O 19: 2D Materials Beyond Graphene II

Time: Monday 16:00–18:30 Location: REC/PHY C213

O 19.1 Mon 16:00 REC/PHY C213

2d Heterojunctions From Non-Local Manipulation of the Interactions: Single and Two-Particle Properties — •Christina Steinke[1,2], Daniel Mourad[1,2], Malte Rösner[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], Gerd Czycholl[1], and Tim Oliver Wehling[1,2] — [1]ITP, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]BCCMS, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

In modern optoelectronics heterojunctions are central building blocks of various applications, which commonly rely on interfaces of different materials. Here, we propose a novel scheme to induce heterojunctions within a single *homogeneous* layer of a two dimensional (2d) material based on Coulomb-interaction effects. Therefore we make use of the fact that in 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to spatially control the band gap by structured dielectric surroundings. We provide a proof of principle by combining a real-space tight-binding description with a many-body formalism for a model system emulating transitionmetal dichalcogenides. We find sizeable spatial band-gap modulations yielding type-II heterojunctions as needed for solar cells or quantum dots and present detailed insights into their excitation-induced two-particle properties. Utilizing the Bethe-Salpeter equation we show that Rydberg-like higher excitonic states can be strongly tuned by the dielectric surroundings. This effect may be used for efficient trapping of these excitonic states upon tailoring of the environment.

O 19.2 Mon 16:15 REC/PHY C213

Growth of Ge and Si on the monolayer silicene on Ag(111) — •Deng-Sung Lin and Han-De Chen — National Tsing Hua University, Hsinchu, Taiwan

Growth of Ge by molecular beam epitaxy on top of silicene monolayer on the Ag(111) surface results in either a dispersed adlayer or a two-dimensional ordered depending on the silicene phases. Scanning tunneling microscopy images show that the ordered adsorbed Ge atoms on the domains occupy directly on top of down-atoms in the buckled silicene layer.[1] By contrast, further growth Si on the silicene up to several MLs results in an atomic flat film with surface structure. We use low-temperature scanning tunneling microscopy to observe the chemical response of the film surface exposed to an atomic deuterium (D) beam. We find D displaces the Ag surfactant adatoms, resulting in a D-terminated (1x1) surface. The displaced Ag atoms migrate on the surface to form Ag(111) crystallites. The results confirm that the surfaces of the few-layer Si films grown on Ag(111) are Ag terminated and suggest that the films have a diamond-like structure [2].

[1]. Chen, H.-D.; Lin, D.-S., ACS Omega 2016, 1, 357-362. [2]. Chen, H.-D.; Chien, K.-H.; Lin, C.-Y.; Chiang, T.-C.; Lin, D.-S. J. Phys. Chem. C 2016, 120, 2698-2702.

O 19.3 Mon 16:30 REC/PHY C213

Direct observation of the conduction bands of single-layer WS_2 on Au(111) — •Philipp Eickholt[1], Marcel Holtmann[1], Charlotte Sanders[2], Philip Hofmann[2], and Markus Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

In the field of 2D materials, single-layer transition metal dichalogenides, especially MoS_2, WS_2, $MoSe_2$ and $WSe2_2$, are among the promising materials due to their exceptional optical and electronic properties [1]. The key to understanding these properties is a profound knowledge of the electronic structure. While there have been many studies of the occupied electronic structure, the crucial information about the dispersion and spin structure of the conduction bands is still missing. Spin- and angle-resolved inverse photoemission (SRIPE) [2] is the ideal technique to study dispersion and spin structure of the unoccupied electronic structure. In this talk we present a SRIPE study of the conduction bands of single-layer WS_2 grown [3] on Au(111).

[1] D. Xiao *et al.*, Phys. Rev. Lett. **108**, 196802 (2012)
[2] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. **85**, 013306 (2014)
[3] M. Dendzik *et al.*, Phys. Rev. B **92**, 245442 (2015)

O 19.4 Mon 16:45 REC/PHY C213

Study of the anisotropic electronic structure of $ReSe_2$ — •Ph. Eickholt[1], C. Langenkämper[1], K. Miyamoto[2], E.F. Schwier[2], J. Noky[3], M. Drüppel[3], P. Krüger[3], M. Rohlfing[3], and M. Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan — [3]Institute of Solid State Theory, University of Münster, Germany

Transition metal dichalcogenides (TMDCs) are heavily studied due to their fascinating optical and electronic properties and possible technical applications. $ReSe_2$ is a new material of the TMDC family. Unlike the well known MoS_2 it grows in a distorted 1T structure. Therefore it has unique anisotropic properties which can be useful in future applications [1]. To develop a fundamental understanding of the optical and electric properties we studied the occupied electronic structure of $ReSe_2$ with the help of angle-resolved photoemission (ARPES) and quasiparticle calculations.

[1] S. Yang *et al.* Nanoscale, **6**, 7226 (2014)

O 19.5 Mon 17:00 REC/PHY C213

Second-harmonic imaging microscopy: a powerful tool for time-resolved investigation of electron dynamics in TMDC heterostructures — •Jonas Zimmermann, Gerson Mette, and Ulrich Höfer — Philipps-Universität Marburg, Germany

Since the discovery of extraordinary luminescence of MoS2 monolayers, 2D transition metal dichalcogenides (TMDC) have been in the spotlight of the materials science community. In particular, heterostructures of different 2D materials attract attention due to their possible application in optoelectronics. As the efficiency of such devices is expected to depend strongly on the relative orientation of the individual layers, experimental techniques to characterize the electron transfer dynamics in dependence on the stacking angle are required.
Here, we present results of our new SHG imaging microscopy setup for time-resolved studies on interfaces of 2D materials. This technique allows us to quantify the crystal structure via polarization dependent measurements and gives us access to the electron dynamics via time-resolved pump-probe experiments. We demonstrate its capabilities with measurements performed on CVD grown WS2 and MoS2 monolayer flakes. The optical excitation tuned to 2.1 eV matches the energies of A- and B-exciton of WS2 and MoS2, respectively. Strong pump-induced features are observed and assigned to exciton generation. The excitonic lifetimes of the two materials correspond to values obtained in linear optical spectroscopy. The results reveal that SHG imaging microscopy is ideally suited to explore the effects of layer stacking on the charge transfer within 2D heterostructures.

O 19.6 Mon 17:15 REC/PHY C213

Electrostatically tuned 2D Heterostructures — •Christian Winkler, Shashank S. Harivyasi, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The family of two-dimensional (2D) materials has been growing rapidly since the discovery of graphene. This creates new scientific challenges as well as opportunities because the properties of layered, van der Waals bonded systems are often different from their 3D counterparts, which offers entirely new strategies for band-structure engineering.

In this work, using first principles approaches, we propose a novel strategy for engineering the level alignment in van der Waals heterostructures. In particular, we focus on the inclusion of self-assembling polar molecules (e.g. Titanyl phthalocyanine) into stacks consisting of 2D transition metal dichalcogenides (TMDCs) sheets (MoX_2 and WX_2, where X = S or Se). For structures of the type TMDC/TiOPc/TMDC we observe a shift in the frontier levels of successive TMDC layers by as much as 0.4 eV. Remarkably, for WSe_2/TiOPc/MoS_2 this allows switching between type I and type II alignment. Using multiple TiOPc layers even quantum cascades can be realized.

Beyond that, we aim to explore the interplay between strain applied to the individual layers (which is known to induce direct to indirect gap transitions) and the electrostatic design approach.

O 19.7 Mon 17:30 REC/PHY C213

Structure determination of silicene nanoribbons on Ag(110)

— •Philipp Espeter[1,2], Christoph Keutner[1,2], Nils Fabian Kleimeier[3], Peter Roese[1,2], Karim Shamout[1,2], Gabi Wenzel[3], Ulf Berges[1,2], Helmut Zacharias[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, D-44227 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [3]Physikalisches Institut - WWU Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster

Since the discovery of graphene much interest came up in graphene analoga from the carbon group. One of the most famous representatives is silicene. Silicene is known to crystallize in different configurations depending on the substrate, such as sheet growth on Ag(111) and nanoribbons on Ag(110). Whereas the structure of silicene sheets is already well known, the structure of silicene nanoribbons remains unclear.

In this study, we demonstrate a structure investigation of silicene nanoribbons on a Ag(110) substrate by means of photoelectron spectroscopy (XPS) and diffraction (XPD). These measurements provide chemical as well as structural information of silicene nanoribbons.

We assess several structure models suggested in literature, ranging from rectangular over pentagonal to hexagonal and from planar over buckled to stacked structures. We will also present a structure model which perfectly fits to the XPD and XPS data.

O 19.8 Mon 17:45 REC/PHY C213

Angle-resolved IPE Study of Silicene Nanoribbons on Ag(110) — •Gabi Wenzel, Nils Fabian Kleimeier, and Helmut Zacharias — Physikalisches Institut - WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Silicene, a two-dimensional buckled honeycomb lattice of silicon atoms, has attracted great interest in the scientific community. To investigate its electronic properties, unoccupied electronic states of silicene nanoribbons grown on Ag(110) were measured by $\vec{k}$-resolved inverse photoemission spectroscopy (KRIPES) in ultra-high vacuum conditions. The IPE setup consisted of a modified Erdmann-Zipf electron gun and an acetone filled Geiger-Müller tube with a CaF_2 window acting as a bandpass filter.

The measurements in $\overline{\Gamma X}$ direction show two main features: one almost linearly dispersing state from 3.2 eV at $\overline{\Gamma}$ to 6.2 eV at $\overline{X}$, the other depicting a linear continuation of the Dirac cone like feature around the $\overline{X}$ point from 0 eV to 5.8 eV.

O 19.9 Mon 18:00 REC/PHY C213

SPM study of atomically thin MoS_2 grown on HOPG via chemical vapor deposition — •Erik Pollmann and Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

Van der Waals heterostructures are material systems based on combinations of different 2D materials such as graphene, hBN and MoS_2 to mix their properties or even create new ones. Monolayers of MoS_2 on HOPG could be used as a model system for the MoS_2-graphene interface and has been studied e.g. by Koós et al. [1].

The aim of our work is to understand the growth mechanism of MoS_2 on this graphene-like surface in order to exploit this knowledge to grow MoS_2 directly on graphene itself. Therefor MoS_2 flakes are grown by chemical vapor deposition and investigated by different Scanning Probe Microscopy techniques. It will be shown, that MoS_2 is more likely to grow at HOPG edges. These one-dimensional defects act as the growth seeds. This would constitute a serious disadvantage for the direct growth on graphene where no step edges are present. Therefore, we investigated if point defects can act as growth seeds as well. To this end, an HOPG crystal was irradiated by highly charged ions to induce quasi zero-dimensional defects [2] before the chemical vapor deposition of MoS_2. The first results obtained from these experiments will be presented.

[1] A. A. Koós et al. *Carbon* **105**, 408-415 (2016)
[2] J. Hopster et al. *2D Materials* **1**, 1011011 (2014)

O 19.10 Mon 18:15 REC/PHY C213

Probing the Bandstructure of MoS_2 on Au(111) using Scanning Tunneling Spectroscopy — •Nils Krane, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Berlin, Germany

Transition metal dichalcogenides (TMCD) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide is especially interesting, since it provides a direct band gap [1] and a strong spin-splitting of the valence band at the K-point.

Here we grow MoS_2 epitaxially on a Au(111) surface as described in [2] and investigate it with a combined STM/AFM at low temperatures. Since STS measures the projected LDOS without information of the parallel momentum $k_\parallel$ in the Brillouin-Zone, it is not possible to assign a band gap to the K- or Γ-point. To get an insight into the band structure of MoS_2, we measure the decay length κ of the tunneling current, which depends on $k_\parallel$ [3]. We find a strong spatial dependence of κ. We ascribe this to the Moiré reconstruction of MoS_2 on Au(111), which differs between fcp- and hcp-stacking at the hollow sides. Furthermore, we investigate the band structure of quasi free-standing MoS_2.

[1] Mak, *et al.*, PRL 105, 136805 (2010)
[2] Sorensen, *et al.*, ACS Nano 8, 6788-6796 (2014)
[3] Zhang, *et al.*, ACS Nano 15, 6494-6500 (2015)