# O 99: 2D materials beyond graphene: TMDCs, silicene and relatives IV

Time: Thursday 15:00–17:45 Location: MA 043

O 99.1 Thu 15:00 MA 043

**Ultrafast Dynamics of Single Layer $TaS_2$** — •Federico Andreatta[1], Antonija G. Čabo[1], Deepnarayan Biswas[2], Charlotte E. Sanders[1], Marco Bianchi[1], Cephise Cacho[3], Alfred Jones[3], Richard T. Chapman[3], Emma Springate[3], Phil D. C. King[2], Jill A. Miwa[1], Søren Ulstrup[1], and Philip Hofmann[1] — [1]Aarhus University, DK — [2]University of St. Andrews, UK — [3]CLF, STFC Rutherford Appleton Laboratory, UK

Metallic transition metal dichalocogenides, synthesized on single crystal metal substrates, have been recently explored down to the single layer limit[1,2]. Here, we synthesize metallic single layer tantalum disulphide ($TaS_2$) on graphene on silicon carbide to create a model two-dimensional van der Waals heterostructure. Not only do we probe the static electronic properties of the single layer $TaS_2$ but also the nonequilibrium carrier dynamics by means of time-and-angle resolved photoemission spectroscopy[3]. We present a novel way to fit the spectral function of the band dispersion at the Fermi level so that the band renormalization is tracked on a femtosecond time-scale.

[1] M. Dendzik, et al. Physical Review B, 92(24), 2015. [2] C. E. Sanders, et al. Physical Review B, 94(8), 2016. [3] S. Ulstrup, et al. ACS Nano, 10(6):6315-6322, 2016.

O 99.2 Thu 15:15 MA 043

**Realistic Description of Competing Interactions in Metallic TMDCs** — Ebad Kamil[1], Gunnar Schönhoff[1], Malte Rösner[1,2], •Jan Berges[1], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany — [2]Department of Physics and Astronomy, University of Southern California, Los Angeles, USA

Two-dimensional transition metal dichalcogenides constitute a prominent showplace for competing many-body instabilities such as superconductivity [Frindt: PRL **28**, 299 (1972)], charge-density waves [Ugeda *et al.*: Nat. Phys. **12**, 92 (2016)] and magnetism [Ma *et al.*: ACS Nano **6**, 1695 (2012)]. In this study, we show that even though the observed phase diagrams are complex, the underlying mechanisms are captured by a compact unifying theoretical framework. We apply the constrained random-phase approximation (cRPA) [Aryasetiawan *et al.*: PRB **74**, 125106 (2006)] and constrained density-functional perturbation theory (cDFPT) [Nomura, Arita: PRB **92**, 245108 (2015)] to the metallic monolayers $H$-$MX_2$ with $M \in \{\mathrm{V}, \mathrm{Nb}, \mathrm{Ta}\}$ and $X \in \{\mathrm{S}, \mathrm{Se}\}$ and summarize the material specifics with a small number of representative Coulomb and electron-phonon interaction parameters. Both cRPA and cDFPT imply a separation of the electrons into a correlated subspace, here an isolated metallic band, and the rest. We find that all relevant physics emerge from interactions within this subspace. Beyond that, the materials can be well described by very similar tight-binding and mass-spring models.

O 99.3 Thu 15:30 MA 043

**Direct determination of monolayer MoS2 and WSe2 exciton binding energies on insulating and metallic substrates** — •Soohyung Park[1,2], Niklas Mutz[1], Thorsten Schultz[1], Ali Han[3,4], Areej Areej[3,4], Lain-Jong Li[3,4], Emil J. W. List-Kratochvil[1], Patrick Amsalem[1], and Norbert Koch[1,2] — [1]Humboldt-Universität, Berlin, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [3]Research Center for Applied Sciences, Taipei, Taiwan — [4]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Two-dimensional transition-metal dichalcogenides (2D TMDCs) are attractive candidates for next-generation optoelectronic devices due to their unique electronic and optical properties. To employ 2D TMDCs in optoelectronic devices, understanding the fundamental physical properties is necessary. In this regard, one key parameter is the exciton binding energy. It is the energy difference between the lowest-energy optical absorption (optical gap) and the charge transport energy gap (transport gap). In this contribution, we will present an experimental study combining angle-resolved direct and inverse photoelectron spectroscopy in order to measure the transport gap, and reflectance measurements for a determination of the optical gap. In this manner we are able to determine the exciton binding energy for two common 2D TMDCs, MoS2 and WSe2, on insulator and metal substrates. In addition, we will show that the dielectric environment of 2D TMDCs strongly impacts the transport gap while the optical gap is barely affected, indicating large exciton binding energy change.

O 99.4 Thu 15:45 MA 043

**One-dimensional states confined within mirror twin boundaries in $MoS_2$** — •Wouter Jolie[1,2], Clifford Murray[1], Philipp Weiss[3], Joshua Hall[1], Fabian Portner[3], Nicolae Atodiresei[4], Arkady Krasheninnikov[5], Hannu-Pekka Komsa[6], Achim Rosch[3], Carsten Busse[1,2,7], and Thomas Michely[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Institute for Theoretical Physics, University of Cologne, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [6]Department of Applied Physics, Aalto University, Finland — [7]Department Physik, Universität Siegen, Germany

We investigate epitaxial, single-layer $MoS_2$ on graphene on Ir(111) with scanning tunneling microscopy and spectroscopy (STM/STS). We find a large bandgap of $2.50 \pm 0.05$ eV in $MoS_2$ showing that it is well decoupled from the substrate. The $MoS_2$ islands feature two types of long, straight, highly symmetric mirror twin boundaries. Along these we measure a small bandgap of the order of 0.1 eV, together with periodic beatings in the local density of states. Using ab initio calculations, these features are traced back to one-dimensional metallic twin boundary states. We will critically discuss the contributions of confinement (finite wire length), Peierls instability (charge density wave formation) and spin-charge separation to explain the observed features.

O 99.5 Thu 16:00 MA 043

**Coupling mechanisms of transition metal dichalcogenides to plasmonic gold nanoparticle arrays** — •Jonas Kiemle[1,2], Sandra Diefenbach[1,2], Sebastian Funke[3], Peter Thiesen[3], Ursula Wurstbauer[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany — [3]Accurion GmbH, Stresemannstr. 30, 87079 Göttingen, Germany

We reveal the manifold interaction mechanisms between monolayers of $MoS_2$ and single layers of plasmon-active gold nanoparticles. The $MoS_2$ shows a ten- to twenty-fold enhanced photoluminescence when it is decorated with the gold nanoparticles. Surprisingly, we detect this enhancement also for excitation energies, which are not resonant to the surface plasmon polaritons of the nanoparticles. Complementary Kelvin probe force measurements indicate a lowering of the work function, when the $MoS_2$ is decorated with the gold nanoparticles. This is in agreement with a reduced band gap for the decorated $MoS_2$ as determined from absorbance measurements. We furthermore demonstrate a dielectric coupling between the two layers by spectroscopic imaging ellipsometry as well as Raman spectroscopy. Combining the various results, we discuss the enhanced photoluminescence in terms of a modified emission pattern of the radiative dipole in the $MoS_2$ monolayers at the presence of the gold nanoparticles.

O 99.6 Thu 16:15 MA 043

**Electronic characterization of the coexisting charge density wave and superconductivity in single-layer NbSe2 at T = 1 K** — •Carmen Rubio-Verdú[1], Deung-Jang Choi[1], Hyejin Ryu[2], Sung-Kwan Mo[2], Zhi-Xun Shen[3,4], José Ignacio Pascual[1,5], and Miguel M. Ugeda[1,5] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [3]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California, USA — [4]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, California, USA — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Single-layer NbSe2 has been studied by means of low-temperature STM/STS. Our STS measurements reveal the coexistence of CDW order and 2D superconductivity at T = 1 K. We spatially mapped the conductivity of the NbSe2 layer at T = 1 K with atomic resolution to

reveal strong oscillations of the depth and width of the superconducting gap with well-defined wavelength of 7 Å, coincident with that of the quasiparticle interference (QPI) patterns visible at the Fermi energy. This phenomenon is accompanied by intriguing spatial dynamics of the QPI patterns for energies within the SC gap.

**15 min. break**

O 99.7 Thu 16:45 MA 043

**Characterization of Collective Ground States in Single-layer NbSe2** — •Miguel M. Ugeda[1,2,3], Aaron J. Bradley[1], Yi Zhang[4], Seita Onishi[1], Claudia Ojeda-Aristizabal[1], Hyejin Ryu[4], Alexander Riss[1], Sung-Kwan Mo[4], Dunghai Lee[1], Alex Zettl[1,5], Zahid Hussain[4], Zhi-Xun Shen[6,7], and Michael F. Crommie[1,5] — [1]Department of Physics, University of California at Berkeley, Berkeley, California, USA. — [2]CIC nanoGUNE, Donostia-San Sebastian, Spain. — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain. — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA. — [5]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA. — [6]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California, USA. — [7]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, California, USA.

In bulk NbSe2 a CDW sets in at 33K and superconductivity at 7.2K and their microscopic formation mechanisms remain controversial. In this talk I will present the electronic characterization of a single layer of NbSe2 by means of STM/STS, ARPES, and transport measurements (1,2). I will show that 3x3 CDW order in NbSe2 remains intact in 2D. Superconductivity also still remains in 2D, but its onset temperature is depressed to 1.9K. Our STS measurements reveal a CDW gap of 4 meV at EF, which is accessible due to the removal of bands crossing EF for a monolayer. [1] Ugeda, Nature Physics 12, 92 (2016). [2]Onishi, PSS B 253, 2396 (2016).

O 99.8 Thu 17:00 MA 043

**Electronic structure of single layer 1T-$NbSe_2$: interplay of lattice distortions, non-local exchange and Mott Hubbard correlations** — •Ebad Kamil, Jan Berges, Gunnar Schönhoff, Malte Schüler, and Tim Wehling — Institut für Theoretische Physik, Universität Bremen, Bremen, Germany.

Transition metal dichalcogenides (TMDCs) often occur in two different crystal phases with octahedral (1T) and trigonal prismatic (2H) symmetry. For $NbSe_2$, the 2H phase has been known to be the most stable and easier to synthesize polymorph. However, recently 1T-$NbSe_2$ in the monolayer limit was synthesized epitaxially on a bilayer graphene and was suggested to be a Mott insulator [Yuki Nakata et al. NPG Asia Materials (2016) 8, e321] with $\sqrt{13} \times \sqrt{13}$ periodic density modulation. We perform ab-initio calculations to understand the emergence of an insulating behavior and charge density wave (CDW) in the monolayer 1T-$NbSe_2$, which otherwise is predicted to be a metal in DFT and GW calculations. We provide an estimate for the local and non-local screened Coulomb interaction within the ab-initio formalism and present the findings of LDA+DMFT simulations that suggest the possibility of opening of a Mott insulating gap in the CDW phase.

O 99.9 Thu 17:15 MA 043

**Two-photon photoemission spectroscopy of the Dirac cone of a stanene-like Sn/Au(111) surface reconstruction** — •M. Düvel[1], M. Maniraj[2], B. Stadtmüller[2,3], D. Jungkenn[2], M. Keunecke[1], S. Emmerich[2,3], D. Schmitt[1], W. Shi[4,5], L. Lyu[2], J. Stöckl[2], J. Kollamana[2], Z. Wei[2], A. Jurenkow[2], S. Jakobs[2], B. Yan[4], D. Steil[1], S. Steil[1], M. Cinchetti[6], M. Aeschlimann[2], and S. Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [3]Graduate School of Excellence Materials Science in Mainz — [4]MPI for Chemical Physics of Solids — [5]School of Physical Science and Technology, ShanghaiTech University — [6]Experimentelle Physik VI, Technische Universität Dortmund

Stanene, the graphene analog of Sn, was recently predicted and has subsequently motivated intense research on the realization of Sn-based ultrathin materials. Using photoelectron spectroscopy, we recently found a superstructure of Sn on Au(111) that reveals a Dirac-like band centered at the Γ-point with anti-parallel spin polarization and a Fermi velocity of $v_F \approx 1 \cdot 10^6$ m/s [Maniraj et al., submitted (2017)]. Using angle-resolved two-photon photoemission spectroscopy, we now access the unoccupied part of the electronic structure of this stanene-like reconstruction. We are able to map the dispersion of the unoccupied part of the surface states and therewith confirm their massless Dirac-like nature. Moreover, we find a series of image potential states, which we analyze in order to determine the interfacial coupling between the stanene-like layer and the Au substrate.

O 99.10 Thu 17:30 MA 043

**First-principles calculations on the electronic, magnetic, and optical properties of $NiPS_3$** — •Tae Yun Kim and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

Magnetic van der Waals layered materials of transition metal phosphorous trichalcogednides ($TMPX_3$) have attracted attention as candidates that can support two-dimensional magnetism [1]. Because of the presence of localized d electrons of transition metals, it is natural to expect that $TMPX_3$ compounds may show some interesting phenomena arising from correlation effects. A recent experimental study revealed that the magnetic structure significantly affects the optical properties of $NiPS_3$, one of $TMPX_3$ compounds that exhibits antiferromagnetic phase below the Neel temperature at 154 K [2]. In this contribution, we discuss the electronic, magnetic, and optical properties of $NiPS_3$ in light of the experimental results based on our first-principles calculations.

[1] J. Park, J. Phys. Condens. Matter 28, 301001 (2016). [2] S. Y. Kim, T. Y. Kim, L. J. Sandilands, S. Sinn, M.-C. Lee, J. Son, S. Lee, K.-Y. Choi, W. Kim, B.-G. Park, C. Jeon, H.-D. Kim, C.-H. Park, J.-G. Park, S. J. Moon, T. W. Noh, arXiv:1706.06259 (2017).