O 47: Poster Session - 2D Materials: Electronic Structure, Excitations, etc.

Time: Tuesday 18:15–20:00 Location: P2/EG

O 47.1 Tue 18:15 P2/EG

Time-resolved and spatially resolved exciton dynamics in a microstructured WSe_2 monolayer investigated by 2D nanoscopy — •Daniel Fersch[1], Sebastian Pres[1], Victor Lisinetskii[1], Robert Schneider[2], Johannes Kern[2], Matthias Hensen[1], Rudolf Bratschitsch[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Atomically flat layers of transition metal dichalcogenides, e.g., WSe_2, are a fascinating material class with potential optoelectronic applications due to their direct bandgap and large exciton binding energies. Mechanical strain on the monolayer can lead to the formation of localized single-photon sources, which are of large interest for quantum-optical applications [1].

As these single-photon emitters are highly localized, it is beneficial to bypass the optical diffraction limit to investigate their physical nature. In this work, we therefore want to employ two-color time-resolved photoemission electron microscopy (TR-PEEM) on a WSe_2 monolayer to inspect local differences in the excited-state dynamics. Furthermore, we plan to use 2D nanoscopy [2,3] to directly probe the electronic structure of the material on a nanometer scale.

[1] J. Kern et al., Adv. Mater. **2016**, 28, 7101.
[2] M. Aeschlimann et al., Science **2011**, 333, 1724.
[3] B. Huber, S. Pres et al., Rev. Sci. Instr. **2019**, 90, 113103.

O 47.2 Tue 18:15 P2/EG

Develop strain manipulation techniques for STM measurement — •Jz-Yuan Juo[1], Bong Gyu Shin[1], Jack Maughan[1], Charlie Shaw[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale deLausanne, CH-1015 Lausanne, Switzerland

An atomic-scale understanding of how strain affects the electronic properties is essential for the implementation of two-dimensional (2D) materials into flexible electronics. However, the combination of low temperature scanning tunneling microscopy (STM) and strain-tunable devices remains challenging due to its technical limitations. The strain controller should fit in the STM sample holder with a maximum size of 1 cm^3 and function at ∼4 K. It should also be compatible with ultrahigh vacuum. Here, we developed a motor-based strain controller, which enabled us to apply uniaxial bending strain in situ. The polyimide film with surface roughness of ∼0.5 nm was chosen to minimize the substrate roughness induced strain. The 2D materials grown by chemical vapor deposition were transferred onto the polyimide film and tighten by clamps to deliver the strain to the 2D material effectively. The uniaxial deformation was confirmed by phonon shifts measured in Raman spectroscopy.

O 47.3 Tue 18:15 P2/EG

Highly ordered metallic phase of Indium on SiC(0001) — •Jonas Erhardt, Maximilian Bauernfeind, Victor Rogalev, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany

Indium thin films attract attention due to diverse electronic properties, which feature for instance a two-dimensional electron gas (2DEG) [1] and superconductivity [2] in the 2D limit or Dirac-electrons in a triangular lattice. Here, we present a combined angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling microscopy (STM) study of highly ordered indium (≈ 2 monolayer) on silicon carbide (SiC). STM reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm assigned as a $(4\sqrt{3} \times 4\sqrt{3})$R30° reconstruction. Additionally, ARPES as well as scanning tunneling spectroscopy (STS) show a metallic band structure with a pronounced electron pocket, indicative of an 2DEG. Interestingly, STS further reveals negative differential conductance (NDC), which is in contrast to the textbook interpretation as local density of states and is possibly related to substrate effects.

[1] E. Rotenberg *et al.*, Phys. Rev. Lett. **91**, 246404 (2003).
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010).

O 47.4 Tue 18:15 P2/EG

Ab-initio simulation of angle-resolved photoemission spectra for transition metal dichalcogenides — •Christoph Dösinger and Peter Puschnig — Universität Graz, Universitätsplatz 5, A-8010 Graz

Angle-resolved photoemission spectroscopy (ARPES) is the most direct experimental technique to investigate the electronic structure of layered materials. ARPES band maps are routinely compared to results from ab-initio band structure calculations. However, simulations of photoemission cross sections including transition matrix element effects which provide additional insights are rare.

In this work, we perform ARPES simulations for single layers of transition-metal dichalcogenides (TMDs). Starting from density functional calculations including spin-orbit coupling, we have computed ARPES intensities within the plane wave final state approach which has proven to work surprisingly well for two-dimensional (mono)-layers of organic molecules adsorbed on metal surfaces. By comparing our simulated band maps and constant binding energy momentum maps with available experimental data for prototypical TMDs, WS2 and WSe2, we assess to what extent the simple plane wave approach can also be applied to this class of materials.

O 47.5 Tue 18:15 P2/EG

Modification of 2D materials by ultra-low energy ion implantation — •Manuel Auge[1], Michael Hennessy[2], Ursel Bangert[2], and Hans Hofsäss[1] — [1]II. Institute of Physics, Georg-August-University Göttingen, 37077 Göttingen, Germany — [2]Bernal Institute, University of Limerick, Limerick, Ireland

A new group of direct semiconductors are monolayer transition metal dichalcogenides (ML TMDs) of the form MX_2 (M = transition metal and X = chalcogen). The high interest in ML TMDs is based on their promising applications in nanoelectronics and photonics [1]. In order to exploit the great potential of the material, it is important to develop a controllable method for modifying the physical properties.

In our study, a unique mass selected ion beam deposition system is used to incorporate low energy ions into two dimensional (2D) lattices. Therefore, a 30 keV ion beam is decelerated in a UHV-chamber down to energies as low as 10 eV. A beam sweep ensures a uniform profile over an area of 1 cm^2 up to 2.5 cm^2. Here, we demonstrate the successful incorporation of Cr into the MoS_2 lattice. The integration of Cr could be verified by energy-dispersive X-ray spectroscopy (EDX) as well as by core loss electron energy loss spectroscopy (EELS). In addition, low loss EELS enables the investigation of the doping effect on the band gap of the material. Financial support by the Volkswagen Stiftung is gratefully acknowledged.

[1] K.F. Mak *et al.*, Phys. Rev. Lett. **105**, 136805 (2010)

O 47.6 Tue 18:15 P2/EG

Optoelectronic properties of point defects in hBN — •Alexander Kirchhoff, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

While pristine hexagonal boron nitride (hBN) is a wide-gap insulator, its point defects are discussed as light emitters in the visible optical spectrum. In this study, we examine two substitutional carbon impurities, C_N and C_B, the nitrogen vacancy V_N and the divacancy V_{NB} in a hBN monolayer from an *ab initio* approach, via the *GW*/BSE approximation. Our results show deep defect states and defect-related excitations with energies in the visible regime. We present a detailed analysis of their spatial structure and energetic composition.

O 47.7 Tue 18:15 P2/EG

p Orbital flat band and Dirac cone in the electronic honeycomb lattice — •Thomas Gardenier[1], Jette van den Broeke[2], Jesper Moes[1], Ingmar Swart[1], Christophe Delarue[3], Marlou Slot[1], Cristiane Morais Smith[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Université de Lille, CNRS, Centrale Lille, Yncréa-ISEN, Université Polytechnique Hauts-de-France, UMR 8520 - IEMN, F-59000 Lille, France

Honeycomb systems have generated much interest in experimental and theoretical physics due to their interesting band structures. The architypical example of a honeycomb lattice is graphene. The electronic structure of graphene close to the Fermi level can be understood by only considering C 2pz orbitals. Bands due to coupling of sp2 hybrid orbitals are either much higher or lower in energy. It has been shown that in the absence of hybridisation, the band structure of honeycomb lattices features a topologically non-trivial flat band, as well as Dirac cones formed by px and py orbitals.

We patterned a Cu(111) surface with CO molecules to confine the surface state electrons into a honeycomb geometry. By careful tuning of the lattice parameters, we created a honeycomb lattice where s- and p-orbital bands are separated. Scanning tunneling spectroscopy and wavefunction mapping are used to determine the band structure and visualise the electron densities. The results are complemented by theoretical muffin-tin and tight-binding calculations.

O 47.8 Tue 18:15 P2/EG

Ultrafast microscopy of charge density wave phase transitions using pump-probe imaging ellipsometry — •Sebastian Rohrmoser, Julius B. Peters, Tobias Heinrich, Murat Sivis, and Claus Ropers — IV. Physical Institute, Georg-August-University Göttingen, Germany

Transition metal-Dichalcogenides (TMDC's) have long been studied as effectively 2D layered systems exhibiting interesting ordering phenomena such as charge density waves (CDW). A variety of experimental techniques in a pump probe fashion have been used to disentangle the fundamental processes leading to the charge ordering including electron diffraction [1], photoemission spectroscopy [2] and transient optical reflectivity [3]. However, spatiotemporal behaviour like domain growth and movement is not well studied.

In this contribution, we present an all-optical approach to measure the complex refractive index of optically excited 1T-TaS2 on a femtosecond temporal and micrometer spatial scale. Specifically, using a pump probe ellipsometry setup with a rotating polarizer we detect the optically driven phase transition between the nearly commensurate (NC) and incommensurate (IC) CDW phase. The scheme will be applied to study the spatiotemporal dynamics of excited CDW states and phase transitions for inhomogeneous excitations.

[1] M. Eichberger et. al., Nature 468, 799-802 (2010)
[2] J.C. Petersen et.al., Phys. Rev. Lett. 107, 177402 (2011)
[3] N. Dean et.al., Phys. Rev. Lett. 106, 016401 (2011)

O 47.9 Tue 18:15 P2/EG

In-plane anisotropy of the elastic properties of monolayer transition-metal dichalcogenides — •Juliane Mörsel, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

Monolayer transition metal dichalcogenides are characterized as two-dimensional materials with hexagonal symmetry. Therefore, the linear elastic properties of these materials are isotropic along the in-plane directions and can be described by only two independent second-order elastic constants (SOECs). The anisotropy of the structure influences, nevertheless, the non-linear elastic properties, which at small values of applied strain can be described in terms of three independent third-order elastic constants (TOECs). In this work, we present an *ab-initio* investigation of the anisotropic behavior of the elastic properties of MoS_2, $MoSe_2$, WeS_2, and $WeSe_2$ monolayers. The SOECs and TOECs are obtained from numerical derivatives of the total energies with respect to the applied Lagrangian strain. For this purpose, total-energy calculations are performed using density-functional theory as implemented in the full-potential all-electron package `exciting` [1]. In order to explicitly exploit the anisotropic elastic behavior of these systems, we calculate the SOECs for non-equilibrium reference structures which are obtained by modifying the equilibrium configuration with uniaxial strains along the principal in-plane directions. Analysis of these results allows us to distinguish different regimes of nonlinearity.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202

O 47.10 Tue 18:15 P2/EG

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

The recent discovery of ferromagnetism in VSe_2 [1] boosted the interest in two-dimensional transition metal dichalcogenides (TMDs), which show peculiar magnetic properties. In this work we discuss the structure and local electronic properties of VS_2 monolayer on Au(111). By means of low-temperature scanning tunneling microscopy we analyze the exact atomic arrangement of VS_2. In spectroscopic measurements we observe a dominant peak at E_F, whose shape and position are dependent on the spatial position within the Moiré unit cell. Bilayer VS_2 islands show the same atomic structure as the monolayer. However, the electronic structure is distinctly different showing a gapped behaviour around E_F. We discuss our findings in conjunction with electron correlation effects in VS_2.

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

O 47.11 Tue 18:15 P2/EG

***In Operando* Soft X-Ray Photoemission Spectroscopy of 2D Materials** — Sanjoy K. Mahatha[1], •Alena Nierhauve[2], Sebastian Rohlf[3], Benedikt Schulte[4], Florian Diekmann[3], Jens Buck[3,5], Matthias Kalläne[3,5], Gregor Praedel[2,4], James McIver[4], and Kai Rossnagel[1,3,5] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, 20355 Hamburg, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [5]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel und Deutsches Elektronen-Synchrotron DESY, 24098 Kiel und 22607 Hamburg, Germany

2D materials provide a fruitful platform for the realization of novel forms of electronics including "Mottronics", "valleytronics", and "twistronics". Specifically, the combination of sub-micrometer position-resolved angle-resolved photoemission spectroscopy (ARPES) with *in operando* electrical control of device-like structures made from 2D materials opens a new avenue toward the direct probing and engineering of novel band-structure and transport phenomena underlying device functionality [1]. Here, we present first *in operando* results obtained from graphene and transition-metal dichalcogenides at our new sub-micrometer ARPES endstation at the soft X-ray beamline P04 of PETRA III.

[1] P.V. Nguyen *et al.*, Nature **572**, 220 (2019).

O 47.12 Tue 18:15 P2/EG

Strain tunable Photodetectors based on 2D materials: A case study of MoS2 monolayers — •Mohammad Bahmani[1], Mahdi Ghorbani-Asl[2], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, Department of Physics, Bremen University, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

In monolayers of transition metal dichalcogenides (ML-TMDs), direct band-gap, weak screening of charge carriers, and a large surface-to-volume ratio facilitate the light-matter interactions in such materials, leading to noticeably high optical absorptions. Synthetic samples usually contain some fraction of intrinsic defects with significant effects on their electrical and optical properties. The localized defect levels have been observed to improve the photoresponsivity of MoS2 MLs by trapping the photoexcited charge carriers, thus increasing the photocurrent. Considering high resilience of ML-TMDs towards mechanical deformations, it was shown that biaxial strain improves the device properties of MoS2-based photodetectors. Recently, we showed the shift of the mid-gap levels of the defects inside MoS2 MLs as a function of various applied strains which could explain the observed improvements in photodetector devices. We study the properties of flexible photodetectors based on phase-engineered MoS2 MLs (1T-2H-1T) under strain. Using sisl tool, we employ a linear response regime to add the electron-photon interactions as a perturbation to the pristine Hamiltonian calculated by TranSIESTA/TBtrans.

O 47.13 Tue 18:15 P2/EG

Modulation of the excitonic behaviour of MoS_2 on gold electrodes with external potential: a sum frequency spectroscopy study — •Tao Yang[1], Erik Pollmann[2], Marika Schleberger[2], Yujin Tong[1,2], and Richard Kramer Campen[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]University of Duisburg-Essen, Faculty of Physics,Lotharstr. 1, 47057 Duisburg, Germany

Two dimensional (2D) materials have recently attracted significant attention because of their unique electronic and optical properties. In particular MoS_2, a transition metal dichalcogenide, has been inten-

sively studied due to its dramatically layer-dependent properties and potential application in electrocatalysis, field-effect transistors and optoelectronics. While the fundamental physics of MoS_2 are increasingly well understood, less attention has been devoted to, and virtually all of these applications require, charge transfer between some other material, often a metal electrode and the MoS_2. Here we use final state resonant sum frequency spectroscopy to study the optical response of MoS_2 deposited on a gold electrode in aqueous solution as a function of applied bias. The data show the evolution of the A and B exciton with electron doping. Together with Raman and electrochemical characterisation, the current study provides important insights into understanding the relationship between electronic structure, atomic configuration and electron transfer at an MoS_2 electrochemical interface.

O 47.14 Tue 18:15 P2/EG

Hot electron dynamics in Stanene/Au(111) — •Marten Düvel[1], Germaine Arend[1], Daniel Franz Walter Marx[1], Jan Philipp Bange[1], Jonas Fredrik Pöhls[1], Marco Merboldt[1], Mahalingam Maniraj[2], Daniel Steil[1], Marcel Reutzel[1], Sabine Steil[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Stanene, the graphene analog with Sn, was recently predicted and has subsequently motivated intense research on the realization of Sn-based ultrathin materials. In our previous work [M. Maniraj et al., Comm. Phys., 2:12, 2019], we found a two-atomic honeycomb superstructure of Sn on Au(111) that shows a Dirac-like band centered at the $\Gamma-$point with anti-parallel spin polarization similar to a topological insulator. Here, we use time- and angle-resolved photoelectron spectroscopy to study the electronic structure and dynamics in the unoccupied regime of the band structure of this stanene-like material system.

O 47.15 Tue 18:15 P2/EG

Metal insulator transition studied with transport on H on epitaxial graphene — •Diana Slawig[1], Markus Gruschwitz[2], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany

The ability of atomic hydrogen to chemisorb on graphene makes it a quite interesting system for hydrogen storage and sensor applications. The introduction of scattering centers via atomic hydrogen chemisorption, the concomitant spin polarization and the opening of a bandgap due to symmetry breaking of the sublattice symmetry makes it particularly interesting for electronic transport measurements.
In this study we performed systematic transport investigations on hydrogen adsorption on epitaxial monolayer graphene on SiC by means of 4-tip STM/SEM. Conductance values were investigated for various surface H-coverages up to the saturation coverage of 0.4 ML, well below the percolation limit. As a function of the H coverage, we observed a metal-insulator transition. Thereby, the sheet resistance increases by three orders of magnitude up to 37 $k\Omega\square$. Temperature dependent measurements on these hydrogen terminated graphene show activated transport behavior with an activation energy of 30 meV. We suspect that upon adsorption of the saturation coverage, the monolayer is neutralized and gapped due charge transfer and breaking of the lattice symmetry.