# O 8: 2D Materials Beyond Graphene I

Time: Monday 10:30–13:00 Location: REC/PHY C213

O 8.1 Mon 10:30 REC/PHY C213

**Transfer of a 2D silica sheet** — •Christin Büchner[1], Kristen M. Burson[2], Markus Heyde[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Hamilton College, Clinton, NY, USA

Two-dimensional (2D) materials hold immense technological potential for creating nanoelectronic devices. Highly conductive materials such as graphene are combined with insulators but the library of 2D materials with large band gap is effectively limited to h-BN. 3D insulators can compromise the electronic properties of graphene due to structural defects and surface roughness.

We present a 2D $SiO_2$ bilayer film, prepared on a Ru(0001) substrate via CVD. The atomic structure has been investigated using scanning probe microscopy.[1] Extended honeycomb structures and glass-like network structures were identified, while DFT calculations and STS measurements indicate a band gap larger than 6.5 eV.[2,3]

Recently, we transferred the bilayer from the growth substrate to a new substrate using a modified mechanical exfoliation procedure. The film maintains its atomically flat structure on the mm-scale after being transferred to a foreign substrate [4]. Low energy electron diffraction, Auger electron spectroscopy, scanning tunneling microscopy and environmental scanning electron microscopy indicate that the structure is maintained throughout the transfer procedure.

[1] DOI: 10.1002/anie.201107097 [2] DOI: 10.1063/1.4939279 [3] DOI: 10.1088/0953-8984/24/35/354010 [4] DOI: 10.1021/acsnano.6b03929

O 8.2 Mon 10:45 REC/PHY C213

**Photocarrier dynamics and interaction effects of interlayer excitons in $WSe_2/MoSe_2$ heterostructures** — •Philipp Nagler, Gerd Plechinger, Alexey Chernikov, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Regensburg, Germany

Atomically thin transition metal dichalcogenides (TMDCs) such as $WSe_2$ or $MoSe_2$ have lately emerged as a promising platform to study the physics of excitons in strongly confined systems. Thereby, the use of transfer techniques allows for the fabrication of van der Waals heterostructures by deterministic stacking of individual monolayers. It is expected that type-II band alignment of the individual monolayers results in the formation of spatially indirect excitons. Here, we present a detailed study of the optical properties of interlayer excitons in a $WSe_2/MoSe_2$ heterostructure using static and time-resolved photoluminescence measurements. At low temperatures, we observe the emergence of an energetically separated (1.4 eV) and spectrally sharp (FWHM $<$ 20meV) feature, which we attribute to the emission of interlayer excitons. Power-dependent measurements show a considerable blue shift of the interlayer exciton peak position due to dipolar exciton-exciton interaction effects. Finally, we employ a streak camera system in order to reveal the photocarrier dynamics of interlayer excitons for varying temperatures. The lifetime at low temperatures amounts to several nanoseconds, which is a consequence of the reduced oscillator strength of the interlayer exciton.

O 8.3 Mon 11:00 REC/PHY C213

**Electronic and atomic structure of the honeycomb lattice of Sn/Au(111) reconstruction** — •Dominik Jungkenn[1], Maniraj Mahalignam[1], Sebastian Emmerich[1], Lyu Lu[1], Jobinson Kollamana[1], Zheng Wei[1], Wujun Shi[2], Binghai Yan[2], Benjamin Stadtmüller[1], Mirko Cinchetti[3], Stefan Mathias[4], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern — [2]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund — [4]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Motivated by recent prediction of Stanene, a honeycomb structure of Sn atoms on a Au substrate [1], we investigated the structure formation of Sn on Au(111) using LEED and STM. In the sub monolayer regime, Sn forms a variety of ordered surface reconstructions depending on Sn coverage and post annealing temperature. One of the most stable structures is the (Sqrt3 x Sqrt3)R30° reconstruction which is characterized by a hexagonal super lattice. Angle resolved photoemission revealed a rich band structure with a Rashba type split band in the vicinity of the Gamma point, in agreement with band structure calculations based on density functional theory. Our results will be compared to the predicted fingerprints of stanene [1]. [1] S. Nigam, et al. Phys. Chem. Chem. Phys., 2015,17, 6705-6712

O 8.4 Mon 11:15 REC/PHY C213

**Electronic properties of single-layer antimony crystals from a tight-binding description: hopping integrals, spin-orbit coupling, and Coulomb interactions** — •Alexander Rudenko — Radboud University, Nijmegen, The Netherlands

Single-layer antimony (Sb) crystals have recently been produced using different methods, including mechanical [1] and liquid-phase [2] exfoliation. Excellent environmental stability and a moderate band gap (∼1.5 eV) make this material promising for electronic and optical applications. Here, we present an analytical tight-binding model for single-layer Sb, derived on the basis of relativistic first-principles calculations within the density functional theory. Significant corrections due to the strong ($\lambda = 0.34$ eV) intraatomic spin-orbit coupling are taken into account perturbatively. The model offers an efficient and accurate description of single-particle electronic states in a wide spectral region up to the mid-UV. The problem of the Coulomb interactions in 2D Sb is also addressed. We find that the screening effects originate predominantly from the $5p$ states, and thus fully captured by the proposed model. The results presented here provide an essential step toward the understanding and rational description of a variety of electronic properties of the novel 2D material.

[1] P. Ares *et al.*, Adv. Mater. **28**, 6332 (2016).
[2] C. Gibaja *et al.*, Angew. Chem. Int. Ed. **55**, 14345 (2016).

O 8.5 Mon 11:30 REC/PHY C213

**Realization of stanene on the surface of Au(111)** — •Mahalingam Maniraj[1], Benjamin Stadtmüller[1], Wujun Shi[2], Dominik Jungkenn[1], Sebastian Emmerich[1], Johannes Stöckl[1], Lu Lyu[1], Jobynson Kollamana[1], Zheng Wei[1], Anatol Jurenkow[1], Sebastian Jakobs[1], Yongli Gao[3], Mirko Cinchetti[4], Binghai Yan[2], Stefan Mathias[5], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — [4]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany — [5]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Stanene was recently predicted and has subsequently triggered intense research on Sn-based graphene-like 2D materials. Combining LEED, STM, spin- and angle-resolved photoemission (ARPES) and DFT calculation, we present clear evidence for the formation of a stanene-like superstructure on the surface of Au(111). Our ARPES results show the existence of Dirac-cone-like bands around the $\bar{\Gamma}$ point with an electron velocity of $1\times10^6$ m/s, which originates from the admixture of Sn $p$ and Au $d$ states. Spin-resolved ARPES measurements reveal a topological insulator-like spin texture. Our realization of a Stanene-like superstructure lays the foundation for the easy fabrication and investigation of stanene as a potential next generation 2D material.

O 8.6 Mon 11:45 REC/PHY C213

**Localized defect states in $MoS_2$ monolayers: Electronic and optical properties** — •Jens Kunstmann, Tsegabirhan B. Wendumu, and Gotthard Seifert — Theoretische Chemie, TU Dresden, Germany

Defects usually play an important role in tuning and modifying various properties of semiconducting or insulating materials. Here we study the impact of point and line defects on the electronic structure and optical properties of $MoS_2$ monolayers using density-functional methods. The different types of defects form electronic states that are strongly localized on the defect. The electronic structure of the monolayer system is quite robust and it is well preserved for point defect concentrations of up to 6%. The impact of point defects on the optical absorption for concentrations of 1% and below is found to be very

small. For higher defect concentrations, molybdenum vacancies were found to quench the overall absorption and sulfur defects lead to sharp absorption peaks below the absorption edge of the ideal monolayer. For line defects, we did not find a considerable impact on the absorption spectrum. These results support recent experiments on defective transition metal chalcogenides. [Kunstmann, Wendumu, Seifert, phys. stat. sol. (b) (2016), doi:10.1002/pssb.201600645]

O 8.7 Mon 12:00 REC/PHY C213

**Chemical and Electronial Repair of Defective $MoS_2$ Monolayers Through Thiols-** — •Anja Förster[1,2], Sibylle Gemming[3,4], Gotthard Seifert[2], and David Tománek[1] — [1]Physics and Astronomy Department, Michigan State Unversity, East Lansing, Michigan 48824, USA — [2]TU Dresden, Center for Advancing Electronics Dresden (cfaed), 01062 Dresden, Germany — [3]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden Rossendorf, Center for Advancing Electronics Dresden (cfaed), Bautzner Landstr. 400, 01328 Dresden, Germany — [4]Insitute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Molybdenum disulfide ($MoS_2$) monolayers are promising candidates for new low-power electronic circuits and sensors. In order to ensure their usability for mass-production, it is necessary to heal the defects that significantly affect the electronic properties of $MoS_2$.

For this purpose, we focus on two defect types: sulfur monovacancies and sulfur-adatoms. We show their effect on the density of states (DOS) of $MoS_2$ and show how thiols can be used to heal these defects.

In detail, the sulfur mono-vacancies introduce defective states near the Fermi-energy to the DOS of $MoS_2$. Thiols are able to cure those defective states by re-inserting the missing sulfur atoms.

In the case of sulfur adatoms, the Fermi-level of $MoS_2$ is shifted by 0.7 eV, bring the conducting band very close to ther Fermi-energy. Thiols are able to remove the sulfur adatoms by forming hydrogen sulfide and disulfides. The latter are adsorbed on the $MoS_2$ surface.

O 8.8 Mon 12:15 REC/PHY C213

**Ion-beam mediated patterning of MoS2 monolayers** — •Mahdi Ghorbani-Asl[1], Silvan Kretschmer[1], Douglas Spearot[2], and Arkady Krasheninnikov[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, Florida 32611, USA — [3]Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, 00076 Aalto, Finland

Using analytical potential molecular dynamics combined with first-principles calculations, we study the production of defects in free-standing MoS2 monolayers under ion irradiation for a wide range of ion energies when nuclear stopping dominates. The probabilities of defect production have been studied for various types of defects. We show that depending on the incident angle, ion type and energy, sulfur atoms can be sputtered away predominantly from the top or bottom layers, providing unique opportunities for ion-beam mediated patterning of MoS2. As an example, we study the stability and electronic properties of mixed MoSX compounds where X are chemical elements from group V or VII. We demonstrate that such systems can show metallic character (e.g. MoSF) and further be used to design metal/semiconductor/metal junctions, which exhibit negative differential resistance.

O 8.9 Mon 12:30 REC/PHY C213

**Van der Waals Epitaxy of Single Layer Transition Metal Dichalcogenides** — •Joshua Hall[1], Borna Pielić[2], Tobias Wekking[1], Marko Kralj[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicherstr. 77, D-50937 Köln — [2]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, HR-10000 Zagreb

We employ molecular beam epitaxy on van der Waals substrates to grow epitaxial mono- to bilayer samples of transition metal dichalcogenides (TMDC). The scalability of the method allows for subsequent investigations such as angle resolved photo emission spectroscopy.

As substrates for our two step synthesis of the TMDC we use in situ fabricated graphene or a monolayer of hexagonal boron nitride. In the first synthesis step, at temperatures in the range from 100 K to 400 K, we expose the substrate to a metal vapor in the background of a sulfur pressure. As signified by low energy electron diffraction, already after this step, the TMDC forms. We find that the ratio of metal to sulfur flux is crucial for the growth mode of the TMDC. As a second step, the sample is annealed in the range of 800 K to 1100 K in a sulfur background. Annealing decreases epitaxial orientation scatter and enlarges domain sizes. It is limited in time and temperature by the onset of TMDC decomposition and intercalation of the educts under the van der Waals substrate monolayer. Our scanning tunneling microscopy studies document the versatility of the two step synthesis by providing examples for excellent quality monolayers of $MoS_2$, $WS_2$, $TaS_2$ and $VS_2$.

O 8.10 Mon 12:45 REC/PHY C213

**Investigation of 2D hBN after ion irradiation** — •Lara Bröckers, Henry Bohnen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

Ion irradiation is a useful tool for the controlled modification of two-dimensional (2D) materials. Previous experiments have revealed characteristic, structural modification of graphene and other 2D materials created by swift heavy ion (SHI) irradiation [1,2]. We could show that the size of these modification, called foldings, vary depending on the irradiation parameters. Typically, the foldings are 50-80 nm in width and more than a micron in length, depending on the angle of incidence of the ions and on the substrate [3]. The main channel for energy deposition in solids by SHIs is the excitation of the target electrons. Therefore, a comparison between 2D materials with different electronic properties can help to reveal the physical mechanisms of defect creation. Comparing the folding of graphene (semiconductor) with the folding of hBN (insulator) we found significant differences. We determine the so-called efficiency, i.e. the number of ions needed to create one folding one average. For graphene this number equals one only for single layer graphene, otherwise it decreases rapidly down to zero with increasing number of layers. In the case of hBN however, also thicker layers are folded with a high efficiency. In addition, we have studied how the efficiency is influenced by the substrate.

[1] Akcöltekin S. et al. *Applied Physics Letters*, 98 (2011) 103103
[2] Ochedowski O. et al. *NimB*, 340 (2014) 39.
[3] Ochedowski O. et al. *Nanotechnology*, 26 (2015) 465302