

## O 18: Poster Monday: 2D Materials 1

Time: Monday 18:00–20:00

Location: P4

O 18.1 Mon 18:00 P4

**Scanning tunneling microscopy and spectroscopy of rubrene on clean and graphene-covered metal surfaces** — ●KARL ROTHE, ALEXANDER MEHLER, NICOLAS NÉEL, and JÖRG KRÖGER — TU Ilmenau, Institut für Physik

Rubrene ( $C_{42}H_{28}$ ) was adsorbed with submonolayer coverage on Pt(111), Au(111) and graphene-covered Pt(111). Adsorption phases and vibronic properties of  $C_{42}H_{28}$  consistently reflect the progressive reduction of the molecule–substrate hybridization. Separate  $C_{42}H_{28}$  clusters are observed on Pt(111) as well as broad molecular resonances. On Au(111) and graphene-covered Pt(111) compact molecular islands with similar unit cells of the superstructure characterize the adsorption phase. The highest occupied molecular orbital of  $C_{42}H_{28}$  on Au(111) exhibits weak vibronic progression while unoccupied molecular resonances appear with a broad line shape. In contrast, vibronic subbands are present for both frontier orbitals of  $C_{42}H_{28}$  on graphene. They are due to different molecular vibrational quanta with distinct Huang-Rhys factors.

Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/12-1 is acknowledged.

O 18.2 Mon 18:00 P4

**The effect of morphology of an intercalated Au layer on electronic properties of Graphene** — ●AMIRHOSSEIN BAYANI and KARIN LARSSON — Department of Chemistry-Ångström laboratory, Uppsala University, Uppsala, Sweden

Thermal Intercalation processes have recently made it possible to produce large quasi free-standing graphene layers on different substrates. One method, which is based on thermal annealing, uses a 4H-SiC (0001) substrate with an attached carbon buffer layer onto the Si-face of the substrate. Various types of metals have then been used with the purpose to intercalate these metal atoms between SiC and the buffer layers, thereby creating a monolayer (ML) of graphene with an intact Dirac point. Moreover, when positioning heavy metal atoms under graphene, the spin-orbit coupling will increase and thereby enhances the Rashba band splitting. This phenomenon comes from the breakage of a mirror symmetry due to interaction with the substrate. To the knowledge of the authors, the role of the morphology of the intercalated layer on the electronic properties of graphene has not yet been considered and it is worth considering this effect when electronic properties of graphene is wanted to be studied after intercalation. Here we show how the morphology of the intercalated Au layer will affect the electronic properties of a ML of graphene. The possibility to induce a band gap at the Dirac point of graphene by manipulating the staggered potential of a 4H-SiC/Au substrate, is thereby looked for. The calculations are based on density functional theory (DFT) + SOC.

O 18.3 Mon 18:00 P4

**Intercalation of epitaxial graphene on SiC(0001) with sulfur** — ●SUSANNE WOLFF, NICLAS TILGNER, TASSILO RAUSCHENDORFER, FLORIAN SPECK, and THOMAS SEYLLER — Chemnitz University of Technology, 09126 Chemnitz, Germany

Epitaxial growth of graphene on SiC in argon atmosphere is a well-established method to produce high quality films. There, the first grown carbon layer is partially covalently bound to the substrate and lacks the graphene-like electronically properties. This so-called buffer layer can be decoupled from the substrate by intercalation. Furthermore, the choice of intercalant manipulates the electronic properties of the decoupled graphene.

We investigated the intercalation of a buffer layer with sulfur by X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). The intercalation process was performed in a two-zone furnace where the  $FeS_2$  precursor and the buffer layer can be heated separately. An argon gas flow transports the sublimated sulfur to the sample. Partial intercalated samples show two sulfur peaks at different binding energies in XPS. They can be attributed to intercalated sulfur and sulfur on top of the not intercalated buffer layer. ARPES measurement in the vicinity of the Dirac point showed that sulfur intercalation results in p-type doped decoupled graphene layers.

O 18.4 Mon 18:00 P4

**twisted graphene on Ir(111) and SiC(0001) studied by**

**SPA- LEED** — ●MOHAMMAD TAJIK<sup>1</sup>, CHRISTIAN BRAND<sup>1</sup>, BIRK FINKE<sup>1</sup>, KARIM OMAMBAC<sup>1</sup>, LAURENZ KREMEYER<sup>1</sup>, FRANK MEYER ZU HERINGDORF<sup>1,2</sup>, and MICHAEL HORN-VON HOEGEN<sup>1,2</sup> — <sup>1</sup>Universität Duisburg-Essen — <sup>2</sup>center for nanointegration duisburg-essen

when graphene is placed on a crystalline surface, the periodic structures within the layers superimpose and a moiré superlattices form. Small lattice rotations between the 2D-layer and the substrate strongly modify the moiré superlattice, upon which many electronic, vibrational, and chemical properties depend. Here we report on such structural modification of epitaxial graphene grown on metallic Ir(111) and semiconducting SiC(0001) surfaces. The spontaneous reorientation in the degree- and sub-degree-range of graphene on Ir(111) depends on the substrate temperature during growth. This effect is described by a 2D coincidence network favored by strain reduction together with the dissimilar thermal expansion of the substrate and graphene. For graphene on SiC(0001) only the oriented  $R0^*$  phase is found due to the higher bonding strength to the substrate. Upon H and Sn intercalation this interaction can be reduced such that the graphene layer is lifted from the substrate. Finally, we present a detailed analysis of an unusually broad diffraction background found for graphene and hex-BN on both substrates.

O 18.5 Mon 18:00 P4

**On the Way to Twisted Bilayer Graphene: Formation and Decoupling of  $0^\circ$ -Rotated Epitaxial Graphene** — ●HAO YIN<sup>1,2</sup>, MIRIAM RATHS<sup>1,2</sup>, MARK HUTTER<sup>1,2</sup>, FRANÇOIS C. BOCQUET<sup>1</sup>, and CHRISTIAN KUMPF<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich and Jülich-Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Jülich, Germany — <sup>2</sup>Experimentalphysik IV A, RWTH Aachen University, Aachen, Germany

On the way to twisted bilayer graphene with a twisting angle of  $30^\circ$ , we investigated the graphene growth on 6H-SiC(0001) using an unconventional epitaxial growth method named 'surfactant-mediated growth', which is based on annealing the SiC surface in borazine atmosphere. Here, we report a LEEM-based study on two different samples, on which we observed different surface morphologies with varying numbers of stacked graphene layers. A large-scale uniform graphene  $R0^\circ$  monolayer is found on the first sample that was annealed to  $1330^\circ\text{C}$ . This sample is a promising candidate for producing  $30^\circ$  TBG. Interestingly, some regions of the graphene  $R0^\circ$  layer exhibit different brightness contrasts at specific start voltages, without showing significant differences in their LEEM-IV curves. The second sample was annealed  $50^\circ\text{C}$  higher, causing the formation of graphene multilayer domains. We utilized LEEM and LEEM-IV in order to determine the number of layers as well as the distribution of multilayer graphene domains. Furthermore, we discuss the influence of the annealing temperatures in terms of the formation and decoupling of the epitaxial graphene layers.

O 18.6 Mon 18:00 P4

**Vertical structure of Sb-intercalated quasi-freestanding graphene on SiC(0001)** — YOU-RON LIN<sup>1,2,3</sup>, SUSANNE WOLFF<sup>4,5</sup>, ●MARK HUTTER<sup>1,2,3</sup>, SERGUEI SOUBATCH<sup>1,2</sup>, TIEN-LIN LEE<sup>6</sup>, F. STEFAN TAUTZ<sup>1,2,3</sup>, THOMAS SEYLLER<sup>4,5</sup>, CHRISTIAN KUMPF<sup>1,2,3</sup>, and FRANÇOIS C. BOCQUET<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — <sup>2</sup>Jülich Aachen Research Alliance (JARA) — <sup>3</sup>Experimentalphysik IV A, RWTH Aachen University, Germany — <sup>4</sup>Institute of Physics, Faculty of Natural Sciences, TU Chemnitz, Germany — <sup>5</sup>Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Germany — <sup>6</sup>Diamond Light Source Ltd., Didcot, Oxfordshire, UK

Using the normal incidence x-ray standing wave (NIXSW) technique, we have investigated the vertical structure of quasi-freestanding monolayer graphene (QFMLG) obtained by intercalation of antimony under the  $(6\sqrt{3} \times 6\sqrt{3}) R30^\circ$  reconstructed graphitized 6H-SiC(0001) surface, also known as zeroth-layer graphene. We found that Sb intercalation decouples the QFMLG very well from the substrate. The distance from the QFMLG to the Sb layer almost equals the expected van der Waals bonding distance of C and Sb. The Sb-intercalation layer itself is mono-atomic, very flat, and located much closer to the substrate, at almost the distance of a covalent Sb-Si bond length. All data is consistent with Sb located on-top of the uppermost Si atoms of the

SiC bulk.

O 18.7 Mon 18:00 P4

**Bi(110) islands on epitaxial graphene** — ●SERGI SOLOGUB<sup>1,2</sup>, JULIAN KOCH<sup>1</sup>, CHITRAN GHOSAL<sup>1</sup>, and CHRISTOPH TEGENKAMP<sup>1</sup> — <sup>1</sup>Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — <sup>2</sup>Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The atomic structure and morphology of ultrathin epitaxial Bi islands grown on the graphene/SiC surface was examined by SPA LEED and STM. Bi films with an average height of a few bilayers were deposited at RT and annealed at 410 K for 30 min afterwards. A Volmer-Weber growth mode with a predominance of the Bi(110) orientation was found. LEED patterns show that the Bi(110) structure has three domains rotated by 60°, with each domain having two subdomains rotated by ±2° with the zig-zag direction of Bi parallel to the arm-chair direction of graphene and four (minority-)subdomains with the zig-zag direction of Bi parallel to the zig-zag direction of graphene. Moreover, STM investigations revealed an elongation of the islands in the zig-zag direction of Bi as well as preferential ("magic") thicknesses (even numbers of Bi monolayers).

Additionally, magneto transport measurements using a 4 T magnet were performed in order to investigate the influence of the Bi islands on the weak localization effect in graphene.

O 18.8 Mon 18:00 P4

**Quantum well states in Bi(110) islands grown on epitaxial graphene** — ●CHITRAN GHOSAL and CHRISTOPH TEGENKAMP — Institut für Physik, TU Chemnitz

The semimetal Bi attracts a lot of interest because of its unique electronic properties such as a low carrier concentrations and large carrier mobilities coming along with mesoscopic Fermi wavelength giving rise to robust quantum confinement effects and spin polarized states in thin films [1]. In this work we studied the growth of Bi on n-type doped monolayer graphene (MLG) on SiC(0001) by means of STS and STM. While for low coverages Bi(110) islands are formed Bi(111) structures were found for higher coverages. This allotropic transition occurs at 10 monolayers (3.3nm) and is significantly larger than the critical coverage reported for Bi on Si(111) [2]. In contrast to Bi/MLG, the deposition of Bi on HOPG results in the formation of islands with an odd number of layers. These differences were attributed to different substrate screening effects. Irrespective of the interface, Bi seems to grow rather in a relaxed bilayers fashion, i.e. supporting the formation of black phosphorous structures [2]. Spectroscopy performed on islands of different heights revealed a large gap opening (750 meV) at the center of 4 ML islands. In addition, we found signatures of edge states, which might refer to a non-trivial topology within these QWS-stabilized nanostructures.

[1] T. Hirahara et al. Phys. Rev. B 75, 035422 (2007); [2] T. Nagao et al. Phys. Rev. Lett. 93, 105501 (2004).

O 18.9 Mon 18:00 P4

**Identification of electronic structures and atomic configuration of Nitrogen defects on graphene/Pt(111)** — ●JEONG AH SEO<sup>1,2</sup>, HYUNMIN KANG<sup>3,4</sup>, YOUNG JAE SONG<sup>3,4</sup>, JUNGSEOK CHAE<sup>1</sup>, and ANDREAS J. HEINRICH<sup>1,2</sup> — <sup>1</sup>Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Korea — <sup>2</sup>Department of Physics, Ewha Womans University, Seoul, Korea — <sup>3</sup>Department of Nano Engineering, Sungkyunkwan University (SKKU), Suwon, Korea — <sup>4</sup>SKKU Advanced Institute of Nano Technology (SAINT), Sungkyunkwan University (SKKU), Suwon, Korea

Nitrogen doped graphene is considered as an effective method for modulating the electronic states and properties of graphene. We have prepared nitrogen doped graphene on Pt(111) surface, grown by deposition of pyridine precursor molecules. We figured out there exist several types of defects including graphitic nitrogen and pyridinic nitrogen structure. The imaging of the defects is performed using low temperature scanning tunneling microscope (STM) and atomic force microscope (AFM). The defects preferred to have strong triangular shape features above certain bias voltage. To figure out the features of nitrogen dopant atom, we measured bias dependent STM images, scanning tunneling spectroscopy and AFM imaging. We have observed prominent difference in spectroscopic feature near the fermi energy between defects and pristine graphene. In addition, we also have observed atomic configuration of defect site using AFM. With the aid of STM simulation based on calculated results from the density functional theory, possible candidates of defect types will be provided.

O 18.10 Mon 18:00 P4

**Bell-shaped Electron Diffraction Component in 2D Materials** — ●HANNAH KOHLER, FRANK MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

In low energy electron diffraction a bell shaped component (BSC) is observed for graphene on SiC and Ir(111) and for hBN on Ir(111) [APL118 (2021) 241902]. The distinctiveness of this broad diffuse intensity appears to be indicative of a highly ordered 2D layer. Several attempts were made to explain the origin of the BSC, but the mechanism remains at large still unclear. In particular, a classification in which 2D systems a BSC exists is missing. Low energy electron microscopy (LEEM) combines the possibility to investigate the BSC with micro-diffraction ( $\mu$ -LEED) and *in-situ* imaging. It was found that the BSC can in fact be detected not only on graphene and hBN, but also on *ex-situ* chemical-vapor-deposition-grown MoS<sub>2</sub>. In graphene on Ir(111) the full width at half maximum (FWHM) of the BSC decreases with an increase in rotational angle of the graphene. Measurements after Cs intercalation of the graphene show a smaller FWHM compared to the non-intercalated graphene layer.

O 18.11 Mon 18:00 P4

**Buffer Layer Characterization of Epitaxial Graphene on Silicon Carbide with Scanning Tunneling Microscopy** — ●BENNO HARLING<sup>1</sup>, ANNA SINTERHAUF<sup>1</sup>, PETER RICHTER<sup>2</sup>, PHILIP SCHÄDLICH<sup>2</sup>, THOMAS SEYLLER<sup>2</sup>, and MARTIN WENDEROTH<sup>1</sup> — <sup>1</sup>IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — <sup>2</sup>Institut für Physik, Technische Universität Chemnitz, Germany

In this contribution, we present a scanning tunneling microscopy study on the buffer layer of epitaxial graphene on 6H-silicon carbide (SiC) at 8 K and room temperature in UHV. The local configurations and properties of the buffer layer still leave many open questions concerning the interactions between graphene and substrate. Our goal is to disentangle the contributions of the graphene and the underlying buffer layer to the tunneling current on a local scale and to establish an understanding of the responsible mechanisms. We employ multibias imaging to investigate buffer layer contributions to the tunneling current. This measurement mode takes quasi-simultaneous STM images line per line at given bias voltages resulting in a connected stack of topography maps. This allows to observe the changes of the topography in dependency of the applied bias voltage, with much lower dependency on tip modifications while scanning. We connect local corrugation changes to relative heights and the overall corrugation tendency within the stack. Financial support of the Deutsche Forschungsgemeinschaft (DFG) is given by project We 1889/13-1 and We 1889/14-1.

O 18.12 Mon 18:00 P4

**Intercalation of Fe under graphene on Ir(110)** — ●JASON BERGELT, AFFAN SAFEER, STEFAN KRAUS, JEISON FISCHER, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany

Graphene on Ir(110) is a single-crystal, where graphene is nearly strain free and the resulting moiré pattern consists of waves with crests and troughs along the [001]-Ir direction. Also it has been shown that the growth of graphene prevents the formation of nano-facets that are present in bare Ir(110) at room temperature. In this work, we intercalated several layers of Fe between Gr and unreconstructed Ir(110). By using scanning tunneling microscopy (STM) and low energy electron diffraction (LEED), we confirm that Fe grows pseudomorphic with respect to unreconstructed Ir(110). Due to strong adhesion of graphene to Ir(110), deposition of Fe on a closed graphene layer results in the formation of clusters on the surface and negligible intercalation at temperatures where alloying of Fe with Ir(110) is absent. Therefore, we implemented a procedure to etch with molecular oxygen small holes of controlled size into graphene. Moreover, we investigated the temperature and evaporation flux dependence of intercalation. Furthermore, we discuss the limit of pseudomorphic growth in view of the formation of a reconstruction at thicker intercalated Fe films.

O 18.13 Mon 18:00 P4

**Strongly correlated boundary states in topologically insulating chiral graphene nanoribbons tuned by contact potential** — ●LEONARD EDENS<sup>1</sup>, FRANCISCO ROMERO<sup>1</sup>, SOFIA SANZ<sup>2</sup>, AMELIA DOMÍNGUEZ-CELORRIO<sup>5</sup>, MANUEL VILAS-VARELA<sup>3</sup>, JINGCHENG LI<sup>4</sup>, DAVID SERRATE<sup>5</sup>, DIEGO PEÑA<sup>3</sup>, and NACHO PASCUAL<sup>1,2</sup> — <sup>1</sup>CIC

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Chiral graphene nanoribbons present a special class of nanographenes in that their distinct edge symmetry causes a topologically nontrivial band dispersion. Truncating such a ribbon results in a pair of symmetry-protected topological end states predicted to be spin-polarized. Metal substrates interact with the molecular orbitals, transferring charge and screening electron-electron correlations. We decouple the nanoribbons by dragging them onto an ultrathin large bandgap insulator using an STM, and also synthesize them on a low-work function surface. Scanning tunneling spectroscopy on the surface intermetallic GdAu<sub>2</sub> reveals a near-neutral ribbon, showing its end state spin-split. On MgO/Ag(001), the ribbons are highly decoupled, leading a greatly enhanced tunneling lifetime, vibronic sidebands, a negative charge and an enhanced correlation gap of opening far in the quantized conduction band.

O 18.14 Mon 18:00 P4

**Structural investigation of Pb intercalated graphene on SiC** — ●SHAISTA ANDLEEB, JULIAN KOCH, CHITRAN GHOSAL, and CHRISTOPH TEGENKAMP — Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz

In order to modify the electronic properties of graphene, intercalation experiments have received a lot of attention recently. In this research, we examined the intercalation of Pb on carbon buffer layer on SiC(0001) using SPA-LEED and STM. The samples were prepared in UHV by several cycles of Pb deposition using MBE at RT followed by annealing at temperatures ranging from 500 to 900°.

In LEED the intercalated phase shows six characteristic spots around the (00)-spots, which we correlated with a striped phase in STM. The local structure on the stripes shows two honeycomb Pb layers with approximately twice the lattice constant of graphene and turned by  $\pm 7.5^\circ$  with respect to graphene. The corresponding spots in LEED coincide with two buffer layer spots. Their energy dependent behavior was analyzed.

O 18.15 Mon 18:00 P4

**Spectroscopic evidence of BCS-BEC crossover in FeSe monolayer** — ●WANTONG HUANG<sup>1,6</sup>, HAICHENG LIN<sup>1</sup>, GAUTAM RAI<sup>2</sup>, YUGUO YIN<sup>1</sup>, LIANYI HE<sup>1</sup>, QI-KUN XUE<sup>1,5</sup>, STEPHAN WOLFGANG HAAS<sup>2,3</sup>, STEFAN KETTEMANN<sup>3,4</sup>, XI CHEN<sup>1,5</sup>, and SHUAI-HUA JI<sup>1,5</sup> — <sup>1</sup>State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — <sup>2</sup>Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA — <sup>3</sup>Jacobs University, Campus Ring 1, 28759 Bremen, Germany — <sup>4</sup>Division of Advanced Materials Science, POSTECH, San 31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea — <sup>5</sup>Frontier Science Center for Quantum Information, Beijing 100084, China — <sup>6</sup>Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

It has been difficult to realize the crossover from Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensates (BEC) in solids. Here we report direct evidence of BEC in a FeSe monolayer. The Fermi energy of the FeSe film can be tuned by graphene/SiC substrate to realize a BCS-BEC crossover. As the Fermi energy drops, the local density of states measured by STM evolves continuously from a BCS gap to a step-like asymmetric spectrum of BEC state. The theoretical calculation based on a two-band model reproduces well the measured spectra and, in particular, identifies features in the quasi-particle density of states that indicate a transition from the BCS to the BEC regime. In addition, the Zeeman splitting of the quasi-particle states is found to be consistent with the characteristics of a condensate.

O 18.16 Mon 18:00 P4

**Investigating the correlated ground state of metallic monolayer MoS<sub>2</sub> with scanning tunneling spectroscopy** — ●CAMIEL VAN EFFEREN, JEISON FISCHER, THOMAS MICHELY, and WOUTER JOLIE — II. Physikalisches Institut, Universität zu Köln, Germany

Using contactless chemical doping [1], we grow metallic monolayer 2H-MoS<sub>2</sub> on a graphene on Ir(111) substrate. Since this method leaves the surface accessible, we perform real space investigations of correlated behavior in metallic monolayer MoS<sub>2</sub> via scanning tunneling microscopy (STM) and spectroscopy (STS). In STS, we find a broad

depression in the density of states around the Fermi level, of about 100 meV. Upon closer inspection, the depression is revealed to consist of a series of small gaps and peaks, spaced by 26-28 meV. This interval corresponds to a flat band in the phonon dispersion of MoS<sub>2</sub>. The appearance of the peaks can be explained by strong coupling between the MoS<sub>2</sub> electrons and phonons at the high-symmetry K-point of the Brillouin zone, and may point to the formation of Holstein polarons. The behavior of the polarons is studied near grain boundaries, edges and defects, where the polaron bands are surprisingly seen to bend under the influence of charge.

[1] C. van Efferen et al., 2D Mater. 9 025026 (2022)

O 18.17 Mon 18:00 P4

**Artificial electronic lattices on InAs(111)A** — ●RIAN LIGHTHART and INGMAR SWART — Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht, The Netherlands

Artificial electronic lattices are a promising tool to elucidate novel effects in the quantum world. The Scanning Tunneling Microscope (STM) allows to build the lattices by manipulating atoms with nanoscale precision and to probe the electronic properties. The electronic lattices consist of artificial atoms on a metallic/semiconducting crystal with a surface state which acts as a 2D electron gas (2DEG). The 2DEG is patterned by scatterers on the surface creating artificial atoms. The versatile artificial atoms are used in lattices to study the effect of structure on electronic characteristics.

An already well-known system is CO on Cu(111), however, this system has a low energy resolution of 80 mV due to coupling of the surface state with bulk states. Here, the promising InAs(111)A surface with native In adatoms is studied since it has a higher energy resolution of around 5 meV. Vertical manipulation allows to place multiple In-adatoms in vicinity of each other. The In adatoms create a potential well that confines the surface state electrons of InAs. The artificial atom created can be coupled into dimers with different bond strengths by varying the distance or by introducing bridge sites. The artificial electronic lattices created on InAs(111)A can help to probe new characteristics in the lattices due to the vastly improved energy resolution.

O 18.18 Mon 18:00 P4

**Resonant photoemission studies at the Fe 3p threshold on thin FeTe/Bi<sub>2</sub>Te<sub>3</sub> and FeSe/Bi<sub>2</sub>Se<sub>3</sub>** — ●MARTIN VONDRÁČEK<sup>1</sup>, TOMÁŠ SKÁLA<sup>2</sup>, KAREL CARVA<sup>2</sup>, GUNTHER SPRINGHOLZ<sup>3</sup>, and JAN HONOLKA<sup>1</sup> — <sup>1</sup>Institute of Physics of the Czech Academy of Sciences, Prague, CZ — <sup>2</sup>Charles University, Faculty of Mathematics and Physics, Prague, CZ — <sup>3</sup>Johannes Kepler University, Institute of Semiconductor and Solid State Physics, Linz, AT

Monolayers (MLs) of tetragonal FeTe and FeSe grow on hexagonal Bi<sub>2</sub>Se<sub>3</sub>(111) and Bi<sub>2</sub>Te<sub>3</sub>(111) substrates as three 60°-rotated domains. In scanning tunnelling spectroscopy, a gap appears at the Fermi level of FeTe/Bi<sub>2</sub>Te<sub>3</sub> suggesting interface-induced superconductivity below T<sub>c</sub> ≈ 6 K [1]. FeSe/Bi<sub>2</sub>Se<sub>3</sub> remains in a gapless state [2]. Unconventional superconductivity in Fe-chalcogenides (FeChs) is believed to be correlated to the texture of the Fermi surface at  $\Gamma$ - and M-points. However, ARPES data of FeCh MLs on Bi<sub>2</sub>Ch<sub>3</sub> is complex due to the superposition of contributions from all three domains. Here we show photon energy dependent UPS data probing k<sub>z</sub> dispersions along the  $\Gamma$ -Z direction. Fano-like modulations of valence band intensities are observed in the energy range 30-80 eV, indicative of a resonant photoemission effect at the Fe 3p edge around 55 eV. Our ML data is compared to previous bulk studies [3].

[1] A. Eich et al., Phys. Rev. B **94**, 125437 (2016). [2] S. Manna et al., Nat. Commun. **8**, 14074 (2017). [3] T. Yokoya et al., Sci. Technol. Adv. Mater. **13** (2012) 054403.

O 18.19 Mon 18:00 P4

**Electron-stimulated photon emission on TMD defects** — ●LYSANDER HUBERICH<sup>1</sup>, JONAS ALLERBECK<sup>1</sup>, FEIFEI XIANG<sup>1</sup>, RICCARDO TORSI<sup>2</sup>, ANNE MARIE TAN<sup>3</sup>, PASCAL RUFFIEUX<sup>1</sup>, ROMAN FASEL<sup>1</sup>, OLIVER GRÖNING<sup>1</sup>, RICHARD HENNIG<sup>3</sup>, YU-CHUAN LIN<sup>2</sup>, JOSHUA ROBINSON<sup>2</sup>, and BRUNO SCHULER<sup>1</sup> — <sup>1</sup>Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland — <sup>2</sup>Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA — <sup>3</sup>Department of Materials Science and Engineering, University of Florida, USA

Due to their exceptionally long electron spin coherence and spin-selective optical readout nitrogen-vacancy centers in diamond are considered a key building block in quantum sensing and quantum-

cryptography applications. However, defects in bulk materials suffer from limited tunability and placement control, poor photon extraction efficiency, and coherence degradation close to the surface. 2D materials such as monolayer transitional metal dichalcogenides (TMDs) are expected to overcome these challenges while offering new synthetic strategies for the bottom-up design of solid-state defects. Here we present an  $NV^-$  center analog in 2D; the dopant vacancy complex ( $Re_{Mo} + Vac_S$ )<sup>-</sup> in  $MoS_2$ . We investigate its electronic states using scanning tunneling spectroscopy and present atomically-resolved photon emission maps of single TMD defects by means of STM luminescence.

O 18.20 Mon 18:00 P4

**Electronic and structural properties of Fe-doped SnS van der Waals crystals** — ●DAMLA YESILPINAR<sup>1,5</sup>, MARTIN VONDRÁČEK<sup>1</sup>, ČESTMÍR DRAŠAR<sup>2</sup>, PATRIK ČERMAK<sup>2</sup>, ONDŘEJ ČAHA<sup>3</sup>, KAREL ČARVA<sup>4</sup>, VÁCLAV HOLÝ<sup>4</sup>, JAN PROKLEŠKA<sup>4</sup>, HARRY MÖNIG<sup>5</sup>, and JAN HONOLKA<sup>1</sup> — <sup>1</sup>Institute of Physics, AV ČR, Na Slovance 1999/2 182 21 Praha 8, CZ — <sup>2</sup>Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, CZ — <sup>3</sup>Department of Condensed Matter Physics, Masaryk University, Žerotínovo nám. 617/9, 601 77 Brno, CZ — <sup>4</sup>Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, 121 16 Prague, CZ — <sup>5</sup>Physikalisches Institute, Wilhelm-Klemm Str. 10, 48149 Münster, DE

We investigate the effect of low concentrations of iron on the physical properties of SnS van der Waals crystals grown from the melt. By means of scanning tunneling microscopy (STM) and photoemission spectroscopy we study Fe-induced defects and observe an electron doping effect in the band structure of the native p-type SnS semiconductor. Atomically resolved and bias dependent STM data of characteristic defects are compared to *ab initio* DFT simulations of vacancy ( $V_S$  and  $V_{Sn}$ ), Fe substitutional ( $Fe_{Sn}$ ) and Fe interstitial ( $Fe_{int}$ ) defects. In line with our EXAFS data, we propose the importance of  $Fe_{int}$  and discuss possible pairing defects, e.g. with  $V_S$ .

O 18.21 Mon 18:00 P4

**In Operando Soft X-Ray Photoemission Spectroscopy of TaS<sub>2</sub> and HfS<sub>2</sub> based memristive devices** — ●TAMMO ZIMMERMANN<sup>1</sup>, ALENA NIERHAUVE<sup>1,2</sup>, MATTHIAS KALLÄNE<sup>1,2</sup>, JENS BUCK<sup>1,2</sup>, ZHANGSONG GENG<sup>3</sup>, CHAO ZHANG<sup>3</sup>, FRANK SCHWIERZ<sup>3</sup>, MARTIN ZIEGLER<sup>3</sup>, and KAI ROSSNAGEL<sup>1,2,4</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, 24098 Kiel, Germany — <sup>2</sup>Ruprecht-Haensel-Labor, DESY and CAU Kiel, 22607 Hamburg and 24098 Kiel, Germany — <sup>3</sup>Department of Electrical Engineering and Information Technology, TU Ilmenau, 98684 Ilmenau, Germany — <sup>4</sup>Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

In neuromorphic engineering interface-based memristive devices (IMDs) are promising candidates to mimic synaptic behavior. A refined understanding of bias-induced changes in the band structure and the underlying transport mechanisms of layered transition-metal dichalcogenide-based IMDs will improve the development toward future applications, e.g., in artificial neural networks. Here, we show first *in operando* position- and momentum-resolved soft x-ray photoemission spectroscopy measurements obtained from transistor-like TaS<sub>2</sub>- and HfS<sub>2</sub>-based IMDs.

O 18.22 Mon 18:00 P4

**Comparison of spin-crossover properties between thin film and bulk sample of a binuclear Fe(II) complex** — ●MARCEL WALTER<sup>1</sup>, SANGEETA THAKUR<sup>1</sup>, CLARA TROMMER<sup>2</sup>, FELIX TUCZEK<sup>2</sup>, SEBASTIEN ELIE HADJADJ<sup>1</sup>, JORGE TORRES<sup>1</sup>, and WOLFGANG KUCH<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — <sup>2</sup>Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Straße 2, 24118 Kiel

Spin-crossover molecules (SCMs) are a promising material in the field of spintronics, due to the reversibility of switching between a high-spin and a low-spin state, which can be triggered by light and temperature [1]. The focus of our research is to deposit large SCMs to explore cooperativity in spin switching on surfaces. A pulsed-valve vapor deposition method is used for thin films. This has the advantage of depositing (sub-) monolayers of SCMs in an UHV environment without applying large amounts of thermal energy, which can decompose the large SCMs. We compare the spin-switching behavior of the dinuclear SCM  $\{[Fe(H_2B(pz)_2)_2]_2(\mu\text{-bipy-ac-bipy})\}$  as thin film on highly

oriented pyrolytic graphite and as bulk sample using X-ray absorption spectroscopy. The spin-crossover properties were examined for thermal-induced spin state switching as well as for light-induced excited spin-state trapping. The results show that the thin films are locked in a mixed spin state while the bulk sample switches completely, although the equilibrium temperature of the spin states is comparable. [1] L. Kipgen et al., *Advanced Materials* 33, 24 (2021)

O 18.23 Mon 18:00 P4

**Neutral and charged excitations in two-dimensional MoTe<sub>2</sub> from first principles** — ●FRANZ FISCHER<sup>1,2</sup>, ABDERREZAK BESTER<sup>1</sup>, and GABRIEL BESTER<sup>1</sup> — <sup>1</sup>University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — <sup>2</sup>Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Atomically thin layers of transition metal dichalcogenides attract remarkable interest due to their extraordinary electronic and optical properties. The lack of inversion symmetry in their crystal structure combined with strong spin-orbit interaction caused by heavy metal atoms gives rise to an extra valley degree of freedom as well as large spin splittings in the Brillouin zone.

We present an effective first-principle formalism that is extendable to study any order of neutral or charged excitation [1]. Our formalism relies on configuration interaction and the GW-approximation and reduces in the case of excitons to the standard form of the BSE. We will present results of the excited states in monolayer MoTe<sub>2</sub> and their emergence from the particular single-particle configurations. In the future we want to extend our methodology to the temporal domain in order to study dynamics of excited states in 2D materials.

[1] *Phys. Rev. B.* **100** 201403(R) (2019)

O 18.24 Mon 18:00 P4

**Relaxation, the moiré potential and excited states for twisted TMDC bilayers** — ●CARL EMIL MØRCH NIELSEN, MIGUEL DA CRUZ, ABDERREZAK TORCHE, and GABRIEL BESTER — University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany

In recent years, the research of transition metal dichalcogenides has amassed much attention due to interesting properties such as strong localisation of excited states. The field of twistronics emerged as twisting provides a new degree of freedom in engineering specific properties. However, the theoretical *ab-initio* approach shows an immediate challenge to overcome; large systems, where the moiré unit cell may hold thousands of atoms.

In this project, the aim is to theoretically study moiré confined optical excitations in twisted TMD vdW-homo and heterostructures. We have successfully integrated a force-field based method of relaxation using LAMMPS as suggested in a paper by Jain et. al. We have re-parameterized the SW and KC potentials seen in this paper and expanded the parameter set to include all possible bilayer TMD combinations. With these we can accurately model the associated local band gap variation, e.g. the moiré potential, taking into effect both lattice corrugation and atomic reconstruction. Our goal is now to investigate the excited state properties with our group-developed code from first-principles.

O 18.25 Mon 18:00 P4

**Tip-induced excitonic luminescence of an atomically-resolved van der Waals heterostructure** — ●LUIS PARRA LOPEZ<sup>1,2</sup>, ANNA ROSLAWSKA<sup>2</sup>, FABRICE SCHEURER<sup>2</sup>, STÉPHANE BERCAUD<sup>2</sup>, and GUILLAUME SCHULL<sup>2</sup> — <sup>1</sup>Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany. — <sup>2</sup>Université de Strasbourg, CNRS, IPCMS, UMR 7504, 67000 Strasbourg, France.

Van der Waals heterostructures (vdWH) made from stacks of transition metal dichalcogenides and other 2D-materials are appealing systems to investigate light-matter interaction. Their optical response is dominated by tightly bound excitons that are sensitive to the presence of atomic-scale inhomogeneities. These inhomogeneities lie at length-scales below the spatial resolution accessible with standard optical spectroscopies. Here, we present an approach using a scanning tunneling microscope to induce the luminescence of an MoSe<sub>2</sub>/FL-graphene vdWH [1]. We correlate the atomic-scale landscape with the locally induced optical response and observe sizeable variations in the excitonic emission between different nm-sized areas. This study paves the way for novel investigations regarding the local properties of vdWH and highly localized excitons. To gain deeper insight into interlayer coupling mech-

anisms on the nanoscale, which occur on sub-ps timescales, requires additional high temporal resolution as well. I thus conclude with an outlook of an experimental setup capable of addressing ultrafast dynamics with fs-temporal and nm-spatial resolution[2]. [1] Parra et al, arXiv:2204.14022(2022). [2] Müller et al, ACS photonics, 7(8), (2020).

O 18.26 Mon 18:00 P4

**Changing structural and electronic properties of h-BN on Ir(111) by potassium intercalation** — •PHILIP GRIMM, FRIEDRICH WANIERKE, FELIX OTTO, MAXIMILIAN SCHAAL, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

2D hexagonal boron nitride (h-BN) is applied in electronics components, e.g., in gate dielectrics for transistors. However, its insulating behaviour is strongly influenced by the growth on metal substrates. One possibility to restore the insulating effect and to decouple h-BN is the intercalation of alkali metals due to their low ionization energies.

In this study, we use h-BN grown by CVD on Ir(111) while potassium is deposited by thermal evaporation. The samples are investigated at various temperatures, the lateral structure by means of LEED as well as the electronic properties by means of XPS and (AR)PES. A  $(\sqrt{3} \times \sqrt{3})R30^\circ$  superstructure of K and a decrease of the moiré pattern originating from h-BN/Ir(111) is observed. In addition, the core levels and the band structure shifts to higher binding energies whereas the work function decreases by the similar value. Another observation is a disappearing band folding of the  $\sigma$ -bands. Due to the metastability of the superstructure at room temperature, we switched to low temperature at 35 K and observed even larger shifts of the core levels as well as of the band-structure ( $\approx 3$  eV). In conclusion, our results indicate an intercalation of K in the 2D-system and consequently h-BN is decoupled from Ir(111).

O 18.27 Mon 18:00 P4

**Adsorption and Reaction of Bromine on h-BN/Rh(111)** — •EVA MARIE FREIBERGER, NATALIE J. WALESKA, FELIX HEMAUER, VALENTIN SCHWAAB, HANS-PETER STEINRÜCK, and CHRISTIAN PAPP — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Due to their unique chemical and electronic properties, rendering them promising for many applications, numerous two-dimensional materials

(2DM) have been predicted, synthesized and characterized. To tailor the properties of 2DM towards possible applications, their chemical modification is of special interest. Hexagonal boron nitride (h-BN), a graphene analogue, exhibits a so-called nanomesh on Rh(111), which can be used as a template enabling spatially defined modification of the 2DM. Using this template, we aim for selective functionalization of h-BN/Rh(111) with halogens, which lead to strong electronic doping. Here, we present a synchrotron radiation-based high-resolution X-ray photoelectron spectroscopy (XPS) study on the adsorption and thermally induced reaction of bromine on h-BN/Rh(111). The adsorption of different amounts of bromine was followed in situ at 170 K, confirming the template effect of the nanomesh for low coverages. Based on temperature-programmed XPS (TPXPS) experiments, we propose covalent functionalization of the pores and a thermally induced on-surface reaction of bromine. Furthermore, the adsorption is observed to be reversible upon heating to 800 K. By shedding light on their controlled chemical modification on the molecular scale, our work paves the way for purposeful tailoring of the properties of 2DM.

O 18.28 Mon 18:00 P4

**Structural investigation of antimony monolayers on Ag(111)** — •STEFANIE HILGERS<sup>1</sup>, JULIAN A. HOCHHAUS<sup>1,2</sup>, MALTE G. H. SCHULTE<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>TU Dortmund University, Department of Physics, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — <sup>2</sup>DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227, Dortmund, Germany

Similar to graphene and further elements of the 4th main group, Group-V elements such as antimony are also predicted to have extraordinary electronic properties. Because of the strong spin-orbit coupling and the resulting topological properties, antimony monolayers are of great interest for future electronic applications. Since the structural configuration of 2D-materials has major influence on the electronic properties of the material, structural investigations are highly relevant. In the here presented research we report on the synthesis and structural investigation of antimony monolayers on Ag(111).

After several cleaning cycles in UHV, antimony is evaporated by a Kudsen cell to deposit monolayers on the Ag(111) surface. The well-known  $(\sqrt{3} \times \sqrt{3})R30^\circ$  superstructure can be identified by low-energy electron diffraction (LEED). In addition, a  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  superstructure can be verified for higher coverages. Furthermore, the real space structure is investigated by scanning tunneling microscopy (STM).