# DS 35: 2D Materials Beyond Graphene IV (jointly with O)

Time: Wednesday 15:00–17:45 Location: WIL A317

**Invited Talk** DS 35.1 Wed 15:00 WIL A317

**Carbon Nanomembranes (CNM) : 2D Materials Beyond Graphene** — •Armin Gölzhäuser — Universität Bielefeld, Physik Supramolekularer Systeme und Oberflächen, Universitätsstr. 25, 33615 Bielefeld

Carbon Nanomembranes (CNMs) are thin (~1nm), synthetic two-dimensional (2D) layers or sheets with tailored physical, chemical or biological function [1]. Their fabrication scheme utilizes a sequence of molecular monolayer assembly on a solid surface and radiation induced cross-linking in two dimensions. The cross-linked 2D-layer is then released from the surface, forming a self-supporting nanomembrane with properties that are determined by properties of the monolayer. Depending on the desired applications, CNMs can be engineered with a controlled thickness, elasticity and surface functionalization. Helium ion microscopy, spectroscopic methods and functional tests are applied to investigate the structure and composition as well as permeation properties. Helium Ion Lithography is used the fabrication of well-defined nanopores [2] and perforated CNMs are tested as ballistic membranes for the separation of gases and liquids.

[1] A. Turchanin and A. Gölzhäuser: Carbon Nanomembranes, Adv. Mater. 28, 6075 (2016).

[2] D. Emmrich, A. Beyer, A. Nadzeyka, S. Bauerdick, J. C. Meyer, J. Kotakoski and A. Gölzhäuser: Nanopore fabrication and characterization by helium ion microscopy, Applied Physics Letters 108, 16310 (2016).

DS 35.2 Wed 15:30 WIL A317

**A hybrid MoS2 material for nanopore sensing: interface and asymmetry** — Ganesh Sivaraman[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3,4], Wanderla L. Scopel[2], Ralph H. Scheicher[3], and •Maria Fyta[1] — [1]Institute for Computational Physics, Stuttgart University — [2]Departamento de Fisica, Universidade Federal do Espirito Santo, Brazil — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden — [4]Departamento de Física, Universidade Federal Fluminense, Brazil

An important class of 2D nanomaterials beyond graphene is the family of transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS2). In MoS2 a semiconducting (2H) and a metallic (1T) phase can co-exist. We investigate the electronic and transport properties of a hybrid MoS2 monolayer composed by a 1T strip embedded in the 2H MoS2 phase. Using density functional theory based calculations with the non-equilibrium Greens functions (NEGF) approach, we study in detail the structural and electronic properties of hybrid MoS2 and its interface. A clear anisotropy in the electronic and transmission properties of the hybrid material was found and linked to the microstructure of its interfaces. We also show the relevance of such a material to sensing DNA with MoS2 nanopores. In order to understand the formation of this nanopore, a single point-defect analysis is performed also assessing the stability of the hybrid system and the different pore terminations. The current modulation around a nanopore when placing DNA in the pore manifests the strong potential of hybrid MoS2 in next generation biosensing devices.

DS 35.3 Wed 15:45 WIL A317

**Semiconductor to Metal Transition in $WS_2$/Ag(111)** — •Charlotte E. Sanders[1], Maciej Dendzik[1], Albert Bruix[1], Matteo Michiardi[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Bjørk Hammer[1], Jill A. Miwa[1], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics and Astronomy, University of British Columbia, Canada

Substrate effects play an important role in determining electronic structure in two-dimensional materials (2DMATs). A common effect of a metallic substrate on a semiconducting 2DMAT is renormalization of the band gap, induced by metallic screening, as recently observed in $MoS_2$/Au(111) [1]. Here we report a substrate effect that goes beyond band gap change due to screening. For $WS_2$/Ag(111), hybridization between electronic states of Ag and $WS_2$ leads to a non-zero density of states at the Fermi level (FL), and thus to a transition of $WS_2$ from a direct band gap semiconductor to a metal. This is evidenced by the asymmetric lineshape observed in core-level photoemission spectra. It is associated particularly with the emergence of states at the FL near the Q point of $WS_2$, as can be seen in measurements by angle-resolved photoemission spectroscopy (ARPES). Meanwhile, ARPES and time-resolved ARPES confirm that the $WS_2$ conduction band minimum at K remains well defined and stays above the FL. Electronic structure calculations based on density functional theory shed further light on the reasons for these strong changes in band structure. [1] Phys. Rev. B 93, 165422 (2016)

DS 35.4 Wed 16:00 WIL A317

**A many-body view on the not-so-passive role of the substrate: trions and screening in transition metal dichalcogenides** — •Matthias Drüppel[1], Thorsten Deilmann[2], Peter Krüger[1], and Michael Rohlfing[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The strongly enhanced Coulomb interaction due to reduced dimensionality has established transition metal dichalcogenides (TMDC) as promising candidates for next-generation opto-electronic devices. However, in almost all experiments and applications, the monolayer is deposited on a substrate for mechanical stability or - in bulk/few layer materials - interacts with neighboring layers. In this talk we show that the surrounding of the monolayer does *not* play a passive role. In contrast, it distinctly modifies the TMDC excitations.

We subsequently apply DFT $\rightarrow$ $GW$ $\rightarrow$ Bethe-Salpeter equation (BSE) to access the optical properties. Our results show how additional charge carriers, that are often induced by substrates, lead to trion formation that might dominate optical spectra. We take our *ab-initio* approach and directly compare trion and exciton spectra, finding that trions split into inter- and intra-valley trions. Additionally, a drastically enhanced screening by a substrate renormalizes both the exciton and trion binding energies and the fundamental band gap. In bilayer and bulk materials, excitons can be excited with electron and hole located on different layers, forming inter-layer excitons.

DS 35.5 Wed 16:15 WIL A317

**Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials** — •Thomas Olsen, Simone Latini, Filip Rasmussen, and Kristian Thygesen — Technical University of Denmark

We present a generalized hydrogen model for the binding energies (E) and radii of excitons in two-dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local. We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for E that only depends on the excitonic mass and the 2D polarizability $\alpha$. The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the binding energy becomes independent of the mass and we obtain $E = 3/4\pi\alpha$), which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the non-hydrogenic Rydberg series in WS2 and can account for screening from the environment.

DS 35.6 Wed 16:30 WIL A317

**Investigation of hexagonal boron-nitride (hBN) on SiC** — •Markus Franke[1,2], François C. Bocquet[1,2], Janina Felter[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Among 2D materials, hexagonal boron-nitride (hBN) seems to be a promising candidate for a new substrate material to achieve a highly ordered layer of free-standing graphene. It forms a flat hexagonal lattice structure with a lattice constant similar to that of graphene, but (in contrast to graphene) has a wide band gap ($> 5\,\mathrm{eV}$) and is therefore insulating. It should be free of charge traps and dangling bonds and its flat surface should prevent overlying 2D materials from corrugating.

Here, we report on the growth of hBN layers on the wide band gap semiconductor silicon carbide (SiC) by annealing SiC wafers in a borazine ($B_3N_3H_6$) atmosphere. The properties of this system are investigated by XPS, ARPES and HREELS.

DS 35.7 Wed 16:45 WIL A317

**Plasmonic Superconductivity in Layered Materials** — Malte Rösner[1,2], Roelof G. Groenewald[1], Gunnar Schönhoff[2], Jan Berges[2], Stephan Haas[1], and •Tim O. Wehling[2] — [1]Department of Physics and Astronomy, University of Southern California, USA — [2]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany

Due to a lack of screening in two dimensions the Coulomb interaction is generally enhanced and consequently plays a major role to understand many-body effects within layered materials. In the field of superconductivity it is usually introduced as an approximate, static, and adjustable parameter $\mu^*$ which describes only effectively the Coulomb repulsion which is therefore responsible for reduced transition temperatures.

Here, we overcome this inadequate handling and present an ab initio based material-realistic Coulomb description for doped single layers of $MoS_2$ which captures simultaneously material-intrinsic, substrate, and dynamical screening processes. Using this model we can reliably describe the resulting plasmonic excitations including both, their coupling to the electrons and their dependence on the environmental screening and doping level. Utilizing Eliashberg theory we show that the low-energy plasmonic modes originating from the dynamically screened Coulomb *repulsion* can actually lead to an effective Coulomb *attraction* and thus to an enhanced transition temperature ($T_c$). Furthermore, we find an optimal ratio between the substrate screening and the electron doping which maximizes $T_c$ of the induced plasmonic superconducting state.

DS 35.8 Wed 17:00 WIL A317

**MoS2 film conductivity change on periodically poled LiNbO3 substrate determined by nano-FTIR spectroscopy** — •Piotr Patoka[1], Georg Ulrich[1], Peter Hermann[2], Bernd Kästner[2], Ariana Nguyen[3], 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]Dept. of Chemistry, Univ. of California Riverside, Riverside, CA 92521, USA — [4]Dept. of Physics and Astronomy, Univ. of Nebraska, Lincoln, Lincoln, NE 68588-0299 USA

Coupling of ultra-broadband synchrotron radiation from the Metrology Light Source (MLS) to a scattering-type scanning near-field optical microscope (s-SNOM) allows for contactless conductivity evaluation in the mid-infrared regime. The system is based on an atomic force microscope, such that the optical signal can be directly correlated with topographic information. Using this method, we investigated the influence of a ferroelectric substrate (LiNbO3) enhanced by its surface phonon on thin films of MoS2. Recent electric transport measurements suggest changes in the carrier density due to substrate polarization.[1] The present findings obtained from s-SNOM studies offer a complimentary way of contactless investigations of conductivity changes.[2]

[1] Nguyen, A. et al., Nano Lett. 15, 3364-3369 (2015).
[2] Hermann, P. et al., Opt. Express 21, 2913-2919 (2013).

DS 35.9 Wed 17:15 WIL A317

**Band gap transition in few-layer $ReS_2$ investigated by photoemission k-space microscopy** — •Mathias Gehlmann[1], Lukasz Plucinski[1], Slavomír Nemšák[1], Irene Aguilera[2], Gustav Bihlmayer[2], Pika Gospodarič[1], Markus Eschbach[1], Ewa Młyńczak[1], Giovanni Zamborlini[1], Vitaliy Feyer[1], Florian Kronast[3], Philipp Nagler[4], Tobias Korn[4], Christian Schüller[4], Stefan Blügel[2], and Claus Michael Schneider[1] — [1]PGI-6, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]PGI-1/IAS-1, Forschungszentrum Jülich GmbH and JARA, D-52425 Jülich, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-12489 Berlin, Germany — [4]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

$ReS_2$ is a promising candidate for novel electronic and sensor applications. The low crystal symmetry of this van der Waals compound leads to highly anisotropic optical and vibrational behavior. However, the details of the electronic band structure of this fascinating material are still largely unexplored. We present a momentum resolved study of the electronic structure of monolayer, bilayer, and bulk $ReS_2$. Using photoemission k-space microscopy in combination with density functional theory calculations we demonstrate a significant 3D delocalization of the valence electrons in bulk $ReS_2$. Furthermore, we directly observe the evolution of the valence band dispersion in our photoemission experiments as a function of the number of layers, revealing a varying character of the band gap.

DS 35.10 Wed 17:30 WIL A317

**Structural Analysis of h-BN on Cu(111)** — •Martin Schwarz[1], Manuela Garnica[1], Jacob Ducke[1], Peter Deimel[1], David Duncan[2], Ari Seitsonen[3], Francesco Allegretti[1], Johannes Barth[1], and Willi Auwärter[1] — [1]Physik Department, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany — [2]Diamond Light Source, Didcot, Oxfordshire, OX11 0DE, United Kingdom — [3]Département de Chimie, École Normale Supérieure, 24 rue Lhomond, F-75005 Paris, France

Atomically thin boron nitride (h-BN) layers on metallic supports represent promising platforms for the adsorption of atoms, clusters, and molecular nanostructures [1-2]. Specifically, STM studies revealed an electronic corrugation of h-BN/Cu(111), guiding the self-assembly of molecules and their energy level alignment. A comprehensive characterization of the h-BN/Cu(111) interface including the spacing between the h-BN sheet and its support - elusive to STM measurements - is crucial to rationalize the interactions within these systems. To this end, we employed complementary techniques including scanning tunneling microscopy (STM), high resolution atomic force microscopy (AFM), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), X-ray standing wave (XSW) and density functional theory (DFT). Thus, our multi-method study yields a complete, quantitative structure determination of the sp2 bonded BN layer on Cu(111).

[1] Joshi, Sushobhan, et al. NL 12.11 (2012): 5821-5828
[2] Urgel, J. I. et al. JACS 137.7 (2015): 2420-2423