O 29: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

O 29.1 Tue 10:30 H8

Line-moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) — •Romana Ganser, Muthu P. T. Masilamani, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

We present angle-resolved photoemission spectroscopy (ARPES) measurements on tunable one-dimensional moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) [1]. In this model system, the moiré structure can be tuned almost continuously in contrast to hardly controllable twist angles in bilayer van-der-Waals heterostructures [2]. We experimentally observe moiré minibands and band gaps of 120 - 170 meV suggesting sizable superlattice potentials. By comparing the experimental data to simple model calculations, we analyze the local character of the potential. This provides important information of interface hybridization effects on the band structure, which may not be limited to the system at hand but rather a broad range of moiré interfaces.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020).
[2] Lisi, S. et al. Nat. Phys. 17, 189-193 (2021).

O 29.2 Tue 10:45 H8

Photoemission Time Scale Determination: the Effect of Crystal Dimensionality and Electronic Correlation — •Fei Guo[1], Dmitrii Usanov[2], Eduardo B. Guedes[2], Mauro Fanciulli[3], Arnaud Magrez[1], Michele Puppin[1], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, 95031, France

Spin polarization of photoelectrons from spin-degenerate dispersive initial states originates from the interference of multiple photoemission channels, measuring the spin polarization with spin- and angle-resolved photoemission spectroscopy (SARPES) allows the estimation of the phases of the interfering channels, and hence the Eisenbud-Wigner-Smith (EWS) time delay of photoemission, which is the amount of time required by the photoelectron to evolve into a free particle final state. While not directly measurable for solid-state photoemission, this time scale has been measured for gaseous photoionization, which is generally in the attosecond (10^-18s) range.

We present investigations with multiple materials of different properties, and by comparing with previous studies, we propose a relationship between the EWS time delay, electronic correlation mechanism, and dimensionality.

O 29.3 Tue 11:00 H8

Disorder effects in the Band Structure of Transition Metal Dichalcogenide alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W) — •Sarath Sasi[1], Aki Pulkkinen[1], Laurent Nicolaï[1], Raphaël Salazar[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

Recent advances in materials synthesis have enabled the creation of 2D TMDC alloys, which offer unique opportunities for tailoring electronic and optoelectronic properties to meet diverse application demands.[1].This study investigates the band structure evolution of $A_xB_{1-x}Se_2$ alloys (A, B = Cr, Mo, W) across varying composition fractions (x). Using the Coherent Potential Approximation (CPA)[2], which accurately models scattering in disordered systems, theoretical calculations were performed with the *SPR-KKR* package[3]. Results reveal that some of the TMDC alloys maintain their band structures without significant disorder effects. Angle-Resolved Photoemission Spectroscopy (ARPES) measurements align closely with one-step model photoemission calculations, confirming theoretical predictions. These insights provide a foundation for tailoring electronic properties, advancing their applicability in next-generation devices.

[1] Zhou, J., Lin, J., Huang, X., et al. Nature, 556, 355-359 (2018).
[2] Soven, P., Phys. Rev., 156, 809(1967).
[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 29.4 Tue 11:15 H8

Unveiling Doping-Induced Electronic Modifications in Antiferromagnetic MPS_3 van der Waals Materials — •Till Willershausen[1], Jonah Elias Nitschke[1], Patrick Merisescu[2], David Janas[1], Lasse Sternemann[1], Michele Capra[1], Mira Arndt[1], Valentin Mischke[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Bath University

Antiferromagnetic van der Waals (vdW) materials, with scalability to monolayer thickness, semiconducting properties, and intrinsic antiferromagnetic ordering, hold promise for spintronic and quantum technology applications. We investigate alkali metal doping effects on the MPS_3 family (M = Mn, Ni, Co, Fe) of 2D antiferromagnetic vdW materials, revealing doping-induced changes in their electronic structure. X-ray Photoelectron Spectroscopy (XPS) shows shifts in oxidation states in $NiPS_3$, $CoPS_3$, and $FePS_3$, while $MnPS_3$ displays no significant changes, indicating distinct charge transfer. Further investigation with Angle-Resolved Photoelectron Spectroscopy (ARPES) reveals new alkali-metal induced bands appearing above the previous valence band maximum. This analysis highlights doping-induced modifications and contrasts in transition metal behavior in MPS_3, providing insights into doping mechanisms and electronic tunability.

O 29.5 Tue 11:30 H8

Enhanced electron-phonon coupling in few-layer $MoTe_2$ from micro-ARPES — •Thomas P. van Waas[1], Julia Issing[2], Marco Gibertini[3], Christophe Berthod[2], Anna Tamai[2], Felix Baumberger[2,4], and Samuel Poncé[1,5] — [1]European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland — [5]WEL Research Institute, Belgium

Bulk orthorhombic T_d-$MoTe_2$ is a type-II Weyl semimetal with a superconducting critical temperature of $T_c = 0.1$ K. Transport measurements show a monotonic increase in T_c as the thickness of multilayer $MoTe_2$ is reduced, reaching $T_c = 7.6$ K in the monolayer. We investigate photoemission kinks in the electron pocket of exfoliated monobi-, and trilayer $MoTe_2$ from micro-focused angle-resolved photoemission spectroscopy. We use a custom code to quantify the electron self-energy $\Sigma_n(E)$ for a parabolic non-interacting dispersion, and obtain from $\Sigma_n(E)$ the Eliashberg spectral function $\alpha^2F_n(\omega)$ using the maximum entropy method. We find two dominant phonon modes in $\alpha^2F_n(\omega)$ for the mono- and trilayer, with a large enhancement of the lower-frequency phonon mode in the former. We also provide tentative results for the bilayer, where quantification is more challenging due to a small splitting of the electronic bands.

O 29.6 Tue 11:45 H8

Electronic structure of V-doped WSe_2 — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics represents a promising and energy-efficient alternative to conventional electronics, with significant potential applications, e.g., in areas such as classical and quantum computing. The vanadium-doped layered transition metal dichalcogenide 2H-WSe_2 is a promising candidate to fulfill the desired properties as a room-temperature magnetic semiconductor with gating tunability. Here, we present a comprehensive electronic structure study of chemical vapor transport-grown pristine and V-doped WSe_2 by soft X-ray, VUV and 11eV-laser ARPES, highlighting the influence of a low V doping concentration on the electronic structure of WSe_2.

O 29.7 Tue 12:00 H8

Unraveling magnetic ordering in a van der Waals correlated

material — Tommaso Pincelli[1,2], •Tania Mukherjee[1,2], Lawson Lloyd[2], Shuo Dong[2,3], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], and Ralph Ernstorfer[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society, 14195 Berlin, Germany — [3]Beijing National Laboratory for Condensed Matter Physics, China

Layered van der Waals (vdW) materials offer a compelling platform to investigate various emergent quantum properties in low dimensions. Fe_3GeTe_2 (FGT), a vdW ferromagnetic metal, is well-known for exhibiting exotic phenomena, ranging from skyrmion formation to heavy fermion behavior. However, an understanding of the magnetic ordering, a key feature for spintronic applications, still remains elusive in this material. In particular, the interplay of both local magnetic moments and an itinerant mechanism in the formation of ferromagnetic ordering in FGT, a non-f-electron correlated system, remains to be clarified. Using time- and angle-resolved photoemission spectroscopy (trARPES) and first-principles calculations, we provide evidence for an ordering mechanism in FGT by observing a pronounced reduction in the Stoner exchange gap. This stands in contrast to earlier temperature-dependent ARPES studies of the electronic structure of FGT, which favored a localized excitation model over the weak-coupling itinerant picture. We also observe the impact of phononic excitations which further confirm our findings.

O 29.8 Tue 12:15 H8

Spin structure of the unoccupied surface state at AgTe/Ag(111) — •Carolin Benfer, Marcel Holtmann, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

The AgTe/Ag(111) surface alloy has recently been investigated as a model system for the role of orbital angular momentum in the formation of spin effects in the electronic structure [1]. Two p-like surface states were detected in ARPES measurements, one shows a Rashba-type spin splitting, while the other one does not. This behavior is attributed to the symmetries of the orbital wave functions of the electrons. For the unoccupied states a third surface state has been predicted. Following the symmetry arguments given in [1], a Rashba-type spin splitting of the state is expected.

We use inverse photoemission (IPE) to directly study the unoccupied state of the surface alloy. Low-energy electron diffraction and scanning tunneling microscopy measurements confirm a homogeneous monolayer film of the surface alloy, which is growing in a honeycomb structure. Angle-resolved IPE measurements detect the predicted surface state with free electron-like dispersion. Spin-resolved IPE measurements reveal a Rashba-type spin structure.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

O 29.9 Tue 12:30 H8

Orbital mixing as key mechanism for ferromagnetism in van der Waals CrI3 — •Alessandro De Vita[1,2], Srdjan Stavrič[3], Roberto Sant[4], Nicholas B. Brookes[4], Giancarlo Panaccione[5], Silvia Picozzi[3], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17 Juni 135, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]Consiglio Nazionale delle Ricerche CNR-SPIN, c/o Università degli Studi G. D'Annunzio, 66100 Chieti, Italy — [4]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [5]Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, km 163.5, I-34149 Trieste, Italy

Van der Waals ferromagnets constitute a versatile platform where exotic quantum states can be realized; among them, CrI3 is a prototypical and widely studied 2D ferromagnet, with promising applications in spin- and orbitronics. Despite that, key information on its electronic occupation and stabilization of the magnetic configuration are missing. By means of complementary absorption and photoemission spectroscopies, and density functional theory calculations, we give a description of the orbital character of bulk CrI3, and demonstrate that the emergence of ferromagnetism in this material is underpinned by the orbital mixing between I p and Cr eg states. Our results have clear impact on the understanding of how microscopic interactions at the orbital level stabilize ordered states in van der Waals ferromagnets.

O 29.10 Tue 12:45 H8

Resonant Photoemission Studies of Transition Metal Sulfides and Selenides — •Yashasvi Mehra[1,2,3], Samuel Beaulieu[4], Mauro Faniculli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Aki I.O. Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Universite de Bordeaux CNRS CEA, CELIA, UMR5107, F33405 Talence, France

By performing resonant ARPES measurements and SPR-KKR photoemission calculations on Transition Metal Selenide, Sulfide and the Vanadium intercalated NbS2 systems, we study the interplay between different decay mechanisms in resonant conditions, radiation-less Raman Auger and Classical Auger emissions. Through a method proposed by Cini and Sawatzky we can determine the on-site Coulomb interaction per element in some cases. On the theoretical front the calculations are performed using the SPR-KKR method, which is based on one-step model, that incorporates the effect of all matrix elements which accounts for the photoemission process. Furthermore, we analyze calculated ARPES, XAS, element and orbital resolved band structure underlining agreement with experimental results and helping with its interpretation.