TT 80: 2D Materials Beyond Graphene: TMDCs, Silicene and Relatives (organized by O)

Time: Wednesday 15:00–17:45 Location: MA 005

TT 80.1 Wed 15:00 MA 005

Imaging spin-valley-layer locking in a transition-metal dichalcogenide — J.-M. Riley[1], F. Mazzola[2], M. Dendzik[3], M. Michiardi[3], T. Takayama[4], L. Bawden[1], C. Granerød[2], M. Leandersson[5], T. Balasubramanian[5], M. Hoesch[6], T. Kim[6], H. Takagi[4], W. Meevasana[7], Ph. Hofmann[3], M.-S. Bahramy[8], J.-W. Wells[2], and •Phil D.C. King[1] — [1]SUPA, University of St. Andrews, UK — [2]Norwegian University of Science and Technology, Norway — [3]Aarhus University, Denmark — [4]Max Planck Institute for Solid State Research, Germany — [5]MAX IV Laboratory, Sweden — [6]Diamond Light Source, UK — [7]Suranaree University of Technology, Thailand — [8]University of Tokyo, Japan

A strong locking between the spin and the valley pseudospin in monolayer transition-metal dichalcogenides (TMDCs) such as MoS_2 and WSe_2 opens unique potential for their use in novel quantum devices exploiting the valley degree of freedom. Here, using spin- and angle-resolved photoemission spectroscopy, we show that such spin-valley coupling persists in bulk 2H-WSe_2 where it becomes further entangled with the layer pseudospin [1]. Enormous spin splittings up to $\sim$0.5 eV result, despite the centrosymmetric nature of the bulk structure which would conventionally preclude the presence of spin polarised states. We argue these occur here due to local inversion symmetry breaking within constituent sub-units of the bulk unit cell, leading to a spin texture that is strongly modulated in both real and momentum space, and allowing us to directly image TMDC spin-valley-layer locking for the first time. [1] Riley *et al.*, Nature Phys. **10** (2014) 835.

TT 80.2 Wed 15:15 MA 005

From optics to superconductivity: Many body effects in transition metal dichalcogenides — Malte Rösner[1,2], Gunnar Schönhoff[1,2], Alexander Steinhoff[1], Frank Jahnke[1], Christopher Gies[1], Stephan Haas[3], and •Tim Wehling[1,2] — [1]Institute for Theoretical Physics, University of Bremen, D-28359 Bremen, Germany — [2]Bremen Center for Computational Material Sciences, University of Bremen, D-28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

We discuss many body effects in MoS_2 ranging from optical properties to the emergence superconductivity (SC) and charge density wave phases (CDW). Combining ab-initio theory and semiconductor Bloch equations we show that excited carriers cause a redshift of the excitonic ground-state absorption line, while higher excitonic lines disappear successively due to a huge Coulomb-induced band gap shrinkage of more than 500 meV and concomitant exciton binding-energy reductions. Upon strong charge doping, we observe a succession of semiconducting, metallic, SC, and CDW regimes. Both, the SC and the CDW instabilities trace back to a Kohn anomaly and related softening of Brillouin zone boundary phonons.

Invited Talk TT 80.3 Wed 15:30 MA 005

2D silcon materials: From single layer silicene to double-layer structures and multi-layer stacks — •Patrick Vogt — Institut für Festkörperphysik,Technische Universität Berlin, Deutschland

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene [1]. Additionally, silicene might have a potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications. However, silicene does not exist in nature and had to be synthesized on a substrate material [2].

We will describe the recent development on the epitaxial formation of single layer silicene on Ag(111), including structural and electronic properties. Based on these results we will look at the growth of silicene double-layer and multi-layer structures and discuss if they can be explained by the stacking of single silicene sheets [3]. If confirmed, such multi-layer structures could open the way towards the technological applicability of silicene.

[1] G.G. Guzmán-Verri, L.C. Lew Yan Voon, Phys. Rev. B 76, 075131 (2007); S. Lebègue and O. Eriksson, Phys. Rev. B, 79 115409 (2009); S. Cahangirov et al., Phys. Rev. Lett. 102, 236804 (2009).

[2] P. Vogt et al., Phys. Rev. Lett. 108, 55501 (2012); C.-L. Lin et al., Appl. Phys. Exp. 5, 045802 (2012); B. Feng et al., Nano Lett. 11, 3507 (2012); A. Fleurence et al., Phys. Rev. Lett. 108, 245501 (2012).

[3] P. Vogt et al., Appl. Phys. Lett. 104, 021602(2014), De Padova et al., Appl. Phys. Lett. 102, 163106 (2013)

TT 80.4 Wed 16:00 MA 005

The electronic band structure of MoS_2 investigated by ARPES — •Mathias Gehlmann[1], Sven Döring[1], Markus Eschbach[1], Ewa Młynczak[1], Irene Aguilera[2], Gustav Bihlmayer[2], Stefan Blügel[2], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]PGI-6, FZ-Jülich — [2]PGI-1/IAS-1, FZ-Jülich

MoS_2 belongs to transition metal dichalcogenides and has drawn a large amount of attention in recent years. While the main area of interest in this material lies in the possibility of integrating it into two dimensional semiconductors and transistor devices, a growing number of researchers focuses on the valley polarization at the edge of the Brillouin zone.

We combine angle-resolved photoemission spectroscopy (ARPES) with density functional theory calculations to perform a thorough analysis of the valence band electronic structure of MoS_2. Our focus lies on the splitting of the valence band around the K point at the edge of the Brilluin zone, and on the comparison of the electronic states of the bulk material and its surface to a free standing monolayer.

TT 80.5 Wed 16:15 MA 005

Photocurrent studies on semiconducting MoS_2 — •Anna Vernickel[1,2], Marina Hoheneder[1,2], Eric Parzinger[1,2], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany

Atomically thin molybdenum disulfide (MoS_2) has gained increasing interest as very promising material for novel and innovative device applications. Its bandgap in the visible range and the transition to a direct semiconductor in the single-layer case make MoS_2 particularly suitable for optoelectronic devices. We report on extensive photocurrent spectroscopy studies of single and few-layer MoS_2 in order to investigate their optoelectronic properties. We discuss the impact of Schottky contacts and thermoelectric contributions to the observed photocurrent. To further investigate the underlying photocurrent dynamics, nanoscale electronic circuits facilitating access to the photocurrent evolution on a picosecond time scale are prepared. We gratefully acknowledge financial support by NIM and BaCaTec.

TT 80.6 Wed 16:30 MA 005

Hot electron dynamics at $2H$-MoS_2 surfaces: Time- and angle-resolved photoelectron spectroscopy results — •Petra Hein, Ankatrin Stange, Kerstin Hanff, Gerald Rohde, Michael Bauer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, Germany

Recent research on the layered semiconductor $2H$-MoS_2 has been concentrated on MoS_2 monolayers: In contrast to the bulk crystal, MoS_2 monolayers are direct bandgap semiconductors without an inversion center, making them an appropriate material for valleytronic devices with hot carrier lifetimes in the picosecond regime. However, $2H$-MoS_2 surfaces could be equally exciting: Due to the symmetry breaking at the surface or a decoupling of the topmost sandwich, similarities to monolayers seem possible. For an investigation of this system, time- and angle-resolved photoelectron spectroscopy is the method of choice, as it provides high surface sensitivity and momentum resolution, while enabling us to map electronic processes on their fundamental time scales. Here, we present a $\vec{k}$-resolved study of the transient photoelectron intensity in the conduction band after excitation of $2H$-MoS_2 surfaces with 3.2 eV pump pulses. Momentum-dependent intensity rise times between 30 fs and 150 fs and decay times of several 100 fs allow us to identify direct electronic excitations and to track the electrons' relaxation pathway into the lowest energy states. The conduction band minima are finally depopulated within $\sim$1 ps. Possible explanations for this observation – such as diffusion processes, optical electron-hole recombination and trapping in defect states – are discussed.

TT 80.7 Wed 16:45 MA 005

Charge carrier trapping and electron-phonon coupling in MoS_2 revealed by μ-Raman spectroscopy — Bastian Miller[1,2], Eric Parzinger[1,2], Alexander Holleitner[1,2], and •Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany

Two-dimensional layered van-der Waals materials are of increasing interest for fundamental research as well as device applications in the areas of electronics, spin- and valleytronics, optoelectronics, and sensing. We utilize power and gate voltage dependent non-resonant and resonant μ-Raman spectroscopy on dual-gate field-effect transistor devices to study doping effects, e-ph coupling and the impact of trap states in mono-, bi- and few layer MoS_2. In non-resonant Raman measurements we observe a strong power- and gate voltage dependence of zone-center Raman modes with contrasting behavior for mono- and bilayer MoS_2. Under resonant excitation, a rich scattering spectra with signatures of multistep scattering processes are observable pointing towards contribution from phonon-phonon and electron-phonon interaction. The origin of the different modes, their dependence on the exciting light energy and evolution with number of layers will be discussed. We acknowledge the financial support by the DFG excellence cluster Nanosystems Initiative Munich (NIM).

TT 80.8 Wed 17:00 MA 005

Newly observed first-order resonant Raman modes in few-layer molybdenum disulfide — •Nils Scheuschner, Roland Gillen, Matthias Staiger, and Janina Maultzsch — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin

We show measurements of two newly observed first-order Raman modes in few-layer MoS_2 with phonon energies of 286 cm^{-1} and 471 cm^{-1}. These modes are strongly resonant and appear only when using excitation energies above $\approx$ 2.4 eV. At 2.7 eV, their intensity is comparable to the second-order Raman modes; their absence thus provides an easy and accurate method to identify single-layer MoS_2. At UV excitation, the intensity of the new modes is even larger than the typically examined A_1'/A_{1g} and E'/E_g modes. We provide a systematic analysis of the phonon modes, their symmetries, and their frequencies in few-layer materials, including the newly observed modes.

TT 80.9 Wed 17:15 MA 005

Near-field microscopy and nano-FTIR spectroscopy on monolayer MoS2 grown on periodically poled LiNbO3 — •Georg Ulrich[1], Piotr Patoka[1], Peter Hermann[2], Bernd Kästner[2], Ariana Nguyen[3], Tom Scott[4], Arne Hoehl[2], Ludwig Bartels[3], Peter Dowben[4], Gerhard Ulm[2], and Eckart Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587 Berlin, Germany — [3]Department of Chemistry, U California Riverside, Riverside, CA 92521, USA — [4]Department of Physics and Astronomy, U Nebraska, Lincoln, NE 68588-0299 USA

Coupling of synchrotron radiation from the Metrology Light Source to a scanning near-field optical microscope (SNOM) has emerged as a possibility for highly sensitive spectroscopic investigations in the mid-infrared regime [1]. It also allows the simultaneous collection of topographic information and optical response from the samples with a spatial resolution below 30 nm. Here we will present the results of nano-FTIR spectroscopy and near-field imaging of monolayer MoS2 islands on a periodically poled lithium niobate (PPLN) sample using synchrotron radiation in the infrared regime and tunable CO2 laser radiation, respectively. The results show the influence of the ferroelectric polarization of the PPLN structure on the MoS2 semiconductor which enhances the surface polarization of the ferroelectric domains only in one direction. [1] P. Hermann et al., Opt. Express 22, 17948 (2014)

TT 80.10 Wed 17:30 MA 005

Growth and Characterization of Epitaxial Single-Layer MoS_2 on Au(111) — •Jill Miwa, Søren Ulstrup, Signe Sørensen, Maciej Dendzik, Antonija Grubišić Čabo, Marco Bianchi, Jeppe Vang Lauritsen, and Philip Hofmann — Dept. of Physics & Astronomy, Aarhus University, Aarhus, Denmark

We present a method for synthesizing epitaxial single-layer MoS_2 on the (111) face of Au. Using scanning tunnelling microscopy (STM) and low energy electron diffraction, the evolution of the growth is followed from nanoscale single-layer MoS_2 islands to a robust high quality epitaxial MoS_2 layer that is stable in air. We investigate the electronic structure of epitaxial single layer MoS_2 by angle resolved photoemission spectroscopy. Pristine and potassium-doped layers are studied in order to gain access to the conduction band. The potassium-doped layer is found to have a (1.39$\pm$0.05) eV direct band gap at $\bar{K}$ with the valence band top at $\bar{\Gamma}$ having a significantly higher binding energy than at $\bar{K}$. A pronounced moiré superstructure of the epitaxial system observed in STM does not lead to the presence of observable replica bands or minigaps. The degeneracy of the upper valence band at $\bar{K}$ is found to be lifted by the spin-orbit interaction, leading to a splitting of (145$\pm$4) meV. Finally, it is shown that the potassium doping does not only lead to a rigid shift of the band structure but also to a distortion, giving rise to the possibility of band structure engineering in single-layers of transition metal dichalcogenides.