

CPP 67: 2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)

Time: Wednesday 10:30–13:45

Location: WIL B321

CPP 67.1 Wed 10:30 WIL B321

Interplay between electronic instability and moiré structure of monolayer V_2S_3 on Au(111) — ●SAHAR PAKDEL¹, UMUT KAMBER², RALUCA-MARIA STAN¹, ANAND KAMLAPURE², BRIAN KIRALY², FABIAN ARNOLD¹, ANDREAS EICH², ARLETTE S. NGANKEU¹, MARCO BIANCHI¹, JILL A. MIVA¹, CHARLOTTE SANDERS¹, PHILIP HOFMANN¹, ALEXANDER A. KHAJETOORIANS², and NICOLA LANATA¹ — ¹Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — ²Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The formation of Moiré superstructures between 2D-materials and their substrates has attracted considerable attention, as it can influence their physical properties. Here we study monolayer V_2S_3 grown on an Au(111) substrate. Scanning tunneling microscopy experiments exhibit multiple domains with different Moiré structures. Comparing the calculated Fermi surfaces with angle resolved photo-emission spectroscopy data, we find that the substrate induces a substantial shift in the chemical potential. We show that the computed Lindhart function of V_2S_3 (at the measured chemical-potential) has a pronounced peak corresponding to a second-order reciprocal point of the prevalent Moiré structure. This suggests that the system tends to favor Moiré structures with modulations able to accommodate underlying electronic instabilities of V_2S_3 . We speculate that this could be the manifestation of a more general mechanism and a promising route for tailoring the electronic structure of 2D-materials.

CPP 67.2 Wed 10:45 WIL B321

Probing the electronic structure of twisted transition metal dichalcogenide bilayers by photoemission — ●BHARTI PARASHAR¹, SVEN BORGHARDT², KEVIN JANSSEN¹, MATEO JUGOVAC¹, VITALIY FEYER¹, DOROTA WILGOCKA SLEZAK³, JÓZEF KORECKI³, LUKASZ PLUCINSKI¹, and CLAUS M. SCHNEIDER¹ — ¹PGI-6, FZ Jülich, Germany — ²PGI-9, FZ Jülich, Germany — ³Polish Academy of Sciences, Kraków, Poland

Moiré bands in twisted transition metal dichalcogenide (TMDC) bilayers are predicted to host novel topological and correlated electronic phases [1]. We performed angle-resolved photoemission studies with few micrometer resolution (μ -ARPES) on several hetero- and homo-bilayers made from MoS_2 and WSe_2 by mechanical exfoliation and dry transfer technique. The twist angle between the layers was determined in a separate experiment by μ -LEED.

We determine the hybridization between the layers through monitoring the formation of new spectral features in normal emission spectra, that are not present in respected monolayers. The existence of hybridization indicates high quality of the interface that is critical to enable formation of interesting moiré bands. Furthermore, our results allow to shed light on whether the valence band maximum is located at Γ or at K at various bilayers. This is important for predicted moiré physics, since only at K the bands are spin-momentum locked.

[1] See e.g.: F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Phys. Rev. Lett. 122, 086402 (2019), and refs. therein.

CPP 67.3 Wed 11:00 WIL B321

Electronic vs Structural Effects in the Moiré Pattern of MoS_2 on Au(111) — CAIO C. SILVA^{1,2}, DANIELA DOMBROWSKI^{1,2}, NICOLAE ATODIRESEI³, WOUTER JOLIE², FERDINAND FARWICK ZUM HAGEN², JIAQI CAI², PAUL T. P. RYAN⁴, PARDEEP THAKUR⁵, VASILE CACIUC³, STEFAN BLÜGEL³, DAVID A. DUNCAN³, THOMAS MICHELY², TIEN-LIN LEE⁵, and ●CARSTEN BUSSE^{1,2,6} — ¹WWU Münster, Germany — ²Universität zu Köln, Germany — ³FZ Jülich and JARA, Germany — ⁴Imperial College London, U. K. — ⁵Diamond Light Source Ltd, U. K. — ⁶Universität Siegen, Germany

The lattice mismatch between a monolayer of MoS_2 and its Au(111) substrate induces a moiré superstructure. The local variation of the registry between sulfur and gold atoms at the interface leads to a periodic pattern of strongly and weakly interacting regions. In consequence, also the electronic bands show a spatial variation.

We use scanning tunneling microscopy and spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS) and x-ray standing wave (XSW) for a determination of the atomic structure and the resulting electronic properties. The experimental results are corroborated by density functional theory (DFT). We deduce the structure of the supercell with high precision, identify the fraction of interfacial atoms that are strongly interacting, and analyze the variation of the electronic structure in dependence of the location within the moiré cell and the nature of the band.

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CPP 67.4 Wed 11:15 WIL B321

Complex moiré structures in rotated monolayer V_2S_3 on Au(111) — ●UMUT KAMBER¹, SAHAR PAKDEL², RALUCA-MARIA STAN², ANAND KAMLAPURE¹, BRIAN KIRALY¹, FABIAN ARNOLD², ANDREAS EICH¹, ARLETTE S. NGANKEU², MARCO BIANCHI², JILL A. MIWA², CHARLOTTE SANDERS², NICOLA LANATA², PHILIP HOFMANN², and ALEXANDER A. KHAJETOORIANS¹ — ¹Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — ²Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Moiré superlattices have led to the emergence of tunable many-body states of matter like superconductivity and Mott insulator states absent in the individual layers [1,2]. For transition metal dichalcogenides (TMDCs), there has been a strong interest in how electronic structure is modified near the single layer limit and potentially affected by the dielectric environment. Here, we show spatially periodic modifications to the electronic structure of single layer V_2S_3 grown on Au(111) varying with the underlying moiré pattern [3]. Similar modifications were observed in multiple moiré patterns, each arising from a different relative orientation between the monolayer and the Au(111) substrate. We characterize these spatial variations in electronic structure with respect to the atomic and moiré lattices via scanning tunneling microscopy and spectroscopy, with the help of ab initio calculations.

[1] Y. Cao et al., Nature, 556, 43 (2018).

[2] Y. Cao et al., Nature, 556, 80 (2018).

[3] F. Arnold et al., 2D Mater. 5, 045009 (2018).

CPP 67.5 Wed 11:30 WIL B321

Screening effects at the internal interfaces of bulk-like MoS_2 — ●PHILIPP MARAUHN, PETER KRÜGER, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The two-dimensional nature of TMDCs is intrinsically linked to reduced screening. This renders the materials sensitive to their dielectric environment. Quasiparticle calculations of MoS_2 deposited on different substrates have shown the importance to account for environmental screening [1]. In this talk we discuss how screening effects modify the electronic structure across the internal interfaces of bulk-like MoS_2 .

In a first step we use a tight-binding model to reproduce the band structure on a level of density functional theory. To include polarization effects, we extend the model by introducing a self-energy operator constructed from layer-resolved quasiparticle corrections calculated within the framework of GW . Using this GW -tight-binding approach, we show that environmental screening has strong impact on the formation of the subbands which originate from interlayer interactions. Most striking, at the K-point, the surface layer decouples from lower lying layers forming a direct gap which is distinctly different from that of the total system.

[1] M. Drüppel et al., Nat. Commun. 8(1), 2117 (2017)

CPP 67.6 Wed 11:45 WIL B321

Charge density wave and superconductivity of single-layer $NbSe_2$ on different screening environments — ●WEN WAN, PAUL DREHER, MARCO GOBBI, and MIGUEL M. UGEDA — Donostia International Physics Center and Centro de Física de Materiales, San Sebastián-Donostia, Spain

Superconductivity and charge density wave order, typical collective electronic phases of transition metal chalcogenides (TMD), are highly sensitive to external perturbations. In the 2D limit, the properties, and even the mere existence, of these phases in monolayers of TMDs become mostly dependent on the supporting substrate due to charge doping/screening and hybridization effects [1,2]. Here, we carry out low-temperature STM/STS (350 mK) measurements to study the electronic structure of single-layer $NbSe_2$ grown on different substrates by molecular beam epitaxy. In particular, we explore and compare the fate and fundamental properties of the superconducting and CDW

states of single-layer NbSe₂ on both highly metallic, semi-metallic and insulating TMD substrates [3].

- [1] M. M. Ugeda, et al. Nature Physics 12, 92 (2016).
- [2] Stan, et al. Phys. Rev. Mat. 3, 044003 (2019).
- [3] W. Wan, et al., in preparation.

CPP 67.7 Wed 12:00 WIL B321

Incorporation of K and Cs into hBN/Ir(111) and hBN/Ru(0001) — ●JIAQI CAI^{1,2,3}, CAIO SILVA^{2,3}, WOUTER JOLIE², THAIS CHAGAS¹, KAI MEHLICH¹, DAVID DUNCAN⁴, CHRISTOPH SCHLUETER⁴, TIEN-LIN LEE⁴, and CARSTEN BUSSE^{1,2,3} — ¹Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — ²II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln — ³Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — ⁴Diamond Light Source, Didcot OX11 0DE, Oxfordshire, United Kingdom

The bi-atomic unit cell of monolayer hexagonal boron nitride (hBN) makes its interaction with the substrate more complex in comparison with its famous cousin, graphene. To probe this interaction, we incorporate alkali metals into hBN/substrate systems. We choose alkali metals for two reasons: i) they tend to lose the electron in the out-most orbitals, thus introducing a strong electronic effect into the hBN/substrate system; ii) the alkali metal ions have full-shell structure, making them unlikely to chemically bond to hBN.

In this talk, we report our experimental results on K as well as Cs incorporation into epitaxial hBN on Ir(111) and Ru(0001). We rely on STM, LEED, XPS, and XSW for the determination of the atomic coordinates with high precision. We report a rich pool of structures (adsorption and/or intercalation of alkali metals), and find that the location of the alkali metal ions are determined by the hBN-substrate interaction strength, and the size of the alkali metal ions.

CPP 67.8 Wed 12:15 WIL B321

Control of interface alloying between silicene and a silver substrate — ●JOHANNES KÜCHLE¹, ALEKSANDR BAKLANOV¹, FELIX HAAG¹, DAVID DUNCAN², PAUL RYAN^{2,3}, ARI SEITSONEN⁴, WILLI AUWÄRTER¹, and FRANCESCO ALLEGRETTI¹ — ¹Physics Department E20, Technical University of Munich, Germany — ²Diamond Light Source, Didcot, UK — ³Imperial College London, UK — ⁴Département de Chimie, École Normale Supérieure, Paris, France

Silicene, the silicon analogue of graphene, is a promising material with unique structural and electronic properties, which has been the focus of intense research in the past decade. The epitaxial growth *via* deposition of silicon on solid substrates is an established strategy for silicene preparation, however, strong interfacial interactions may modify the functional properties of the resulting layer. On metal substrates, interfacial alloying may occur, but surprisingly, its role is often underestimated. Here, we present our recent experiments with soft X-ray photoelectron spectroscopy (SXPS) at various Si coverages, indicating that during the growth of the most commonly studied (4 × 4) superstructure of silicene on Ag(111) a Si-Ag surface alloy is formed. Our scanning tunneling microscopy studies resolve a yet unreported phase, which we relate to the Si-Ag alloy. Notably, we show that the alloy related component in SXPS can be largely suppressed by growing silicene on a GeAg₂ surface alloy on Ag(111). In this case, a number of distinct structures are observed by low-energy electron diffraction, which differ significantly from all previously reported superstructures of silicene.

CPP 67.9 Wed 12:30 WIL B321

Curvature-Induced Charge Baskets in Two-Dimensional Semiconducting Monolayers — ●BONG GYU SHIN¹, JZ-YUAN JUO¹, SOON JUNG JUNG¹, and KLAUS KERN^{1,2} — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569 Stuttgart, Germany — ²Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization and quantum confinement in monolayer MoS₂ on a SiO₂/Si substrate using a gate-tunable home-built scanning tunneling microscope at ~4.9K. Monolayer MoS₂ follows surface roughness of the substrate, which exhibits a bending strain with band gap reduction. This band gap reduction at a local regime acts like a potential well leading to charge localization. When the bending strain in MoS₂ is larger than 2% at a local region of ~4 nm, quantum-confined energy

levels are observed near the conduction or valence band edge due to the significant band gap reduction of ~1 eV. Moreover, our theoretical results show that spatial flattening of the conduction (valence) band edge occurs by heavy electron- (hole-) doping of over ~10¹³ cm⁻². The strain-induced quantum confinement in 2D materials can play an important role in the future development of quantum devices.

CPP 67.10 Wed 12:45 WIL B321

Long-range charge order induced by strain in layered IrTe₂ revealed by ARPES — ●CHRIS W. NICHOLSON¹, MAXIME RUMO¹, GEOFFROY KREMER¹, THOMAS JAOUEN¹, BAPTISTE HILDEBRAND², MARIE-LAURE MOTTAS¹, BJÖRN SALZMANN¹, AKI PULKINEN², BERNARDO BARBIELLINI², TIMUR KIM³, SAUMYA MUKHERJEE³, CEPHISE CACHO³, MATTHIAS MUNTWILER⁴, FABIAN VON ROHR⁵, PHILIPP AEBI¹, and CLAUDE MONNEY¹ — ¹University of Fribourg, Switzerland — ²LUT University, Finland — ³Diamond Light Source, UK — ⁴Swiss Light Source, Switzerland — ⁵University of Zurich, Switzerland

Uniaxial strain combined with ARPES offers a relatively new route to studying the interplay between the lattice and electronic structure. The wide range of properties displayed by layered transition metal dichalcogenides makes them intriguing candidates for exploring this.

Here we present ARPES data revealing the influence of tensile strain on the electronic structure of IrTe₂, which exhibits a complicated mixture of one dimensional charge ordered phases at low temperatures but very broad electronic bands [1]. The application of strain induces a single, long-range ordered phase, with clear quasi-1D features at the Fermi level and sharp bands over a wide binding energy range. By comparison with electronic structure calculations, we will discuss the mechanism of this strain-induced stabilization with reference to the redistribution of charge between Ir and Te bonds [2].

- [1] Ko et al, Nat. Comm 6, 7342 (2015)
- [2] Nicholson et al, in preparation

CPP 67.11 Wed 13:00 WIL B321

Seeking 2D Ferromagnets among TMD materials — ●PAUL DREHER^{1,2}, WEN WAN^{1,2}, ADOLFO O. FUMEGA⁵, MD N. HUDA⁴, SHAWULIENU KEZILEBIEKE⁴, SANTIAGO BLANCO^{2,3}, VICTOR PRADO⁵, HANNU-PEKKA KOMSA⁴, MARCO GOBBI^{2,3}, PETER LILJEROTH⁴, and MIGUEL M. UGEDA^{1,2} — ¹Donostia International Physics Center, San Sebastián, Spain — ²Centro de Física de Materiales, San Sebastián, Spain — ³CIC nanoGUNE, San Sebastián, Spain — ⁴Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland — ⁵Departamento de Física Aplicada, Universidade de Santiago de Compostela, Campus Sur s/n, E-15782 Santiago de Compostela, Spain

We study the magnetic character of various monolayer TMD candidates (VSe₂, CrSe₂) grown by MBE on different substrates (NbSe₂, graphene, graphite) by combining various characterization techniques. Our findings reveal that the substrate plays a crucial role on the magnetic order in the grown TMD monolayer. The CDW order in single-layer VSe₂ causes a strong reduction in the DOS at EF incompatible with ferromagnetism. When grown on graphene substrates, the CDW persists VSe₂ and it becomes paramagnetic [1]. Instead, the electronic structure of single-layer VSe₂ on a superconducting substrate (NbSe₂) shows features compatible with magnetism [2]. Finally, XMCD measurements on Cr-based TMD monolayers indicate the presence of an uncompensated spin in Cr, which retains a paramagnetic behavior even at low temperatures. [1] J.Phys.Chem.C, 123, 27802 (2019), [2] ArXiv:1909.10208 (2019).

CPP 67.12 Wed 13:15 WIL B321

Signatures of strong coupling between WS₂ excitons and surface plasmon polariton waves — MORITZ GITTINGER¹, SVEN STEPHAN¹, TRUNG NGUYEN¹, ANTONIETTA DE SIO¹, ●MARTIN SILIES¹, CHRISTOPH LIENAU¹, ALISON CADORE², ILYA GOYKHMAN², and ANDREA FERRARI² — ¹Institute of Physics and Center of Interface Science, Carl von Ossietzky Universität Oldenburg — ²Cambridge Graphene Centre, University of Cambridge, UK

All-solid-state strong coupling systems with large vacuum Rabi splitting energies are of great potential in future technologies such as quantum information processing. Here, atomically thin layers of transition metal dichalcogenides in close vicinity to metallic nanoparticles have recently been explored as excellent candidates for the observation of this coherent energy transfer from the exciton to its localized surface plasmon counterpart [1]. We here present first results of the interaction between surface plasmon polariton (SPP) waves induced in

focused-ion beam written gratings in planar silver films with excitons from atomically-thin WS₂ flakes. By using confocal angle-resolved reflectance spectroscopy, the dispersion relation of the coupled system is mapped at room temperature. We observe a clear anti-crossing of the exciton and the SPP resonance with a normal mode splitting of up to 50meV. We take this splitting as a first signature for a strong coupling between the WS₂ exciton and the SPP wave in the silver grating [2].

[1] Schneider C. et al, Nature Comm. 9, 2695 (2018) [2] Vasa P, and C. Lienau, ACS Photonics 5, 2-23 (2018)

CPP 67.13 Wed 13:30 WIL B321

Substrate-dependent charge transfer mechanisms between monolayer MoS₂ and molecular dopants — ●PATRICK AMSALEM¹, SOOHYUNG PARK^{1,2}, THORSTEN SCHULTZ^{1,3}, XIAOMIN XU¹, BERTHOLD WEGNER^{1,3}, AREEJ ALJARB⁴, ALI HAN⁴, LAIN-JONG LI^{4,5}, VINCENT C. TUNG^{4,6}, and NORBERT KOCH^{1,3} — ¹Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Berlin, Germany — ²Korea Institute of Science and Technology

(KIST), Seoul, South Korea — ³Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — ⁴King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — ⁵The University of New South Wales, Sydney, Australia — ⁶Lawrence Berkeley National Lab, Berkeley, CA, USA

2D transition metal dichalcogenides monolayer films have recently gained enormous attention. Yet, to extend the range of applications of these emerging materials, tuning their Fermi level is of crucial importance. Here, we report on the adsorption of a strong p-type organic dopant, F6TCNNQ, as an efficient route for doping of MoS₂ [1]. More specifically, we employ angle-resolved UV and X-ray photoelectron spectroscopy to reveal the charge transfer (CT) mechanisms taking place at a TMDC/organic interface as a function of the electrical properties of the employed supporting substrate, here sapphire, graphite and gold. The present findings can be exploited for the design of advanced hybrid heterostructures with tailored electronic properties. [1] S. Park et al., Communications Physics 2, 109 (2019).