

## DS 31: 2D Materials Beyond Graphene III (jointly with O)

Time: Wednesday 10:30–13:00

Location: WIL A317

DS 31.1 Wed 10:30 WIL A317

**Band structure and excitons of monolayer and bulk ReSe<sub>2</sub>: A many-body view** — ●JONATHAN NOKY<sup>1</sup>, MATTHIAS DRÜPPEL<sup>1</sup>, PHILIPP EICKHOLT<sup>2</sup>, THORSTEN DEILMANN<sup>3</sup>, KOJI MIYAMOTO<sup>4</sup>, PETER KRÜGER<sup>1</sup>, MARKUS DONATH<sup>2</sup>, and MICHAEL ROHLFING<sup>1</sup> — <sup>1</sup>Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — <sup>2</sup>Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany — <sup>3</sup>Center for Atomic-Scale Materials Design (CAMD), Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — <sup>4</sup>Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

Transition metal dichalcogenides (TMDCs) are a fascinating new class of semiconductors, which attracted a lot of interest in the past few years. They are promising materials for new optical and electronic devices on the nanoscale. Here, we focus on one of the less studied members of this group: ReSe<sub>2</sub>. In contrast to other TMDCs, it grows in a distorted 1T structure, which leads to new anisotropic properties.

We present electronic and excitonic spectra for both monolayer and bulk ReSe<sub>2</sub> within many-body perturbation theory (MBPT). For this, we apply the *GW*-BSE (Bethe-Salpeter equation) approach within the efficient LDA+*GdW* approximation [1]. Our results on the quasiparticle band structure are complemented with experimental ARPES data. Based on the band structure we investigate the excitons. The lowest four states show distinct dipolar characteristics, which is in contrast to many other TMDCs.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

DS 31.2 Wed 10:45 WIL A317

**Fabrication and characterization of coupled TMDC heterostructures** — ●BORJA V. PANO<sup>1,2</sup>, BASTIAN MILLER<sup>1,2</sup>, ALEXANDER W. HOLLEITNER<sup>1,2</sup>, and URSULA WURSTBAUER<sup>1,2</sup> — <sup>1</sup>Walter Schottky Institute and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching — <sup>2</sup>Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Atomically thin transition metal dichalcogenides (TMDC) have emerged as an exciting class of two-dimensional (2D) semiconductors with unique electronic and optoelectronic properties, and are of interest for both fundamental research and novel device applications.

We investigate heterostructures of four different TMDC monolayers (MoS<sub>2</sub>, WS<sub>2</sub>, MoSe<sub>2</sub>, WSe<sub>2</sub>). Due to the formation of a type II band alignment between the layers and the strong Coulomb binding energy in 2D TMDC, these devices open a promising path for studying long-lived interlayer excitons, where bound electrons and holes are localized in different layers.

A polymer-based dry transfer technique is used to vertically stack micromechanical cleaved monolayers with angle alignment of the crystal axes. We characterize the heterostructures through optical and atomic force microscopy, Raman and photoluminescence spectroscopy. We observe strong signatures of interlayer coupling.

We acknowledge the financial support by the DFG and the excellence cluster Nanosystems Initiative Munich (NIM).

DS 31.3 Wed 11:00 WIL A317

**Switchable white graphene: electrochemical surface science of the boron nitride nanomesh** — ●STIJN MERTENS — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstraße 8-10/134, 1040 Vienna, Austria — KU Leuven, Chemistry Department, Celestijnenlaan 200F, 3001 Leuven, Belgium

On Rh(111), a monolayer of hexagonal boron nitride (h-BN) forms a so-called nanomesh superstructure [1] with a 3.2-nm lattice constant and strong electronic corrugation, useful for trapping atoms and molecules [2,3].

We show by electrolyte-to-vacuum transfer experiments and thermal desorption spectroscopy that hydrogen underpotential deposition (H upd) [4] leads to submonolayer quantities of hydrogen intercalated between the h-BN overlayer and Rh(111). In situ STM reveals that this lifts the corrugation of the nanomesh and is fully reversible under potential control. Copper upd is used to quantify the defect density in the nanomesh, and to determine the electrochemical window where the nanomesh is stable. Dynamic contact angles of an electrolyte drop show that the microscopic change within the 2-dimensional material leads to a macroscopic effect related to a 10% change in adsorption en-

ergy [4]. The static friction on the other hand, which can be extracted by extending the Young equation for non-equilibrium effects, remains unchanged for the surface in the two states.

[1] Corso et al., Science 303 (2004) 217. [2] Berner et al. Angew. Chem., Int. Ed. 46 (2007) 5115. [3] Dil et al. Science 319 (2008) 1824. [4] Mertens, Greber et al. Nature 534 (2016) 676.

DS 31.4 Wed 11:15 WIL A317

**In-situ LEEM investigation of the growth of hexagonal boron nitride on metal surfaces** — ●JANINA FELTER, MARKUS FRANKE, and CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

Hexagonal boron nitride (hBN) is a prominent and frequently studied member of the family of two-dimensional (2D) materials. Due to its structural and electronic properties, in particular its insulating nature, it is of highest interest as part of hetero-epitaxial systems in conjunction with other 2D materials or organic thin films. However, the production of high quality hBN monolayers and organic thin films on hBN necessitates a deep understanding of nucleation and growth of these materials. Here, we present a detailed in-situ and real-time study of the growth of hBN monolayers on Cu(111) using Low-Energy Electron Microscopy (LEEM). We correlate the results with structural information obtained by  $\mu$ LEED and discuss the influence of substrate temperature, growth rate and movement of step edges.

DS 31.5 Wed 11:30 WIL A317

**Time-of-Flight Secondary Ion and Neutral Mass spectrometry of particles ejected from 3D and 2D materials during irradiation with highly charged and swift heavy ions** — ●PHILIPP ERNST<sup>1</sup>, FLORIAN MEINERZHAGEN<sup>1</sup>, MATTHIAS HERDER<sup>2</sup>, STEPHAN SLEZIONA<sup>1</sup>, ANDREAS WUCHER<sup>2</sup>, and MARIKA SCHLEBERGER<sup>1</sup> — <sup>1</sup>University Duisburg-Essen, AG Schleberger, Germany — <sup>2</sup>University Duisburg-Essen, AG Wucher, Germany

We have studied the ionization probability for strontium titanate bombarded by energetic ions, i.e. swift heavy ions (SHI) and highly charged ions (HCI). Strontium titanate is a dielectric and as such is known to be very sensitive to both, SHI and HCI irradiation, which result in characteristic surface modifications [1,2]. Therefore, it has been postulated that both projectile types trigger similar mechanisms leading to these modifications. To test this hypothesis, we compare time-of-flight mass spectra taken during irradiation with SHI at different electronic stopping powers (dE/dx) and with HCI with varying potential energy (<sup>129</sup>Xe ions with a potential energy from  $E_{\text{pot}}$  4.5 up to 59 keV by constant kinetic energy  $E_{\text{kin}}$ ), respectively. Both, emitted secondary ions (SIMS) and secondary neutrals (SNMS), were detected in order to determine differences of the ionization probability. To further test if the spatial distribution of the energy deposition (HCI a few nm, SHI up to tens of microns) does play a role, exemplary measurements with a 2D dielectric have been performed.

[1] F. Meinerzhagen, et al. Rev. Sci. Instr. 87 (2016) 013903.

[2] F. Aumayr, et al. J. Phys. Condens. Matter, 23 (39) (2011).

DS 31.6 Wed 11:45 WIL A317

**A monolayer of MoS<sub>2</sub> on Au(111) as a decoupling layer for single molecules** — ●CHRISTIAN LOTZE, NILS KRANE, ROBERT STEYRLEUTHNER, ROBERT BITTL, JAN BEHREND, and KATHARINA J. FRANKE — Fachbereich Physik, Freie Universität Berlin

Thiophene based molecules are commonly used for semiconducting devices like solar cells or light emitting diodes. In order to optimize these, a detailed understanding of the molecules electronic structure and the environmental influence on the latter is of great interest.

Scanning tunneling spectroscopy (STS) allows to address individual molecules in a precisely known surrounding. However, it bears the drawback that it requires a conductive substrate. Deposition of organic molecules on a metal substrate leads to strong hybridization of the electronic states. Preservation of the molecular character requires the inclusion of thin band-gapped materials.

Here, we present STS experiments performed on 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene-*n* (BTn-*n*; *n*=1,2) molecules adsorbed on a single layer molybdenum disulfide (MoS<sub>2</sub>) on

Au(111). We show that it acts as an effective decoupling layer. Differential conductance spectra of the molecules exhibit a multitude of sharp characteristic peaks, that are connected to the highest occupied molecular orbital. We propose that these originate from a surprisingly effective excitation of vibronic resonances by the tunneling electrons.

DS 31.7 Wed 12:00 WIL A317

**Surface-confined Mott transition in the strongly correlated compound 1T-TaSe<sub>2</sub>** — ●FLORIAN DIEKMANN, CHRISTIAN SOHRT, KERSTIN HANFF, LARS-PHILIP OLOFF, ARNDT QUER, MATTHIAS KALLÄNE, and KAI ROSSNAGEL — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The surface associated modification of the electronic structure of 1T-TaSe<sub>2</sub> in the commensurate charge density-wave (CDW) state is examined by utilising photon energy dependent X-Ray photoemission spectroscopy. In particular, the CDW-induced splitting of the Ta 4f core levels is probed over a wide range of photon energies from 80 eV to 6 keV corresponding to a variation of the information depth from extreme surface to effective bulk sensitivity. The measured depth-dependent core-level splitting corroborates the idea of a surface-confined Mott transition due to a modified CDW at the surface [1,2].

[1] L. Perfetti *et al.*, Phys. Rev. Lett. **90**, 166401 (2003).

[2] C. Sohrt *et al.*, Faraday Discuss. **171**, 243 (2014).

DS 31.8 Wed 12:15 WIL A317

**Insights into structure and binding of micron-sized hexagonal boron nitride islands on Ir(111)** — ●MARIN PETROVIĆ, MICHAEL HORN-VON HOEGEN, and FRANK-J. MEYER ZU HERINGDORF — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Single-layer hexagonal boron nitride (hBN) islands have been synthesized on Ir(111) via chemical vapor deposition (CVD) of borazine at various temperatures. By using low-energy electron microscopy (LEEM) as the main experimental tool, two types of hBN islands were identified which differ in their shape (triangular and trapezoidal) and in their rotational registry with respect to the iridium. Moreover, photoemission electron microscopy (PEEM) and IV-LEEM spectroscopy measurements show that the two island types exhibit different work functions and interaction strengths with iridium, which is proposed to be the origin of their divergence in shape and growth modes. In addition, it is found that for CVD synthesis above  $\approx 950$  °C additional boron islands are formed on the iridium surface, which is a result of increased decomposition of hBN and significant solubility of boron in iridium at high temperatures.

DS 31.9 Wed 12:30 WIL A317

**Intervalley scattering dynamics in MoS<sub>2</sub> imaged by two-photon photoemission with a high-harmonic probe** — ●ROBERT

WALLAUER, JOHANNES REIMANN, NICO ARMBRUST, JENS GUEDDE, and ULRICH HOEFER — Fachbereich Physik und Zentrum für Materialwissenschaften Philipps-Universität, 35032 Marburg, Germany

We will report on the application of time- and angle-resolved two-photon photoemission (2PPE) with a high-harmonic probe for the investigation of the electron dynamics of MoS<sub>2</sub> in momentum space. For this purpose, we combined a high-repetition rate high-harmonic source with tunable femtosecond pump pulses and a 3D ( $k_x$ ,  $k_y$ , E) electrostatic electron spectrometer. At our high-harmonic photon energy of 23.5 eV we essentially probe only the first layer, which is not necessarily equal to a bulk sample.

We used this setup to study the electron dynamics in the conduction band of MoS<sub>2</sub> after optical excitation with different pump photon energies. Thereby we showed that optical excitation above the A exciton resonance at 1.8 eV with 2.05 eV pump pulses results in an immediate occupation of the conduction band at K followed by an ultrafast transfer to the conduction band minimum at  $\Sigma$  [1]. Subsequently, the occupation at both high-symmetry points decays slowly on a ps timescale. We will present new data for pump photon energies in the range of 1.8 - 2.1 eV and show how the dynamics of this transfer depend on the excess energy above the exciton resonance.

[1] R. Wallauer *et al.*, Appl. Phys. Lett. **109**, 162102 (2016).

DS 31.10 Wed 12:45 WIL A317

**Theoretical aspects in the investigation of intrinsic magnetic order in monolayer FePS<sub>3</sub>** — ●PILKWANG KIM<sup>1</sup>, JAE-UNG LEE<sup>2</sup>, SUNGMIN LEE<sup>1,3</sup>, JI HOON RYOO<sup>1</sup>, SOONMIN KANG<sup>1,3</sup>, TAE YUN KIM<sup>1</sup>, CHEOL-HWAN PARK<sup>1,4</sup>, JE-GEUN PARK<sup>1,3</sup>, and HYEONSIK CHEONG<sup>2</sup> — <sup>1</sup>Department of Physics and Astronomy, Seoul National University (SNU), Seoul 08826, Korea — <sup>2</sup>Department of Physics, Sogang University, Seoul 04107, Korea — <sup>3</sup>Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea — <sup>4</sup>Center for Theoretical Physics, Seoul National University (SNU), Seoul 08826, Korea

It has been a while since Onsager established that there can be a phase transition at a finite temperature in the two-dimensional (2D) Ising system. However, experimental verification of such long-range magnetic order has been mostly limited to the magnetism arising from extrinsic effects such as defects and chemical dopants. Bulk iron phosphorus trisulfide (FePS<sub>3</sub>) is a van der Waals material with an Ising-type antiferromagnetic order. In this presentation, we discuss the results of our first-principle calculations on the electronic structure and vibrational spectrum of monolayer FePS<sub>3</sub>. The calculations are compared with the experimental Raman spectra that exhibit several new peaks emerging below the Néel temperature. We demonstrate that the drastic changes in the Raman spectra can be understood in terms of the zone-folding effects, which suggests that monolayer FePS<sub>3</sub> exhibits intrinsic anti-ferromagnetic order.