O 87: 2D Materials IV: Charge Density Waves and Electronic Properties

Time: Thursday 15:00–17:30 Location: H25

O 87.1 Thu 15:00 H25

The 3×3 charge density wave in quasi-freestanding monolayer 2H-TaS_2 — •Joshua Hall[1], Camiel van Efferen[1], Clifford Murray[1], Matthias Rolf[1], Niels Ehlen[1], Jun Li[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], Alexander Grüneis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany

We report on the 3×3 charge density wave (CDW) in a quasi-freestanding monolayer of TaS_2, as grown by molecular beam epitaxy on graphene on Ir(111) [1]. Investigated by scanning tunnelling microscopy, the 3×3 periodicity of the CDW is visible at liquid helium temperatures, and allows analysis of spatial CDW amplitude variations and the influence of point and line defects. Performing low temperature scanning tunnelling spectroscopy (STS) reveals a decreased density of states at the Fermi energy, indicating partial gapping of the Fermi surface. In constant current STS maps, an energy dispersive standing wave pattern is found, which firstly illustrates the quasi-freestanding nature of the TaS_2 islands and secondly allows partial determination of the band structure, which is compared to data from angle resolved photoemission spectroscopy of the same system.

[1] Hall et al., 2D Materials **5** 025005 (2018)

O 87.2 Thu 15:15 H25

Structure determination of the commensurate charge density wave phase of 1T-TaS_2 — Gevin von Witte[1], Tilman Kisslinger[2], Jan-Gerrit Horstmann[1], Kai Rossnagel[3], Alexander Schneider[2], Claus Ropers[1], and •Lutz Hammer[2] — [1]IV. Phys. Inst., Univ. Göttingen — [2]Ls. f. Festkörperphysik, Univ. Erlangen-Nürnberg — [3]Inst. f. Exp. u. Angew. Physik, Univ. Kiel

The transition metal dichalcogenide 1T-TaS_2 consists of van-der-Waals stacked S–Ta–S trilayers with tetrahedrally coordinated Ta atoms. Depending on temperature several charge-density wave (CDW) states are observed. Here, we present a structural analysis of the low-temperature $(\sqrt{13} \times \sqrt{13})R13.9°$ CDW-phase (C-phase) by quantitative LEED-IV.

From an UHV-cleaved single crystal, we collected a large total data base comprising 128 inequivalent beams which allows to determine 78 structural parameters safely (redundancy factor $\rho = 10$). The excellent fit quality achieved is expressed by a Pendry R-factor of $R_P = 0.12$.

The C-phase shows a strongly modulated superstructure with Ta atoms arranged in Star-of-David shaped clusters. LEED-IV reveals that the CDW distortion of the topmost trilayer is practically bulk-like with only tiny vertical atomic relaxations ($\leq$0.06 Å): The clusters of Ta atoms contract laterally by up to 0.25 Å and also rotate within the superstructure cell, causing respective distortions as well as heavy bucklings (≈0.20 Å) in the adjacent sulphur layers. Most importantly, we find a stacking sequence of A–A–B of the three outermost trilayers, i.e., a vertical stacking of the top trilayer and a shift by two units of the basic hexagonal lattice (6.73 Å) between the 2^{nd} and 3^{rd} layer.

O 87.3 Thu 15:30 H25

Atomic-scale and ultrafast melting of a charge density wave — •Mohamad Abdo[1,2,3], Shaoxiang Sheng[1], Moritz Tritschler[1], Steffen rolf-Pissarczyk[2,3], Luigi Malavolti[1,2,3], Gregrory McMurtrie[1,2,3], Max Hänze[1,2,3], Jacob Burgess[4], and Sebastian Loth[1,2,3] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]University of Manitoba, Winnipeg, Canada

NbSe2 is a layered transition metal dichalcogenide (TMD) that features CDW phases between 33K and 7K. These phases exhibit collective modes in phase and amplitude. The CDW is disturbed by atomic defects that act as pinning centers [1-2]. Here we use a THz-coupled scanning tunneling microscope (STM) [3] to measure the picosecond dynamic response of the CDW locally at individual atomic defects. Pairs of THz pulses excite the CDW and probe the response in the sample*s density of states with a time resolution better than 200 fs. We find an efficient excitation mechanism driven by the tip-enhanced THz electric field in the STM junction. This excitation melts the CDW by an ultrafast displacement current and triggers a rich dynamical response that varies on the scale of one unit cell of the CDW.

[1] P. Soumyanarayanan, PNAS 110, 1623-1627 (2013). [2] X. Xi, et al. Nature Nanotechnology 10, 765-769 (2015) [3] T. Cocker, et al., Nature Photonics 7, 620-625 (2013).

O 87.4 Thu 15:45 H25

Using microARPES to measure the charge density wave gap of 1T-VSe_2 — •Alfred J. H. Jones[1,2], Jude Laverock[1], Charles J. Sayers[3], Mattia Cattelan[4], Simon J. Bending[3], Liam S. Farrar[3], Enrico Da Como[3], and Neil A. Fox[1,4] — [1]H. H. Wills Physics Laboratory, University of Bristol, UK — [2]Department of Physics and Astronomy, Aarhus University, DK — [3]Centre for Nanoscience and Nanotechnology, University of Bath, UK — [4]School of Chemistry, University of Bristol, UK

Charge density wave (CDW) order, as seen in a number of the layered two dimensional (2D) transition metal dichalcogenides (TMDCs), leads to many and varied changes to the lattice and electronic structure. Such phenomena continue to be poorly understood for a number of strongly correlated metals, including the metallic TMDCs. Within this class of TMDCs, 1T-VSe_2 is especially interesting due to the strong 3D character of the CDW.

Here I will report on measurements of the electronic structure of VSe_2 taken from a single domain of the bulk crystal using microARPES. These measurements were made using the NanoESCA, an energy filtered PEEM instrument capable of analysing the band structure of materials from regions as small as three microns. I will present the momentum and temperature dependence of the gap that opens in the spectral function of VSe_2, and show that the observed behaviour is in good agreement with a mean-field weak coupling description.

O 87.5 Thu 16:00 H25

Electronic properties and magnetism of sulphur-deficient VS_2 on Au(111) — Sabina Simon, Felix Förschner, Jannik Dornseiff, Julia Tesch, and •Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Monolayers of two-dimensional transition metal dichalcogenides (TMDs) have recently received considerable scientific interest due to their unique properties making them prospective materials for novel device applications. Among a large variety of TMDs, VS_2 and VSe_2 monolayers gained specific attention as possible 2D materials with peculiar magnetic properties. The recent discovery of ferromagnetism in VSe_2 [1] boosted the interest in this materials even further.

In this work we discuss the structure and local electronic properties of sulphur-deficient VS_2 nanoribbons on Au(111). By means of low-temperature scanning tunneling microscopy we analyze the exact atomic arrangement within the VS_2 nanoribbons, showing stabilization of the atomic structure with every second sulphur atomic row missing in the upper layer. We observe very strong atomic level variations in the local density of states, which are discussed with respect to emergent magnetism in VS_2.

[1]. M. Bonilla et al., Nature Nanotechnology **13**, 289 (2018).

O 87.6 Thu 16:15 H25

Electronic structure and charge order of monolayer VSe_2 — Jiagui Feng[1], •Deepnarayan Biswas[1], Akhil Rajan[1], Matthew D. Watson[1], Federico Mazzola[1], Oliver J. Clarke[1], Kaycee Underwood[1], Igor Marković[1], Martin McLaren[1], Andrew Hunter[1], David M. Burn[2], Liam B. Duffy[3], Sourabh Barua[4], Geetha Balakrishnan[4], François Bertran[5], Patrick Le Fèvre[5], Timur K. Kim[2], Gerrit van der Laan[2], Thorsten Hesjedal[3], Peter Wahl[1], and Phil D. C. King[1] — [1]University of St. Andrews, UK — [2]Diamond Light Source, UK — [3]University of Oxford, UK — [4]University of Warwick, UK — [5]Synchrotron Soleil, France

The electronic states and phases of many monolayer (ML) transition metal dichalcogenides (TMDs) found to be different from its bulk properties and this evolution of electronic properties with thickness in TMDs are still a key open question. Here we show the results of our study on molecular beam epitaxy (MBE) grown ML VSe_2 film on bi-layer graphene/SiC. We have measured the detail band dispersion of this material using angle resolved photoelectron spectroscopy (ARPES). The low energy electron diffraction (LEED), along with the ARPES data show an enhanced charge density wave order compare to

its bulk form. Our density functional theory (DFT) calculation and X-ray magnetic circular dichroism (XMCD) measurements suggests no magnetic ordering in ML VSe_2.

O 87.7 Thu 16:30 H25

Growth and properties of VS_2 nanostructures on Au(111) — •Sabina Simon, Felix Förschner, Jannik Dornseiff, Julia Tesch, and Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Transition metal dichalcogenides present enormous scientific interest due to their diverse properties, which can be uniquely tailored by the nature of the components, number of layers or the stacking order of the crystal. Recent theoretical calculations predict an intricate magnetic behaviour for 2D monolayers of VS_2 [1,2], which depends on its structure and chemical composition, thus propelling this material into the focus of an active research.

In this work we discuss the epitaxial growth of VS_2 nanostructures (nanoislands and nanoribbons) on Au(111). By means of low-temperature scanning tunneling microscopy we investigate the influence of growth parameters upon the structure and chemical composition of the VS_2 nanostructures. Local spectroscopic measurements reveal strong variations of the electronic properties at the atomic level due to the interaction with the substrate and the presence of sulphur defects.

[1] Y. Ma *et. al.*, ACS Nano **6**, 1695 - 1701 (2012).
[2] D. Gao *et al.*, J. Mater. Chem. **1**, 5909 - 5916 (2013).

O 87.8 Thu 16:45 H25

Material Realistic Description of Coulomb Engineering in Two-dimensional Materials — •Christina Steinke[1,2], Malte Rösner[3], and Tim Wehling[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Heterojunctions are building blocks of various applications in modern optoelectronics. Common heterojunctions rely on interfaces of different materials in order to gain the desired spatial band-gap modulations. We investigate a new type of lateral heterojunction imprinted externally into an otherwise homogeneous monolayer of a 2d material. [1,2] In 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to tune the local band gaps within a monolayer by laterally structured dielectric surroundings and leads to characteristics of a heterojunction in the local density of states with a spatially sharp band gap modulation. By means of material realistic models based on ab-initio calculations we study the nature and tunability of this band-gap modulation in 2d semiconductors in dependence of the chosen environment and identify optimal candidates for Coulomb engineered 2d systems.

[1] M. Rösner et al., Nano Lett. 16(4) (2016), 2322-2327
[2] A. Raja et al., Nature Communications 8 (2017), 15251

O 87.9 Thu 17:00 H25

Coulomb engineering of two-dimensional Mott insulators — •Erik van Loon[1], Malte Schüler[1], Daniel Springer[2], Jan Tomczak[2], Giorgio Sangiovanni[3], and Tim Wehling[1] — [1]Universität Bremen, Bremen, Deutschland — [2]TU Wien, Wien, Österreich — [3]Julius-Maximilians-Universität Würzburg, Würzburg, Deutschland

Substrates provide a convenient tool for manipulating two-dimensional materials. One way the substrate affects the material is via the screening of the Coulomb interaction. Here, we investigate the impact of this substrate screening on two-dimensional Mott (that is: Coulomb interaction-driven) insulators. This requires a theoretical description of the interplay of internal and external screening and correlation. We address the metal-insulator transition in the presence of substrate screening and how the size of the gap is altered.

O 87.10 Thu 17:15 H25

Ab initio study of environmental stability, reactivity and heterostructures formation in 2D materials. — •Clotilde Cucinotta — Imperial College London

I will discuss strategies and examples on how to address, from a theoretical and computational standpoint, the description of key properties and processes occurring in different layered materials of deep technological interest (BP, TiS2, MoS2). I will illustrate how progress in the understanding of exfoliation, basal plane functionalization, chemical reactivity and heterostructures formation in this new class of materials can be achieved by adopting a comprehensive and concerted approach, i.e. combining multidisciplinary competences of experimental and theoretical research.