simultaneously with the transition to metal. Our study constitutes key evidence to support the narrative of spin state excitation to explain the MIT within $FeSb_2$.

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Keywords: X-ray spectroscopy, correlated semiconductor, spin-state excitation, metal-insulator transition

Mo-09

Inducing Itinerant Ferromagnetism by Manipulating Van Hove Singularity in Epitaxial Monolayer 1T-VSe_2

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The itinerant ferromagnetism can be induced by a van Hove singularity (VHS) with a divergent density of states at Fermi level. Utilizing the giant magnified dielectric constant ε_r of $SrTiO_3$(111) substrate with cooling, here we successfully manipulated the VHS in the epitaxial monolayer (ML) 1T-VSe_2 film approaching to Fermi level via the large interfacial charge transfer, and thus induced a two-dimensional (2D) itinerant ferromagnetic state below 3.3 K (Fig. 1). Combining the direct characterization of the VHS structure via angle-resolved

photoemission spectroscopy (ARPES), together with the theoretical analysis, we ascribe the manipulation of VHS to the physical origin of the itinerant ferromagnetic state in ML 1T-VSe_2. Therefore, we further demonstrated that the ferromagnetic state in the 2D system can be controlled through manipulating the VHS by engineering the film thickness or replacing the substrate. Our findings clearly evidence that the VHS can serve as an effective manipulating degree of freedom for the itinerant ferromagnetic state, expanding the application potentials of 2D magnets for the next-generation information technology. [1]

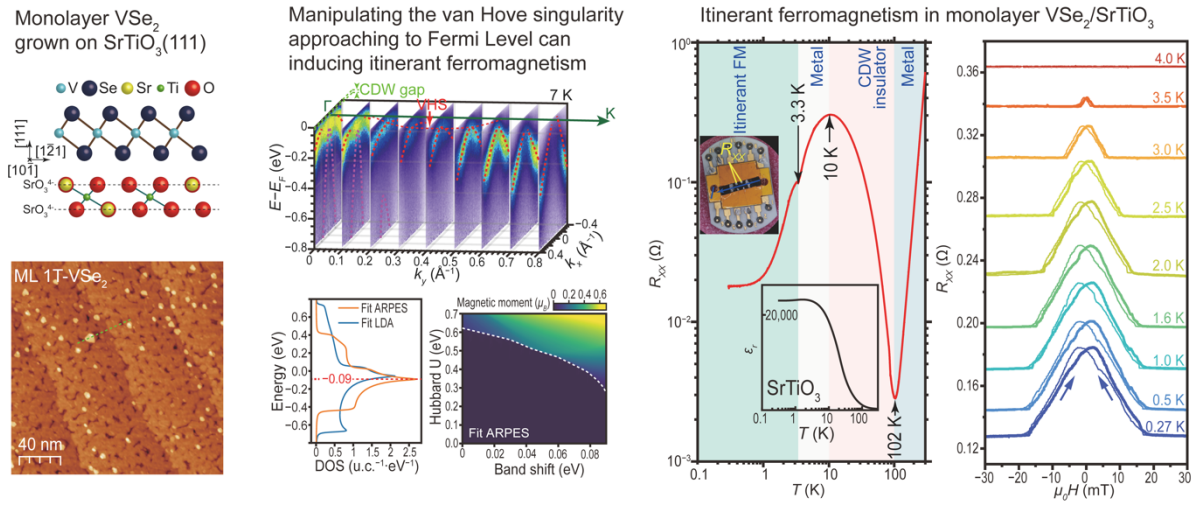

Fig. 1: *MBE growth, van Hove singularity structure and itinerant ferromagnetism in monolayer 1T-VSe_2/$SrTiO_3$(111).*

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Mo-10

Recent Advances in Physics and Materials Science of Magnetic Topological Insulators and Strong Spin-Orbit Coupled Materials

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Topological insulators (TIs) are narrow–gap semiconductors characterized by the gapless Dirac-like surface state and protected by time-reversal (TR) symmetry. Introduction of a magnetic field (external or internal) breaks TR symmetry and causes splitting of the topological surface state at the Dirac point thus making the surface insulating. Internal magnetic field in TIs can be created in various ways, in particular, by doping with 3d-transition metal atoms [1], displaying magnetic semiconductors as well as bulk materials on the surface of three- or two-dimensional TIs [2]. Magnetic field effect on the TI surface state (SS) can be also realized due to extension of the TI SS into the magnetic overlayer [3,4]. Antiferromagnetic TIs can realize such intriguing effects as magnetoelectric effect [5] and axion insulator phase [6]. Here we present and discuss recent results of the study of ferromagnetic TIs and intrinsic antiferromagnetic TIs, van der Waals magnetic multilayers with high Chern number and some strong spin-orbit coupling materials [7-11].

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Mo-11

New Spin-Momentum Locking and Strong Correlations in Chiral Semimetals

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Spin-orbit coupling in noncentrosymmetric crystals can lead to a directional relationship between the electron's spin angular momentum and its linear momentum. While Rashba- and Dresselhaus-type spin-momentum locking have been studied for decades and inspired many important applications, their natural counterpart, Weyl-type parallel spin-momentum locking (see Fig 1), has remained elusive in experiments until now. This is because until recently, all known Weyl-semimetals had mirror symmetries, which suppresses parallel spin-momentum

locking [1]. However, we have recently detected the first experimental signature of truly parallel spin-momentum locking in a chiral topological semimetal by probing its bulk and surface spin-texture with spin-ARPES [2]. These chiral materials could therefore find applications as energy-efficient memory devices for field-free switching of magnets with perpendicular magnetic anisotropy [3] and new types of Josephson diodes [4].

Moreover, we recently also discovered the first evidence of strong electron correlations in a chiral topological semimetal. Specifically, we observed a spin-dependent loss of quasiparticle weight in the vicinity of a Berry curvature monopole near the Fermi level. This intriguing discovery presents a unique opportunity to investigate the robustness of topological band crossings against strong electron interactions. Moreover, we also observed the presence of chiral surface states in this material, which suggest a suprising violation of the topological bulk-boundary correspondence due to the existence of topological edge states even in the absence of long-lived topological quasiparticles in the bulk.

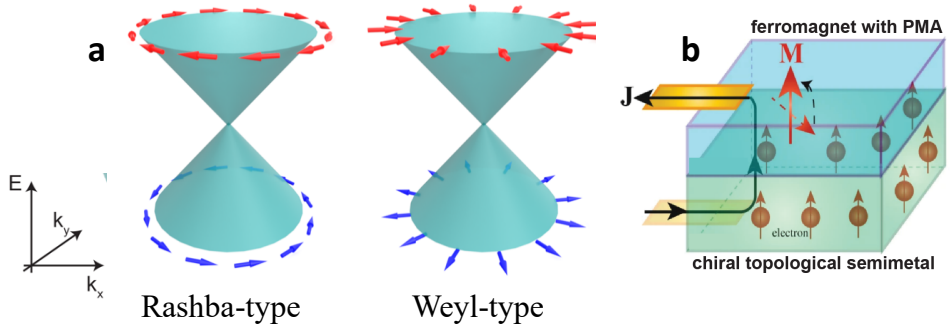

Fig. 1: (a) *Orthogonal Rashba-type spin-momentum locking vs. parallel Weyl-type spin-momentum locking.* **(b)** *Proposed interface for a memory device, adapted from Ref. [3].*

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Mo-12

The Pseudochiral Fermi Surface of α-RuI_3

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In search for potential quantum spin liquids (QSL), the compound RuI_3 has been recently synthesized in small single crystal [1-4]. In this study we carry-out a micro-ARPES measurement to resolve its 3D electronic structure.

We unambiguously demonstrate that RuI_3 is a moderately correlated metal with two bands crossing the Fermi level, implying the absence of any QSL phase. Interestingly, we find that the Fermi surface 2D (kx, ky) slice at any k_z lacks mirror symmetry, i.e. is pseudochiral. We link this phenomenon to the ABC stacking in the $R\bar{3}$ space group of α-RuI3, which is achiral but lacks any mirror or glide symmetries and discuss the generalities of when such a pseudochiral electronic structure may be observed in different space group.

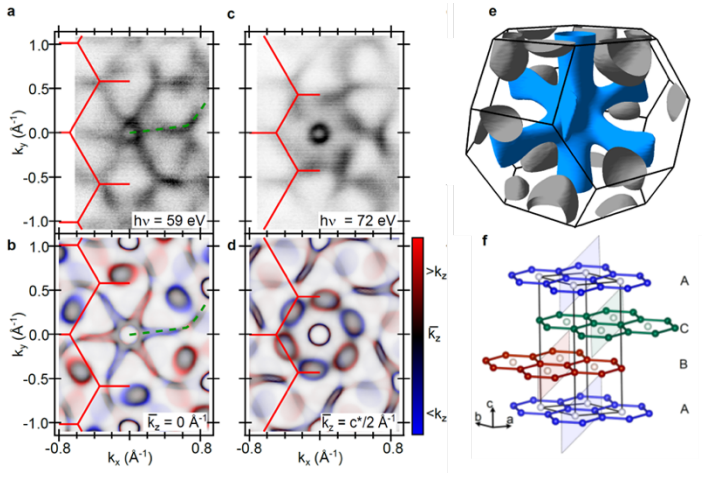

Fig. 1: a, c *Measured Fermi Surface corresponding to k_z = 0 and c*/2 respectively.* ***b, d*** *Simulated Fermi surface obtained by convolution of the DFT calculations with an energy and k_z Lorentzian broadening. Red and blue color indicates if the intensity comes mainly from a band above or below $\bar{k}_z$.* ***e*** *3D representation of the Fermi surface with the electron pocket in blue the holes pockets in grey.* ***f*** *Illustration of the Ru-plane showing the absence of global (1-10) mirror (or glide) symmetry due to the ABC stacking order.*

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Mo-13

Spectroscopic evidence for spin splitting in altermagnetic MnTe

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The Anomalous Hall effect (AHE) has been understood in close relation to nontrivial band topology. Recently, it has been proposed that AHE can arise in compensated collinear magnets with opposite-spin sublattices connected by rotational symmetry. This distinct magnetic phase, so-called 'altermagnetism', is characterized by time-reversal symmetry (TRS) broken electronic structure with non-relativistic spin-momentum locking. We performed angle-resolved photoemission spectroscopy (ARPES) on MnTe, an altermagnetic candidate. Spin-split electronic structure with a large splitting of ~1 eV is clearly resolved. The breaking of Kramers' degeneracy at the Neel temperature provides evidence for the spin-split ground state of altermagnetic MnTe. The compensated magnetic semiconductor with TRS-broken electonic structure opens up a new platform for novel topological spintronics.

Mo-14

Spin-Polarized Electronic States in $CoTe_2$

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The broad class of layered transition metal dichalcogenides (TMDs) has attracted significant attention in the last decades due to their novel electronic, optical, and topological properties, combined with their potential for various applications [1]. The TMX_2 family of TMDs has attracted notable interest due to the observation of Lorentz-symmetry violating, type-II Dirac fermions associated with a tilted Dirac cone near the Fermi energy. We present a detailed investigation of the electronic structure of 1*T* -$CoTe_2$ by combining first-principles calculations with spin-polarized ARPES experiments. We find that similar to other TMX_2 compounds, $CoTe_2$ is also a topological semimetal supporting a type-II Dirac crossing in the vicinity of the Fermi energy. In addition to the bulk electronic structure, we demonstrate that $CoTe_2$ hosts a ladder of topological surface states. In contrast to the surface states which typically display Rashba-type in-plane spin splitting, we find that $CoTe_2$ hosts interesting out-of-plane spin polarization as well. Our work establishes $CoTe_2$ as a potential candidate for

the exploration of Dirac fermiology and applications in spintronic devices, infrared plasmonics, and ultrafast optoelectronics. [2]

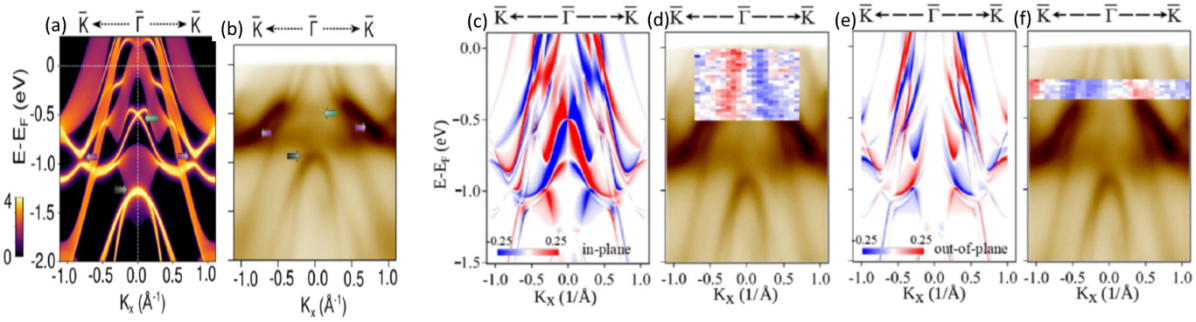

Fig. 1*: Theoretically calculated momentum-resolved spectral density plot (a) and experimentally measured ARPES plots along the K path. Calculated in-plane spin polarization (c) and measured spin polarization with spin-ARPES (d). Calculated out-of-plane spin polarization (e) and measured spin polarization with spin-ARPES (f)*

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Tu-01

Long-ranged charge order conspired by magnetism and lattice in antiferromagnetic Kagome metal FeGe

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A charge order (CO) has been discovered to emerge deep into the antiferromagnetic phase of the kagome metal FeGe. We have performed systematical experiments to study its origin, using transport, single crystal x-ray diffraction (SCXRD), scanning tunneling microscopy (STM), and angle-resolved photoemission spectroscopy (ARPES). We observed a first-order structural transition by transport and a long-ranged CO by STM in high-quality FeGe samples [1], in contrast to the previously reported short-ranged ones [2] that we show is due to the existence of certain defects. The distorted $2 \times 2 \times 2$ CO superstructure was precisely refined by SCXRD, which is characterized by a strong dimerization along the c-axis of 1/4 of the Ge1-sites in the Fe_3Ge layers [1]. Our ARPES experiments observe neither signatures of nesting of Fermi surfaces or van-Hove singularities nor sizeable electronic energy gaps around the Fermi level that can induce a 100 K CO, which excludes a conventional CDW mechanism driven by saving electronic energies for the CO in FeGe. Instead, we find the sudden upward shift of an electron-like band dominated by Ge-4p orbitals around the A point, as well as the upward shift of another electron-like band dominated by Fe-3d orbitals around the K point after the CO phase transition in the ARPES spectra [3]. These experimental results are well reproduced by our DFT calculations, which predicts that the CO in FeGe is driven by primarily saving magnetic energies via a first-order structural transition involving large partial Ge1-dimerization along the c-axis [4]. Our results have provided a comprehensive understanding of the puzzling CO behavior in FeGe, and established a novel CO mechanism conspired by magnetism and lattice, in contrast to the conventional nesting mechanism.

I will also briefly introduce the two new ARPES beamlines in Hefei Advanced Light Facility (HALF), a new 4th generation synchrotron facility that is under construction.

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Tu-02

First-principles Materials Design of Nickelate and Palladate Superconductors

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Motivated by the recent discovery of superconductivity in layered nickelates [1,2], we derived effective low-energy models for $NdNiO_2$ from first principles [3]. We found that the electronic structure of $NdNiO_2$ shares a characteristic commonality with high-T_c cuprates in that the $3d_{x2-y2}$ band forms a large two-dimensional Fermi surface. On the other hand, nickelates and cuprates have several distinct differences: The charge transfer from the oxygen p orbitals to the Ni 3d orbitals is much smaller than that in the cuprates. The $3d_{x2-y2}$ band is not half-filled due to the charge transfer from the Nd layer to the NiO_2 layer. We then performed an extensive materials search by replacing the Nd block layer with other block layers. We found several dynamically stable Ni- and Pd-compounds whose low-energy electronic structure better mimics the electronic structure of high-T_c cuprates [4,5]. By solving the resulting low-energy models by means of the dynamical vertex approximation [6,7], we found that the ratio between the Coulomb interaction and the kinetic energy of Pd compounds is better for realizing high T_c superconductivity than Ni compounds [8,9,10].

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Tu-03

Magnetic Weyl semimetal in Kagome lattice $Co_3Sn_2S_2$

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Weyl semimetal is a novel topological quantum state with emergent relativistic Weyl fermions of opposite chiralities and surface Fermi arcs in the electronic structure. Such distinct electronic structure leads to many exotic physical properties. It can be realized in a symmetry with inversion symmetry broken or time reversal symmetry broken. The latter is very sensitive to the magnetic structure so that the manipulation of the topological phase transition and the physical properties can be easily induced by external magnetic or electric field, that has great potential applications in the field of spintronics. In this talk, I will show the ARPES study on the magnetic Weyl semimetal phase in Co3Sn2S2, including the

observation of the surface Fermi arc, bulk Weyl point[1], spin-orbital coupling effect[2] and the topological phase transiton[3]. These results not only can help to understand the exotic physical properties of Co3Sn2S2, but also provide insights into the interplay between the magnetism and the topology.

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Tu-04

Electronic Properties of Atomically Thin Correlated Material Films

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2D systems can not only have physical properties distinct from those of 3D materials but also allow control/manipulation of their properties through stacking. For example, Mott insulating and superconducting states, unavailable in single layer graphene, are realized in twisted bilayer graphene. While these novel 2D systems are mostly obtained through exfoliation of van der Waals materials, a more conventional approach through thin film growth. In this presentation, I wish to introduce our research efforts to measure and manipulate electronic properties of a few unit-cell (uc) thick thin films by using thin film growth and *in situ* angle resolved photoemission (ARPES).

We started with ARPES on a few uc thick film of $SrRuO_3$ (SRO), a prototypical metallic ferromagnet with spin-orbit coupling. It was found that nodal lines and quadratic band crossing points are generic features of ultrathin perovskite films. These symmetry-protected nodal lines and quadratic band crossing points are sources of Berry curvature that causes the sign changing anomalous Hall effects [1]. By using additional 'conducting layer', we were able to obtain the electronic structure of 1 uc thick SRO films. Our results show that 1 uc films are not insulators but remain metallic. Dosing experiments reveal that 1 uc films are correlated Hund metals caused by the high density of states near E_F from the van Hov singularity [2]. We further controlled the strain and octahedron distortion of 1 uc films by using various substrates. We demonstrate that the electronic state of 1 uc films can be manipulated from a good metal to a correlated Hund metal, and finally to a Mott insulator [3][4].

Meanwhile, we were able to grow and measure the electronic structure of $SrIrO_3$ (SIO) films down to 1 uc. 1 uc SIO films has the same crystal structure of that of 1 uc Sr_2IrO_4. Not surprisingly, it is found that SIO 1uc films have the electronic structure of Sr_2IrO_4: relativistic Mott insulating state with (short) AF order. I will discuss the signature of AF order in the electronic structure of 1 uc SIO films

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Tu-05

Softening of a Flat Phonon Mode in the Kagome ScV_6Sn_6

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The long range electronic modulations recently discovered in the geometrically frustrated kagome lattice have opened new avenues to explore the effect of correlations in materials with topological electron flat bands [1]. Here, we present ARPES and IXS data that demonstrate a complete melting of the ScV_6Sn_6 (166) kagome lattice. The low energy phonon with propagation vector 1/3 1/3 1/2 collapses at 98 K, without the emergence of long-range charge order, which sets in with a propagation vector 1/3 1/3 1/3. The CDW is driven (but locks at a different vector) by the softening of an overdamped phonon flat plane at $k_z=\pi$. We observe broad phonon anomalies in momentum space, pointing to (1) the existence of approximately flat phonon bands which gain some dispersion due to electron renormalization, and (2) the effects of the momentum dependent electron-phonon interaction in the CDW formation [2]. Ab initio calculations corroborate the experimental findings to indicate that the weak leading order phonon instability is located at the wave vector 1/3 1/3 1/2 of a rather flat collapsed mode. Our data report the first example of the collapse of a softening of a flat phonon plane and promote the 166 compounds of the kagome family as primary candidates to explore correlated flat phonon-topological flat electron physics.

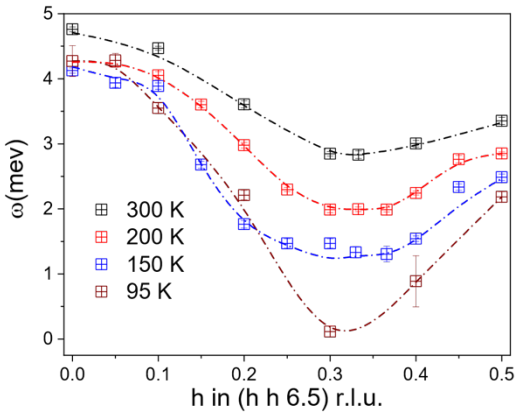

Fig. 1: *Momentum dependence of the 1/3 1/3 13/2 phonon frequency at selected temperatures, highlighting the large momentum softening.*

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Tu-06

The Role of van Hove Singularities in Kagome Metals

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The topology of a van Hove singularity (vHS) in two-dimensional materials is that of a saddle point connecting the electron-like and hole-like bands. When the vHS is aligned with the Fermi level, the electron-like and hole-like conduction can coexist, giving rise to an enhanced density of states as well as an attractive component of the Coulomb interaction. Therefore, the vHS has been considered as a driving source for unconventional electronic orders in correlated materials.

Recently, Kagome metals have attracted a lot of attention. The existence of multiple vHSs in the electronic structure of Kagome metals [1-3] provides a fertile territory to explore the possible manifestation of van Hove scenario in Kagome materials. This expectation is also in accord with the experimental observations of superconductivity and charge density wave in Kagome metals, which are the two leading instabilities of the two-dimensional vHS. However, despite the exciting theoretical proposals, the role of vHSs in Kagome metals remains to be examined experimentally. In this talk, I will present our recent studies on AV_3Sb_5 (A=Cs, Rb, K) and related Kagome metals. Using angle-resolved photoemission spectroscopy, we have unveiled the relationship between vHSs and electronic orders in these Kagome materials.

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Tu-07

Spin and Charge Dynamics of Doped One-Dimensional Mott Insulators

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Motivated by a recent angle-resolved photoemission spectroscopy (ARPES) experiment for a doped one-dimensional (1D) Mott insulator $Ba_{2-x}Sr_xO_{3+\delta}$ [1], we calculate ARPES spectrum, dynamical spin structure factor, and dynamical charge structure factor for 1D extended Hubbard models with long-range interactions, by using dynamical density-matrix renormalization group (DDMRG). We use the extended Hubbard models with not only a nearest-neighbor attractive interaction proposed in Ref. [1] but also long-range repulsive interactions up to third neighbors proposed by the analysis of biexciton in 1D Mott insulators [2]. In the repulsive model, ARPES spectrum exhibits a tendency toward the ARPES data in $Ba_{2-x}Sr_xO_{3+\delta}$, but the agreement with the ARPES data is worse than in the case of the attractive interaction. We find a clear difference of dynamical spin and charge structure factors between the attractive and repulsive modeld. In particular, the momentum dependence of dynamical charge structure factor shows a very contrasting behavior between the two models. Therefore, resonant inelastic x-ray scattering that can detect momentum dependent charge dynamics will be a good tool to identify a proper model for describing doped 1D Mott insulator $Ba_{2-x}Sr_xO_{3+\delta}$.

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Tu-08

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

Yulin Chen

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.

Tu-09

Anomalies at the Dirac point in graphene

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Study of graphene attracted enormous attention due to its rich physics and application in the next-generation electronic devices. Curiously, angle-resolved photoemission spectroscopy (ARPES) studies show anomalies at the Dirac point suggesting possibilities of energy gap with intense in-gap states, plasmaron excitations, electron correlation and electron-phonon induced effects, etc. We studied the properties of the Dirac states in pristine and hole-doped graphene employing ARPES and density functional theory. Employing symmetry-selective ARPES measurements for each band, we discover dispersive linear energy bands crossing at a distinct Dirac point within the anomalous region. No gap is observed even after 5% boron substitution that reduced the carrier concentration significantly suggesting protection of the internal symmetries even after boron substitutions. We show that apparent anomalies at the Dirac point appear due to the lifetime and momentum broadenings. The substitution of boron at the graphitic sites essentially leads to a band renormalization and a shift of the Dirac point towards the Fermi level. These results suggest that SiC-graphene is a good platform to realize interesting science as well as advanced technology where the carrier concentration, mobility, etc. can be tuned keeping the Dirac Fermionic properties protected.

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Tu-10

Orbital and wavevector dependence of the Moiré potential in a semiconducting heterobilayer

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Moiré semiconductors emerged as tunable quantum simulators for strongly correlated phases [1]. The single-particle low-energy physics is ruled by the moiré-periodic superpotential that develops by twisting or stacking layers with different lattice parameters. Signatures of this modulation are observed in the spectral function measured by angle-resolved photoemission spectroscopy (ARPES) in the form of replicas and gaps opening at the nascent zone boundary. In moiré transition metal dichalcogenides (TMDs), flat bands are reported at the Brillouin zone center and their dispersion is associated to the effective moiré potential experienced by electronic states with large out-of-plane orbital character [2,3]. Here, we extend this analysis and present the orbital and wave vector dependence of this interaction over the whole Brillouin zone by comparing quantitatively our ARPES data on a TMD heterobilayer with an extended tight-binding model. Our results set the fundaments for future spectroscopic studies of the electronic correlations in moiré systems.

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Tu-11

Tailoring Dirac fermions by in-situ tunable high-order moiré pattern

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Moiré superlattices provide a promising playground for explorations of novel quantum phases and phase transitions. We report an experimental study of a high-order moiré pattern formed in graphene-monolayer xenon heterostructure (G/mXe). The moiré period is in situ tuned from few nanometers to +∞, by adjusting the lattice constant of the xenon monolayer through annealing. Using angle-resolved photoemission spectroscopy, we observe that Dirac node replicas move closer and finally overlap with a gap opening, as the moiré pattern expands to +∞ and evolves into a Kekulé distortion. A moiré Hamiltonian coupling Dirac fermions from different valleys explains experimental results and indicates narrow moiré band. Our Letter demonstrates a platform to study continuous evolution of the moiré pattern, and provides an unprecedented approach for tailoring Dirac fermions with tunable intervalley coupling.

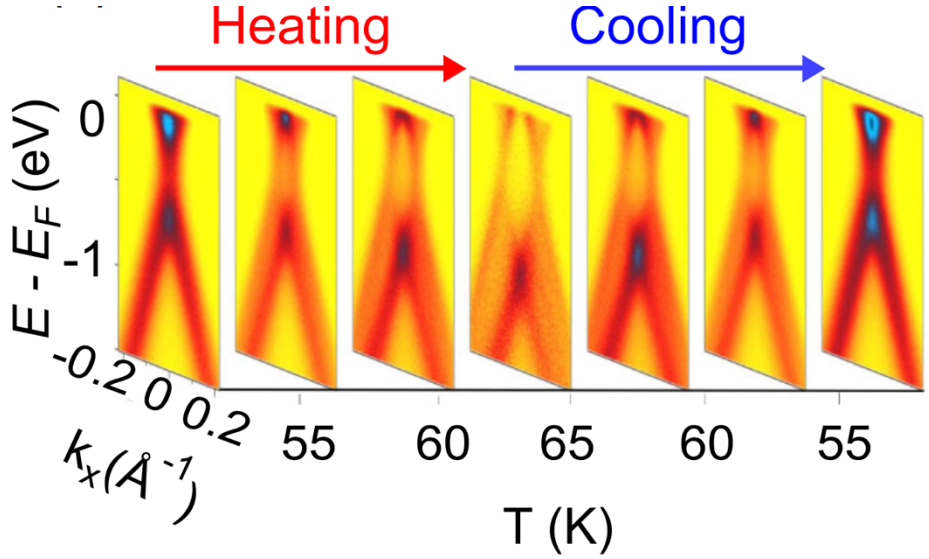

Fig. 1: *In-situ tuning the Dirac cone replicas in G/mXe by annealing processes.*

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We-01

Ultrafast Photoinduced Phase Transitions in Quantum Materials Revealed by Time- and Angle-Resolved Photoemission Spectroscopy

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The manipulation of the macroscopic properties of quantum materials through ultrafast photoexcitation is a fascinating field in condensed matter physics. Exciting coherent phonon mode optically provides a new pathway for driving nonequilibrium phase transitions and realizing novel states that are not accessible in thermal equilibrium conditions. If photoinduced coherent atomic motion could stop at metastable positions away from equilibrium, the material could possibly enter a novel metastable state different from its original state. Here, we systemically study the ultrafast electronic dynamics of the three-dimensional charge density wave (CDW) material 1T-$TiSe_2$ using time- and angle-resolved photoemission spectroscopy (TRARPES). We discovered multiple metastable states on different time scales in 1T-$TiSe_2$ by optical exciting the coherent motions of specific atoms. Firstly, we observed an ultrafast switching from the CDW phase to a metastable metallic state after photoexcitation, which is significantly different from its thermal equilibrium phase. The lifetime of this photoinduced metallic metastable state is tunable by varying the pump fluence and could be longer than 1 picosecond for the highest pump fluence in our studies. Combining with the phenomenological Ginzburg-Landau simulation, we demonstrate the emergence of the metastable state is due to transient modification of the double-well potential in the CDW phase and halting of the coherent phonon motions. Our results highlight the potential of optical modulation of atomic motion as an alternative pathway for realizing novel metastable states and as a useful approach for manipulating quantum materials via optical excitation of coherent phonon modes.

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We-02

Theoretically describing pump-probe experiments in electron-phonon coupled systems out to ps time scales

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In this talk, we describe coupled nonequilibrium electron-phonon systems semiclassically—using Ehrenfest dynamics for the phonons and quantum mechanics for the electrons—via a classical Monte Carlo approach that determines the nonequilibrium response to a large pump field. The semiclassical approach is quite accurate, because the phonons are excited to average energies much higher than the phonon frequency, eliminating the need for a quantum description of their behavior. The energy for the electrons is still in a quantum-degenerate regime, so quantum mechanics is critical to describe their behavior. The numerical efficiency of this method allows us to perform a self-consistent time evolution out to very long times (tens of picoseconds) enabling us to model pump-probe experiments of a charge density wave (CDW) material. Our system is a half-filled, one-dimensional (1D) Holstein chain that exhibits CDW ordering due to a Peierls transition. The chain is subjected to a time-dependent electromagnetic pump field that excites it out of equilibrium, and then a second probe pulse is applied after a time delay. By evolving the system to long times, we capture the complete process of lattice excitation and subsequent relaxation to a new equilibrium, due to an exchange of energy between the electrons and the lattice, leading to lattice relaxation at finite temperatures. We employ an indirect (impulsive) driving mechanism of the lattice by the pump pulse due to the driving of the electrons by the pump field. We identify two driving regimes, where the pump can either cause small perturbations or completely invert the initial CDW order. Our work successfully describes the ringing of the amplitude mode in CDW systems that has long been seen in experiment, but never successfully explained by microscopic theory. We also describe the fluence-dependent crossover that inverts the CDW order parameter and changes the phonon dynamics.

As observed in experiments (see, e.g., Ref. 1), the lattice motion causes the gap energy to oscillate, which is reflected in the computed PES at low temperatures in Fig. 1. The equilibrium spectrum before the pump is gapped (due to the Peierls distortion), which implies that only the lower band is populated. After excitation, the system will stabilize to a new equilibrium with a reduced gap energy. Increasing the temperature of the lattice has two major effects on the computed PES. The first is the evident damping of the gap oscillations, so the system relaxes faster to a new equilibrium PES for higher initial temperatures. The second effect is the "washing out" of the finer details in the spectrum at higher temperatures, increasing at longer times. The period of initial PES oscillations in Fig. 1(a) is much larger (around 1000 $\hbar/\gamma$) than what one would expect for $\Omega = 0.01\ \gamma/\hbar$ which is a clear sign that electron-phonon interaction significantly modifies the intrinsic phonon frequency. The advantage of our self-consistent MC approach is evident from the time scale of Fig. 1, where the time resolution must be kept at $0.1\ \hbar/\gamma$ to capture the electron dynamics, still the fast evolution scheme allows us to average over 3000 MC configurations. Translating these units to the ones in experiments, for $\gamma = 1$ eV, the time step is $\Delta t \approx 0.07$ fs, while the simulation time is around 7 ps. Most other methods can only approach maximal times on the order of 10s to 100s of fs.

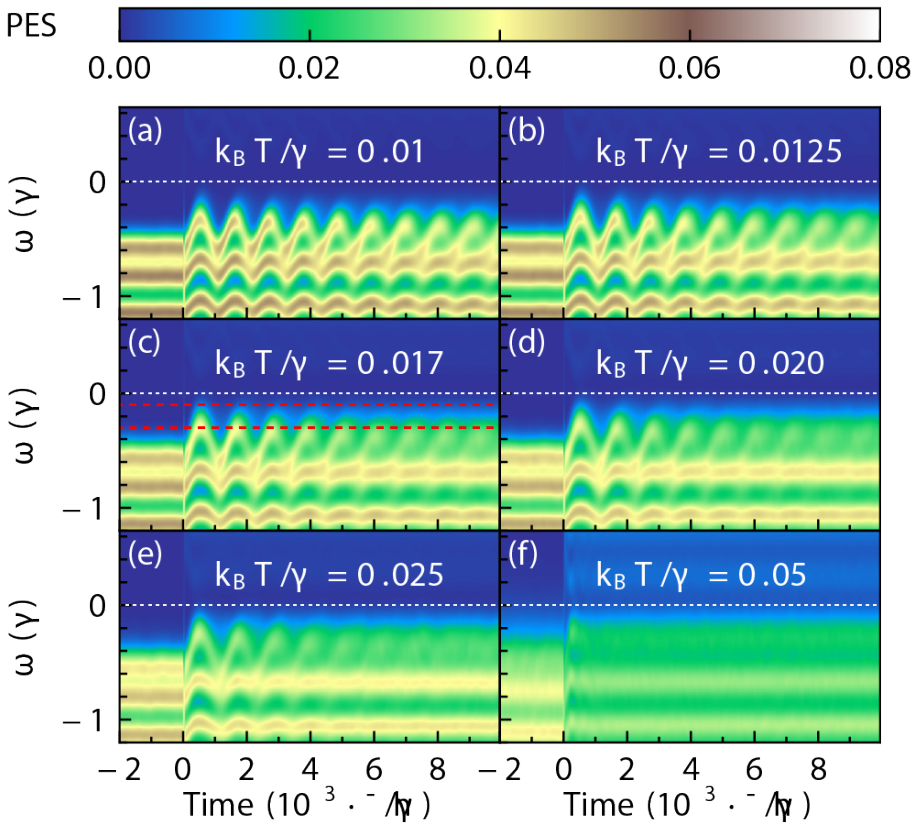

Fig. 1. Photoemission spectra for a chain of L = 30 sites at different temperatures. The electron-phonon coupling is λ = 0.6 and the phonon frequency is Ω = 0.01 γ/ħ. The pump parameters are E0 = 0.33, σp = 10 ħ/γ, and ωp = 0.1 γ/ħ.

As one can see in Fig. 1, exciting the electron impulsively excites the amplitude mode phonon as well, whose oscillation is damped as a function of time. The band edges of the PES oscillate with the frequency of the amplitude mode (which is renormalized from its bare value). As the initial temperature is raised, the damping is more rapid. In the talk, I will discuss this phenomenon and describe more pump/probe experiments on electron-phonon coupled systems.

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We-03

Ultrafast Dynamics of Hot Carriers in Pristine and Electron Accumulation Layers of Indium Selenide

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The dynamics of hot carriers in pristine and electron accumulation layers of InSe are monitored by time-resolved and angle-resolved photoemission spectroscopy (time-resolved ARPES). In pristine surface of InSe, the electrons excited by photons of 3.12 eV experience a manifold relaxation. First, they thermalize to electronic states degenerate with the M valley. Subsequently, the electronic cooling is dictated by Fröhlich coupling with phonons of small momentum transfer. Ab initio calculations predict cooling rates that are in good agreement with the observed dynamics [1]. The electron accumulation layer at the surface of InSe can lead to a formation of 2D electron gas (2DEG). In such a cause, the cooling rate of excited carriers can be monitored at doping level spanning from the semiconducting to the metallic limit. We observe that screening of LO phonons is not as efficient as it would be in a strictly 2D system. The large discrepancy is due to the remote coupling of confined states with the bulk. Our data indicate that the effect of such a remote coupling can be mimicked by a 3D Frohlich interaction with Thomas– Fermi screening [2]. The far-reaching outcomes provide insights on the screening of electron–phonon coupling in constrained dimensions and will be of high relevance for the development of aggressively downscaled circuits.

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We-04

Real-time observation of phonon-electron energy flow in laser-heated Nickel

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After driving a solid-state system out of equilibrium, the pathways the system takes to restore the ground state can lead to new functionalities. Examples range from all-optical magnetic switching [1] to insulator-metal transitions [2]. Typically, femtosecond laser

excitation of solids creates out-of-equilibrium hot electrons that cool down by transferring their energy to other degrees of freedom and ultimately to lattice vibrations of the solid. We often describe this behavior by assigning average thermodynamical properties, such as temperature in the so-called 3-temperature model, to electron, spin and lattice quasiparticles. Recently we observed for the prototypical ferromagnet Nickel that the momentum-dependent transient phonon occupation does not follow this simplified behavior and deviates significantly from thermal predictions [3]. In this talk I will give an overview how momentum-resolved phonon spectroscopy and time-resolved ARPES leads to a complete understanding of the intriguing electron-phonon scattering events at the heart of the non-equilibrium energy transfer dynamics from laser-heated electrons over spins to phonons and back.

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We-05

Sub-10 meV Time-Resolved ARPES Setup Using High-Harmonic Generation

Maciej Dendzik[1], Qinda Guo[1], Antonija Grubišić-Čabo[1], Magnus H. Berntsen[1], Cong Li[1], Wanyu Chen[1], Bharti Matta[2], Ulrich Starke[2], Björn Hessmo[1], Jonas Weissenrieder[1] and Oscar Tjernberg[1]

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Time-resolved ARPES is a powerful experimental technique enabling to study electronic band structure of quantum materials under out-of-equilibrium conditions. However, detailed studies of subtle electronic effects, such as presence of a superconducting gap, require excellent energy resolution and sufficiently high probe energy to map the whole surface Brillouin zone. Here, we present a high repetition rate, narrow bandwidth, extreme ultraviolet photon source for time-resolved ARPES recently developed at the BALTAZAR laboratory (KTH) [1]. The narrow bandwidth pulses for photon energies of 10.8, 18.1 and 25.3 eV are generated through high harmonic generation using ultra-violet laser pulses with relatively long duration. The high harmonic generation setup employs an annular drive beam in tight focusing geometry at a repetition rate of 250 kHz providing overall temporal resolution of ca. 200 fs. Photon energy selection is provided by a series of selectable multilayer bandpass mirrors, thin film filters, or a low-density normal-incidence grating [2]. A two-stage optical-parametric amplifier provides < 100 fs tunable pump pulses from 0.65 to 9 μm. During the talk, developed instrumentation and the first experimental results on cuprate superconductors will be discussed.

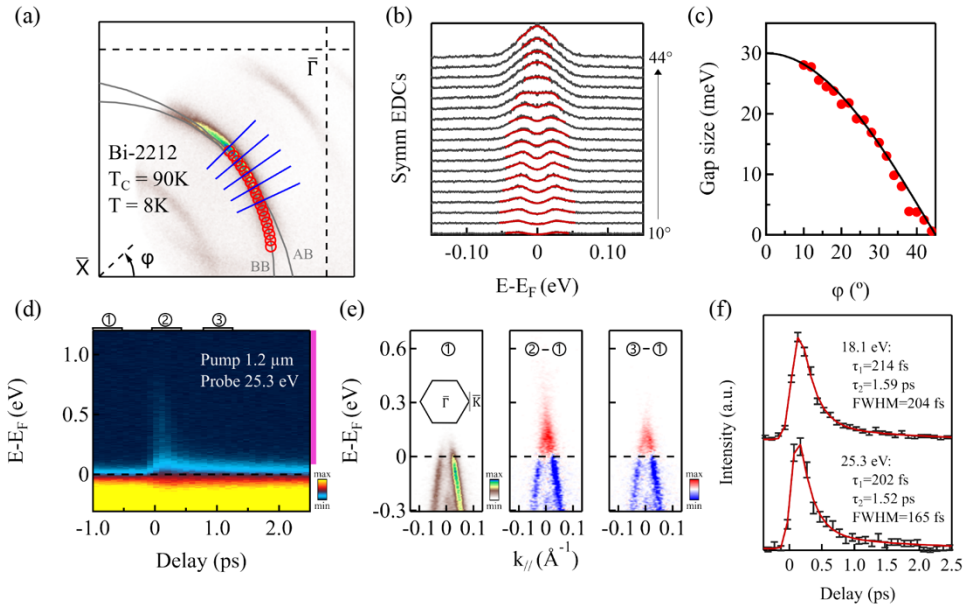

Fig. 1: *(a-c) ARPES spectra of Bi-2212 superconductor. (d-f) Time-resolved ARPES of graphene/SiC.*

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We-06

Observation of Ultrafast Interfacial Meitner-Auger Energy Transfer in a Van der Waals Heterostructure

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Interlayer charge- and energy-transfer processes in atomically thin, layered van der Waals heterostructures are of fundamental importance for determining their properties in novel device concepts based on single active crystalline layers. In our work, we study the ultrafast excitation, relaxation and transfer processes in an epitaxial grown monolayer WSe_2/graphene heterostructure using time- and angle-resolved photoemission spectroscopy [1]. By measuring the non-equilibrium electronic structure, we identify a novel interfacial energy transfer mechanism: Meitner-Auger energy transfer, which describes the conversion of an exciton in the semiconductor to an intraband electron-hole pair in graphene, characterized by the excitation of deep-lying valence holes in graphene. Based on a systematic microscopic calculation of interlayer couplings, we identify Meitner-Auger energy transfer as the dominant transfer process surpassing the efficiency of the established Förster- and Dexter-type transfer.

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Th-01

Revealing the Momentum-dependent Heavy Quasiparticles in Ce-based Kondo Lattice Systems

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The localized-itinerant transition of 4*f* electrons plays a key role in the rich physics of Ce-based heavy fermion systems. It is normally realized by the many-body Kondo effect, i.e., hybridization between the conduction and *f* electrons (*c-f* hybridization), but the importance of momentum-dependent *c-f* hybridization, as well as its competition with other interactions, remains open questions. Here we report our recent ARPES studies on some Ce-based heavy fermion systems, including $CeCu_2Si_2$ [1] and $CeRh_6Ge_4$ [2], where we found expperimental evidences of anisotropic *c-f* hybridization that could be closely related to their unconventional superconductivity or quantum criticality [3]. In epitaxial Ce films, the simplest Kondo lattice system, we found evidence of bandwidth-controlled Mott physics for 4*f* electrons [4], which is often observed in d-electron systems. Our results demonstrate that the momentum-dependent (and band-dependent) *c-f* hybridization, as well as their intricate interactions with long-range magnetic order [5] or Mott physics, can be important to understand the emergent phenomena in Kondo lattice systems.

*In collaboration with F. Steglich, H.-Q. Yuan, C. Cao, Y.-F. Yang, J. Denlinger, M. Smidman, J. Kroha, M. Shi, N. C. Plumb, B. Thiagarajan, J. Adell, D.-W. Shen, Y.-B. Huang.

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Th-02

Imaging the itinerant-to-localized transmutation of electrons across the metal-to-insulator transition in V_2O_3.

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According to the "Standard Model of Condensed-Matter Physics", the Bloch theory, metal or insulator are mutually exclusive states of matter. In insulators the highest occupied

quantum-mechanical energy band is totally filled with electrons, while in metals it is partially filled. Thus, as temperature cannot change the number of electrons in a solid, it should not change either its intrinsic nature, i.e. metallic or insulating. However, V_2O_3, a metal at room temperature, shows a first-order metal-to-insulator transition (MIT) when cooling below $T_{\mathrm{MIT}} \approx 160\,\mathrm{K}$, with an abrupt resistivity change of over six orders of magnitude. The very existence of a metal-to-insulator transition shakes the foundations of the well-tested Bloch model!

In fact in V_2O_3, as in many other transition-metal oxides, the last partially filled band is formed out of *d*-orbitals, which are rather localized in space. Thus, electrons in these bands can hardly avoid each other, and are subject to their strong mutual repulsion –the electron correlations, neglected in Bloch theory. The strong repulsion between electrons can inhibit their movement and result in a "Mott" metal-to-insulator transition (MIT), a fundamental phenomenon whose understanding has remained a challenge for over 50 years. A key issue is how the wave-like itinerant electrons in the metallic state change into a localized-like state in the insulator due to increased interactions. However, observing the MIT in terms of the energy- and momentum-resolved electronic structure of the system, the only direct way to probe both itinerant and localized states, has been elusive.

In this talk, I will discuss our recent experimental studies of the MIT in V_2O_3 [1] using angle-resolved photoemission spectroscopy. We found that in this material the temperature-induced MIT is characterized by the progressive disappearance of the conduction band of itinerant electrons, without any change in its energy-momentum dispersion, and the simultaneous shift to larger binding energies of a quasi-localized state initially located near the Fermi level. Only when the state of itinerant electrons crossing the Fermi level has vanished, a complete gap of about 700 meV is observed, associated to the final energy position of the quasi-localized state. Furthermore, the spectral weights of the itinerant and quasi-localized states show a clear thermal hysteresis that tracks the one observed in resistivity data across the MIT.

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Th-03

Antiperovskite X_3SnC: A new platform for quantum phase transition (X = lanthanide)

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Antiperovskites, the electronically inverted structures of perovskites, are rare despite their simple crystal structure due to the synthetic challenge and thermodynamic constraints. Their peculiar bonding feature and unusual oxidation states of the constituent elements, as clearly distinct from the conventional crystal system, allow the exotic physical phenomena. Here, we report X_3SnC antiperovskite family with a variety of quantum phase transitions assisted by antiperovskite frameworks. The crystal structure of the antiperovskite X_3SnC is composed of a network of corner-sharing X_6C octahedra and is stabilized by the strong covalent X–C bonds.

We found Ce_3SnC shows devil's staircase behavior in heavy fermion states with antiferromagnetic ordering due to the unusual spin interaction of the Ce 4f electron and a high Sommerfeld coefficient in Gd_3SnC with the non-fermi liquid behavior while keeping the ferromagnetic ordering of Gd 4f electrons due to the unusual banding nature of antiperovskite. We expect this discovery will expand the spectrum of the crystal system as a platform to study strongly correlated physics and trigger the further exploration of unusual crystal structures for emerging novel physical phenomena.

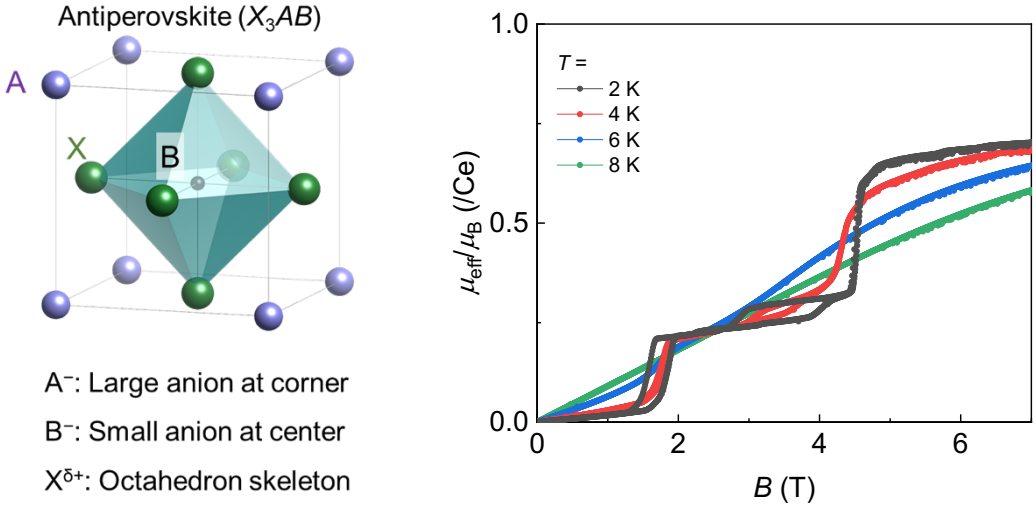

Fig. 1: *The crystal structure of X_3SnC antiperovskites and devil's staircase behavior of Ce_3SnC in low temperatures.*

References can also be given in the abstract [1]. Abstract text is allowed to flow around the graph.

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Th-04

Evidence for Single-Band Mott Insulator State in Nb_3Cl_8 and Excitonic Insulator State in $Ta_2Pd_3Te_5$

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In non-interacting or weakly interacting electron systems, the single-electron band theory can describe the electronic structures of materials well. However, electron correlation can significantly alter the electronic structures and even cause the failure of the single-electron band theory. Band calculations show that Nb_3Cl_8 has a metallic state with a weakly dispersive

band that is half-filled at the Fermi level, but experiments show that it is an insulator. By combining experimental and theoretical analysis, we have discovered that the Coulomb interaction on the half-filled band far exceeds the electronic kinetic energy, leading to a Mott transition. This Mott insulating state is only related to one half-filled band and can be straightforwardly described by the single-band Hubbard model. Similarly, band calculations show that $Ta_2Pd_3Te_5$ is a semimetal with a small overlap between the valence and conduction bands, but experiments show that it is a semiconductor. Based on experimental and theoretical analysis, we have revealed that spontaneous condensation of excitons leads to a metal-insulator transition. Unlike other candidate excitonic insulators, no structural phase transition is observed in $Ta_2Pd_3Te_5$, indicating that its insulating state is purely driven by electron correlation.

Th-05

How quasiparticle die in a bad metal

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Strongly interacting Fermi liquids often turn into bad metals at elevated temperature. How this crossover proceeds is largely unknown, as is the nature of the bad metal state. Here, we address this question by studying how low-temperature quasiparticles in the model Fermi liquid Sr_2RuO_4 disappear with increasing temperature on approaching the bad metal state. In contrast to common ARPES folklore, our experiments show that quasiparticles do not disappear via a vanishing residue *Z*. To the contrary, we find that the residue *Z* increases with increasing temperature and gradually diminishing coherence. Quasiparticles eventually disappear not by losing weight but by dissolving via excessive broadening. These findings are in semi-quantitative agreement with dynamical mean field theory calculations.

We further study the non-Fermi-liquid state of Sr_2RuO_4 observed in transport measurements under uniaxial strain [1]. To this end, we introduce a new method for precision ARPES experiments under continuously varying strain. Our data monitor the tuning the of a van Hove singularity across the chemical potential and show that quasiparticles remain intact at the critical strain. This suggests that non-Fermi liquid behavior emerges in Sr_2RuO_4 from subtle changes in the scattering rate rather than from a breakdown of the concept of quasiparticles.

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Th-06

Analyzing ARPES Data on a Fermi Surface Crossing Path in k-Space

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Many-body correlations are commonly extracted from ARPES data via the sudden approximation. This framework involves a square matrix $\mathbb{G}(k,\omega)$ of Green functions in thermal equilibrium and a column vector $\mathbb{M}$ of dipolar matrix elements, defining a scalar, complex function $G(k,\omega)=\mathbb{M}^{+}\mathbb{G}\,\mathbb{M}$. The intrinsic, k-resolved spectral function is derived from Im(G), taking the limit $\mathrm{Im}(\omega) \rightarrow 0$. The exact matrix $\mathbb{G}$ being unknown for any quantum model of interest for material science, an ansatz for the scalar G has to be made. The principle of causality requires G to be holomorphic as function of ω in the two open half plains where Im(ω) is finite and has a definite sign. A causal ansatz obeys the criterion $\mathrm{sgn}(\mathrm{Im}(G(\omega)))=-\mathrm{sgn}(\mathrm{Im}(\omega))$, called the Herglotz property. The real ω-axis does not belong to either domain of analyticity but forms the boundary between them. By analytical continuation onto the boundary and beyond, one encounters singularities that influence the physical spectrum more or less, depending on their distance from the boundary.

A point $k=k_F$ on the Fermi surface (FS) is characterized by a singularity in the analytic continuation of $G(k_F,\omega)$, positioned exactly at $\omega=0$. Since thermal broadening already pushes the singularity beyond the boundary, a FS is only sharply defined at temperature T=0. The analytical structure of $G(k,\omega)$ is constrained by the hermiticity of the self energy, combined with the Herglotz property. In particular, the spectral intensity at the Fermi edge diverges for $k=k_F$ but drops to zero for other points k in the Brillouin zone.

Assuming T=0, the singular behavior expected on a FS crossing path is still masked in the ARPES data by extrinsic broadening. Two sources of broadening can be modeled analytically: (i) The convolution with a Lorentzian noise spectrum of half width δ_L is obtained by evaluating the holomorphic $G(k,\omega)$ at a distance δ_L from the real ω-axis. A well known example is the Voigt profile, derived from the same holomorphic function as the unconvoluted Gaussian, in this case the complex error function. (ii) The finite angular resolution of ARPES is modeled by convoluting $G(k,\omega)$ with a smooth distribution $k+\Delta k$, centered on the nominal momentum k. Mechanisms (i) and (ii) cap the divergence in different ways. By systematically increasing their strength, either independently or in combination, a surprising variety of line shapes is generated. This allows to assess, whether the experimental resolution is sufficient to have confidence in the many-body parameters extracted from the data, particularly near a fixed point of strong correlations.

To generate various line shapes, an ansatz for the intrinsic $G(k,\omega)$ at T=0 is made, using the two band periodic Anderson model [1]. An isolated pole is assumed as singularity, causing a

Fermi liquid scenario. Other singularities, causing non-FL scenarios, are briefly reviewed [2-4].

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Th-07

Circular Dichroism and Orbital Angular Momentum in Chiral Weyl Semimetals PdGa/PtGa

Yun Yen[1,2] ,MengYu Yao[3], Jonas A. Krieger[4], Qun Yang[5], Iñigo Robredo[3], Maia G. Vergniory[6], Niels B. M. Schröter[4], and Michael Schüler[1,7]

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In recent years, there has been some development on using direct spectroscopic experiments to diagnose topology in quantum materials. For instance, circular dichroism (CD) can be directly connected to Berry curvature in 2D topological insulators with angle resolved photoemission spectroscopy (ARPES)[1]. On the other hand, nonsymmorphic chiral Weyl semimetals can host multifold crossings with large Chern numbers[2,3], where both orbital angular momentum (OAM) and Berry curvature have radial hedgehog structure close to these multifold Weyl nodes.

In this work, we show that CD-ARPES measurements can indeed map fingerprints of topology in chiral Weyl semimetals PdGa/PtGa, where CD exhibits radial structure as OAM. To simulate the CD intensity, we use Wannier function based tight binding model and plane-wave approximated photoelectron states, which we get from our in-house open source code dynamics-w90[4]. The simulation and the experiment show remarkable agreement. To examine the relationship between CD and topology, we theoretically check the correspondence between local OAM and dipole matrix elements, which we find to depend on both orbital characters and experimental geometry. According to our analysis, Pd/Pt local OAM can be measured by CD, where d orbital contribution is dominated by magnetic quantum number $m=\mp 2$ complex orbitals. Although the total CD signal consists of many interatomic interference terms, which can lead to deviation between CD and OAM, all the interference terms still exhibit radial structure Using CD to detect band topology in 3D

topological semimetals is indeed complicated, but we conclude that one can still see the reminiscence of radial OAM structure, which directly comes from the topological nature of the Weyl nodes.

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Th-08

Mott Quantum Critical Points and phase separation at finite doping in Hund metals

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"Hund metals" are multi-orbital paramagnetic metals with sizeable effects due to the intra-atomic exchange energy or Hund's coupling, and are characterised by strong, orbital-selective correlations and large fluctuating local magnetic moments. Their physics is relevant for iron-based superconductors and other materials like transition metal oxides.
A general feature found in models and realistic simulations of these materials, and corroborated by experimental data, is a frontier crossing the doping-interaction strength plane, and originating from the Mott transition point of the half-filled system, across which the aforementioned defining features are strongly enhanced.

This frontier is a cross-over at large doping while approaching half-filling it becomes a first-order transition between two metals. It features a phase separation zone ending in a quantum critical point at finite doping.

I will show that all this phenomenology is due to the first-order nature of the Mott transition and can be back-tracked to a small energy scale splitting the atomic ground-state multiplet, in this case the Hund's coupling.

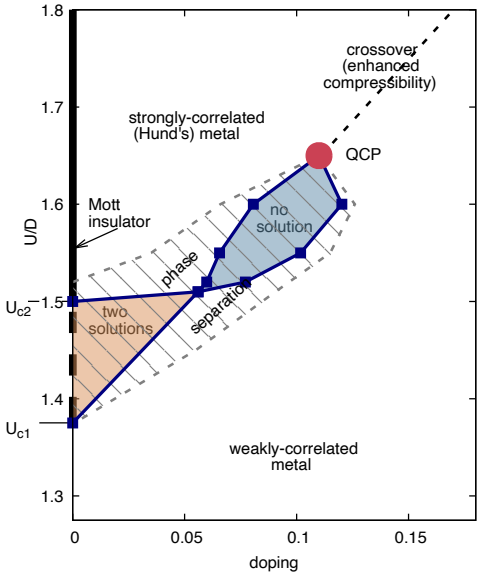

Fig. 1: *Phase diagram of the 2-orbital Hund-Hubbard model with nonzero Hund's coupling in the interaction strength/doping plane.*

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Th-09

Scattering Rates of Quasi-Particles: from Fermi Liquids via Marginal Fermi Liquids to "Super-Planckian" Systems.

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The scattering rate of quasi-particles determines transport, thermal, and magnetic properties of metals. Conventional superconductivity is related to scattering of charge carriers by the excitation of phonons. Unconventional superconductivity is often believed to be mediated by scattering processes caused by electronic excitations such as spin fluctuations. ARPES is a valuable method to measure the energy, temperature, momentum, and spin dependence of electron scattering rates.

Here we report on measurements of the energy, momentum, and spin dependence of scattering rates in various metals: nearly-free electron systems Na and Na suboxide, Ni metal, and Fe-based superconductors.

Na and Na suboxide, the latter with a reduced number of charge carriers, show a perfect quadratic increase of the scattering rate as a function of energy in a wide energy range of 2 eV: $\Gamma=\alpha E^n$, n=2. The derived α value in Na does not support the often-discussed importance of spin fluctuations in alkali metals. Theory predicts for nearly-free electron systems a strong dependence on the charge carrier density, usually expressed by the unit-sphere radius of the

electron r_s in units of the Bohr radius. For both, Na and Na suboxide we derive in good agreement with theory $\alpha \sim r_s^{5/2}$ [1,2].

In Ni the scattering rates are linear in energy and spin dependent due to Stoner excitations. The energies of the observed kinks are related to the on-site Coulomb interaction U and to the Hund exchange interaction J_H [3].

In the electron-doped ferropnictides, maximal scattering rates close to a marginal Fermi liquid ($\Gamma=\beta E$, $\beta=1$) were derived. In the optimally hole-doped ferropnictides, a "super-Planckian" slope $\beta\sim3$ was observed for specific sections of the Fermi surface which also show the largest superconducting gap [4-6]. Measurements as a function of doping concentration indicate that the size of the slope and thus the electronic scattering rate is linked to the superconducting transition temperature [5]. This result strongly supports the model of s^{+-} superconductivity. Recent ARPES studies of iron chalcogenides also showed an orbital dependent scattering rate [7], the energy dependence of which is for particular bands close to the Fermi level beyond the Planckian bond.

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Th-10

Nodal s± Pairing Symmetry in an Iron-Based Superconductor with only Hole Pockets

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The origin of the high temperature superconductivity in the iron-based superconductors remains elusive after being extensively studied for more than a decade. In the iron-based superconductors that have hole pockets around the Brillouin zone center and electron pockets around the zone corners, the pairing symmetry is generally considered to be s±. For the iron-based superconductors with only hole pockets, however, a couple of pairing scenarios have been proposed but the exact symmetry is still highly controversial. By taking laser-based angle resolved photoemission measurements with super-high resolution and at ultra-low temperature, we have precisely determined the superconducting gap distribution of KFe_2As_2 which is a prototypical iron-based superconductor with hole pockets both around the zone center and around the zone corners. The complete superconducting gap structure, in combination with the observation of the spin resonance in neutron scattering, provides strong evidence on the s± pairing symmetry in KFe_2As_2 with a gap sign reversal between the hole pockets around the zone center and the hole pockets around the zone corners. These results

unify the pairing symmetry in the hole doped iron-based superconductors and point to the spin fluctuation as the pairing glue in generating superconductivity.

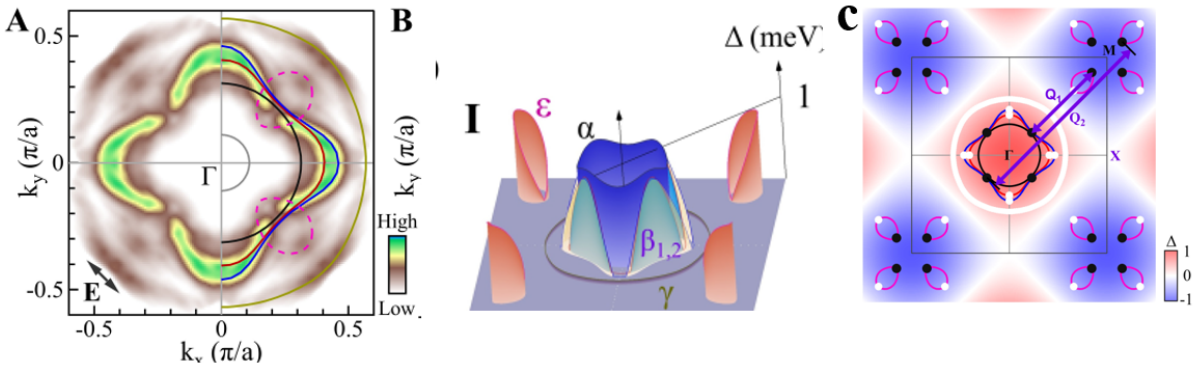

Fig. 1: *Fermi surface, momentum dependence of superconducting gap and possible nesting vectors in* KFe_2As_2

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Th-11

Ab Initio Studies, Spectroscopic Signatures, and Fractionalization in Cuprate High-T_c Superconductors

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Understanding of the microscopic origin of the material dependence of copper oxide superconductors with a diversity of the superconducting critical temperature T_c ranging from 10K to above 130 K at ambient pressure and even to 164K under pressure is a major challenge in condensed matter physics. We derived a number of *ab initio* Hamiltonians for the cuprate superconductors, carrier doped CaCuO2, Bi2Sr2CuO6, Bi2Sr2CaCu2O8, and HgBa2CuO4 without adjustable parameters [1] and solved them by state-of-the-art quantum many-body solvers [2]. The solutions reproduced detailed materials dependence in experiments as well as the common properties, from which the principal component that controls the superconducting amplitude is revealed and a scaling relation to predict the optimum T_c is proposed at the optimum doping. The result also supports electron fractionalization [3] that has a close relationship to the severe competition of the *d*-wave superconductivity and charge inhomogeneity such as the charge/spin stripe. The fractionalization is represented by the two-component fermion model in its simplest form [4], which well accounts for the pseudogap formation. It also well describes the elusive angle

resolved photoemission spectroscopy (ARPES) results [5]. There, the main and direct origin of the high-T_c superconductivity is identified to be originated from the dark fermions emerging as a consequence of the fractionalization, which generates a prominent peak in the imaginary part of anomalous self-energy, while the peak completely cancels with the normal self-energy contribution in the total spectral function and hidden in the ARPES and STM measurements. The fractionalization also predicted the enhancement of the excitonic resonance in the resonant inelastic X-ray scattering (RIXS) [6], which was verified in the measurement [7].

The series of this work were performed in collabotations with Jean B. Moree, Michael T. Schmid, Motoaki Hirayama, Shiro Sakai, Marcello Civelli, Takahiro Misawa, Youhei Yamaji, Teppei Yoshida, Atsushi Fujimori, Amol Singh, Di-Jing Huang and group of NSRRC, Taiwan, China.

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Th-12

Phonon-Mediated Attractive Interaction and Its Impact on Cuprate Superconductors

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Unconventional superconductivity comprises a large part of the innovative landscape due to rich applications and mysterious pairing mechanisms. Establishing a minimal microscopic model is a crucial step in designing and discovering these materials. In this talk, I will introduce a joint effort of ARPES and quantum many-body simulations about the necessary components of microscopic models in unconventional superconductors. In the ARPES spectra of 1D cuprate chains, we identified a prominent folding feature beyond the predictions of the Hubbard model [1]. Through multiple numerical methods, we provided a quantitative explanation through the coexistence of strong correlations and electron-phonon coupling [2]. Based on this model and extracted parameters, we found an instability of *p*-wave superconductivity in heavily doped 1D cuprates and an enhancement of *d*-wave superconductivity in optimally doped quasi-1D ladders [3,4]. The coexistence and interplay between these two interactions provide a possible reason for unconventional superconductivity and a control knob to turn it [5].

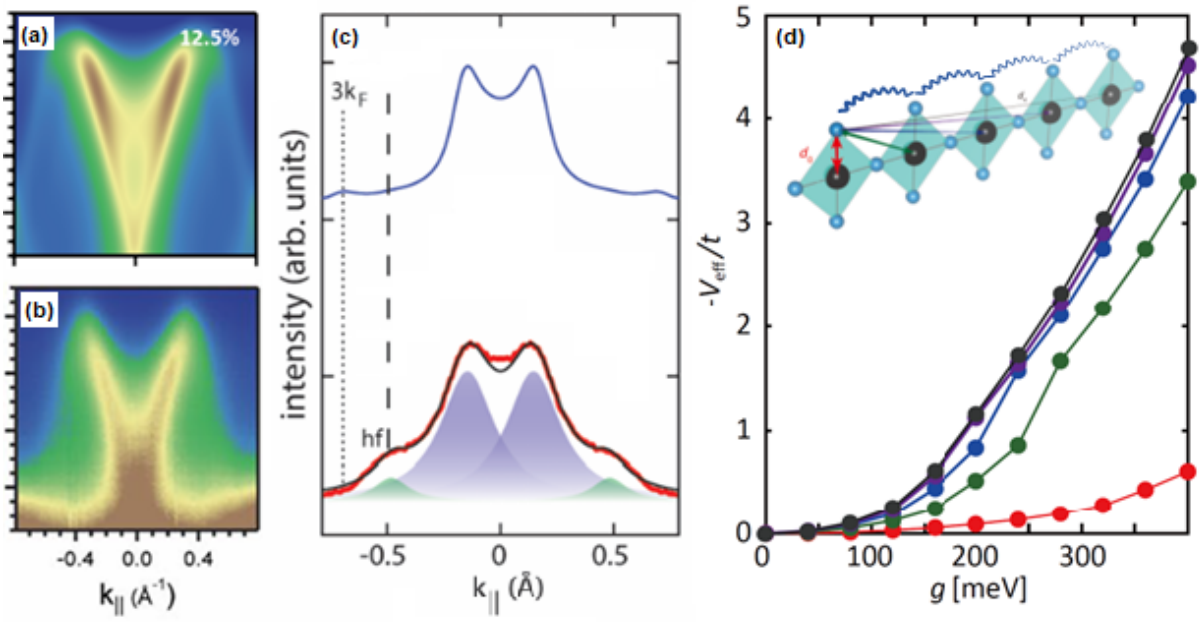

Fig. 1: *(a) Simulated spectral function for a doped 1D cuprate chain using the Hubbard model. (b) ARPES experimental spectrum for the same system with similar doping. (c) The comparison of the two spectra MDCs at E=-0.7eV, where the dashed lines highlight the mismatched features. (d) The explanation using the nearest-neighbor attractive interaction mediated by phonons.*

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Th-13

Electronic Origin of High-Tc Maximization and Persistence in Trilayer Cuprate Superconductors

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In high temperature cuprate superconductors, it was found that the superconducting transition temperature T_C depends on the number of CuO_2 planes (n) in the structural unit and the maximum T_C is realized in the trilayer system (n=3). It was also found that the trilayer superconductors exhibit an unusual phase diagram that T_C keeps nearly constant in the overdoped region which is in strong contrast to the T_C decrease usually found in other cuprate superconductors. The electronic origin of the T_C maximization in the trilayer superconductors and its high T_C persistence in the overdoped region remains unclear. By taking high resolution laser-based angle resolved photoemission (ARPES) measurements, here we report our revelation of the microscopic origin of the unusual superconducting properties in the trilayer superconductors. For the first time we have observed the trilayer splitting in $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$ (Bi2223) superconductor. The observed Fermi surface, band structures, superconducting gap and the selective Bogoliubov band hybridizations can be well described by a three-layer interaction model. Quantitative information of the microscopic processes involving intra- and interlayer hoppings and pairings are extracted. The electronic origin of the maximum Tc in Bi2223 and the persistence of the high T_C in the overdoped region is revealed. These results are qualitatively consistent with the composite picture where high-Tc can be realized in an array of coupled planes with different doping levels such that a high pairing strength is derived from the underdoped planes while a large phase stiffness from the optimally or overdoped ones. They provide key insights in understanding high Tc superconductivity and pave a way to further enhance Tc in the cuprate superconductors.

Th-14

Probing a Bose Metal via Electrons:

Inescapable Non-Fermi Liquid Scattering and Pseudogap Physics

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Non-Fermi liquid behavior and pseudogap formation are among the most well-known examples of exotic spectral features observed in several strongly correlated materials such as the hole-doped cuprates, nickelates, iridates, ruthenates, ferropnictides, doped Mott organics, transition metal dichalcogenides, heavy fermions, *d*- and *f*-electron metals, etc. We demonstrate that these features are inevitable consequences when fermions couple to an unconventional Bose metal[1] mean field consisting of lower-dimensional coherence. Not only do we find both exotic phenomena, but also a host of other features that have been observed *e.g.* in the cuprates including nodal anti-nodal dichotomy and pseudogap

asymmetry(symmetry) in momentum(real) space. Such a generic emergent Bose liquid also display the observed large energy distribution of the underlying self-energy, and the corresponding kink formation. Most significantly, it explains the observed proportionality between the low-temperature superconducting gap and the high-temperature scattering rate. Obtaining these exotic and heretofore mysterious phenomena via a mean field offers a simple, universal, and therefore widely applicable explanation for their ubiquitous empirical appearance.

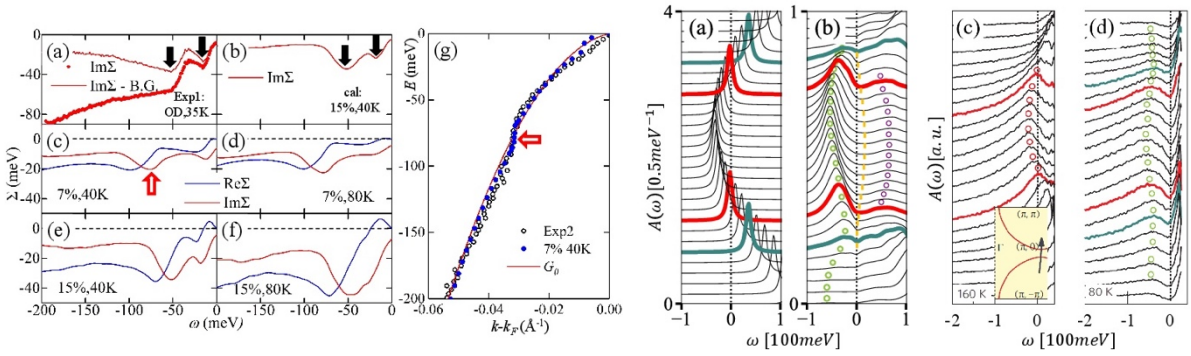

Fig. 1: (left panel) self-energy resulting from scattering against emergent Bose liquid showing non-Fermi liquid scattering rate at zero frequency, and structures that produces the kink in the one-body spectral function. (right panel) pseudogap formation from scattering against a Bose metal.

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Th-15

Several revealing ARPES measurements that should be conducted on the high-Tc cuprate superconductors

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Here we argue that the following set of ARPES measurements on the high-Tc cuprate superconductors can be very revealing. More specifically, (1)A thorough investigation of the unoccupied electron spectral function dozens of meV above the Fermi energy can be extremely revealing on the origin of the pseudogap(PG) phenomena and can help to identify the anomalous self-energy related to electron pairing fluctuation. (2)A systematic comparison on the way that the Fermi arc phenomena emerge with decreasing temperature among different family of cuprate superconductors can help to establish the potentially universal relation between such a phenomena with other PG signatures, especially the spin gap

phenomena observed in NMR measurement. (3)A re-investigation of the quantum critical scaling of the electron self-energy with a much higher momentum and energy resolution than available about 20 years ago is important to check the consistency of claim of the Marginal Fermi liquid phenomenology made then. This measurement can be especially illuminating around the newly discovered PG end point where strong evidence for quantum criticality is found. (4)A thorough investigation of the doping and temperature evolution of the anti-nodal dispersion in the superconducting state, especially on how and when the exceptionally flat anti-nodal dispersion evolves into the standard d-wave BCS dispersion, may hold the key to answer the mechanism of superconductivity in a non-Fermi liquid normal state background. (5)A thorough investigation of the so called "waterfall" phenomena across different family of cuprate superconductors may provide important clue on the origin of the non-Fermi liquid behavior in these strongly correlated electron systems. (6)A systematic comparison on the role of the VHS doping among different family of cuprate superconductors may offer new clues for theoretical understanding of these systems.

Fr-01

Floquet engineering of a model semiconductor

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Time-periodic light field can dress the electronic states, providing fascinating opportunities for manipulating the electronic band structure of two-dimensional materials and topological materials in the ultrafast timescale with intriguing light-induced emergent phenomena [1]. In this talk, I will present our recent progress in time- angle-resolved photoemission spectroscopy (TrARPES) instrumentation [2,3] with tailored pump and probe pulses. I will also present our recent progress on the ultrafast dynamics and Floquet band engineering of a model semiconductor - black phosphorus [4]. By pumping resonantly with the band gap, we demonstrate the ultrafast manipulation of its electronic structure of black phosphorus in the femtosecond timescale, which shows interesting coupling with the pseudospin degree of freedom.

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Fr-02

Visualizing Band Hybridization and Moiré Effects in Gate-Tunable Twisted Graphene Layers Using NanoARPES

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Twisted graphene layers have emerged as an intriguing class of quantum materials that display surprising correlation effects, including superconductivity, Mott insulators as well as

strange metal phases [1-4]. The possibility to tune these states using twist angle and electrostatic doping provides a promising route to interrogate the underpinning interactions between the electronic states. Here, we use angle-resolved photoemission spectroscopy with spatial resolution at the new micro- and nanoARPES branch at the ASTRID2 synchrotron light source at Aarhus University in Denmark to visualize the electronic states of twisted graphene layers integrated in device architectures. Specifically, we reveal the flat band in twisted double-bilayer graphene around the magic angle of 1.3° and systematically track the evolution of hybridization effects and moiré bands with small twist angles up to 6°. The interactions in the systems are further tuned by *in situ* electrostatic doping using a back-gate electrode. Our study paves the way for directly engineering band structure and correlation effects in twisted two-dimensional materials.

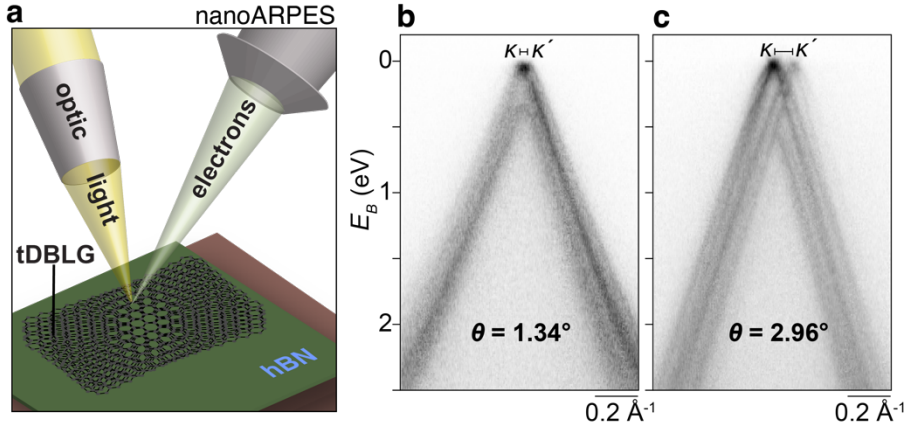

Fig. 1: *NanoARPES experiment on twisted double bilayer graphene (tDBLG): **(a)** Sketch of nanoARPES experiment on a heterostructure device composed of tDBLG on hBN. **(b)-(c)** NanoARPES spectra of tDBLG with interlayer twist angles of (b) 1.34° and (c) 2.96°, respectively.*

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Fr-03

Recent Progress of the High-resolution Micro-focused ARPES beamline at Shang Synchrotron Radiation Facility

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Recent progress in angle-resolved photoemission spectroscopy (ARPES) has made it essential for condensed matter physics. With greatly improved energy and momentum resolution in recent decades, ARPES can now simultaneously observe electronic states beyond energy and momentum, e.g. in spin- and time-degree of freedom. Meanwhile, the need to measure local band structures is growing, such as the edge states of topological materials (e.g. 2D/higher-order topological insulators), quantum phase transitions in micro/nano-heterostructures (e.g. twisted bilayer graphene), localized states on inhomogeneous surfaces, and hard-to-cleave single crystals/microsamples, making the spatially-resolved ARPES an important frontier.

In this talk, I will introduce the recent progress of the high-resolution micro-focused ARPES beamline and station at Shanghai Synchrotron Radiation Facility (BL03U at SSRF). By using a novel type of APPLE-Knot undulator, the headload from the inserting device to the beamline optics has been greatly suppressed, resulting in a high energy resolution which is close to the theoretical limits. Moreover, an optimized ultra-high precision elliptical mirror realized a micro-focused beam spot of 15×15 μm^2 size at sample position with a single focusing optics that maximizes the incident photon flux to sample. This endstation has been successfully applied to the measurements of several recently discovered quantum materials with multiple cleaved plans (Fig. 1), rough surface as well as micro-size crystal. As the second part of this talk, a new endstation at the branch-line of BL03U that aims for sub-micron focusing by capillary optics will be introduced, along with newly obtained commissioning results.

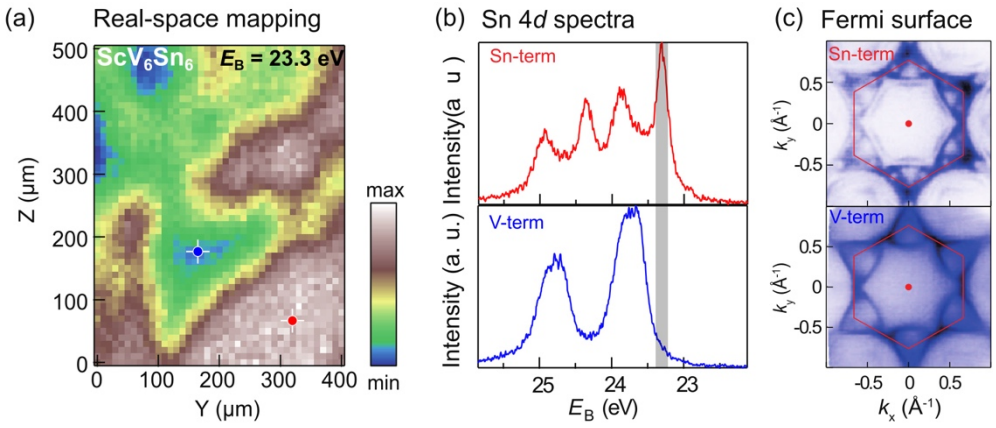

Fig. 1: *(a) Real-space mapping of photoelectron intensity of Sn 4d core states (E_B = 23.3 eV) on in-situ cleaved ScV_6Sn_6 surface with step-size of 10 μm; Sn 4d spectra (b) and Fermi surfaces (c) acquired at Sn- and V-terminated domain at the positions indicated by red and blue circles in (a).*

Fr-04

Topological excitonic states and their fingerprints on electronic structure

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Excitons, bound states of electrons and holes, are fundamental quasiparticles induced by coherent light–matter interactions. Time and angle resolved photoemission spectroscopy has been recently shown to be a powerful tool to reveal exciton formation in the single particle spectral function, opening up the exciting frontier to study momentum dependent exciton driven band structure renormalization, and ultimately search distinctive signature of exciton condensation in the band structure. Here I will discuss our recent work utilizing XUV and UV time resolved ARPES to study exciton formation in real time. I will show how their formation can uniquely modify the band structure in a k dependent way and will reveal under which conditions these excitonic state can be driven in the presence of topological invariants, what properties of the topological state persists and what are their fingerprints in the material's band structure. I will also discuss the potential of these materials to drive excitonic condensation.

Fr-05

Controlling charge density order in 2H-$TaSe_2$ using a van Hove singularity

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The understanding and manipulation of correlated states of matter like superconductivity or ferromagnetism are amongst the principal challenges in physics. From magnetic phases, high-temperature to topological Kagome superconductors and magic-angle twisted bilayer graphene, the correlated states often appear alongside a high density of electron states induced by van Hove singularities (vHs) [1-5]. We report on the interplay between a vHs and a charge density wave (CDW) state in 2H-$TaSe_2$. We use angle-resolved photoemission spectroscopy to investigate changes in the Fermi surface of this material under surface doping of a bulk crystal with potassium. At high doping, we observe modifications which imply the disappearance of the (3×3) CDW and formation of a different correlated state at the surface. Using a tight-binding-based approach as well as an effective model, we explain our observations as a consequence of coupling between the single-particle Lifshitz transition, during which the Fermi level passes through a vHs, and the charge density order. The high electronic density of states associated with the vHs induces a change in the periodicity of the CDW from the known (3×3) to a new (2×2) superlattice [6]. Our observation of the (2×2) phase validates a prediction from almost 50 years ago: we present the first spectral evidence of saddle-point nesting-driven CDW in transition metal dichalcogenides as originally proposed [1]. Moreover, the tunability of our system opens a new avenue to explore the interrelationships between CDW, van Hove singularities and superconductivity.

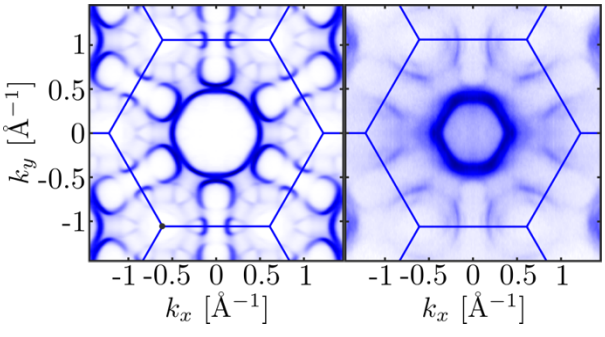

Fig.1. *Comparison of Fermi surface photoemission maps for pristine (left) and surface-doped (right) 2H-$TaSe_2$.*

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