

## TT 9: Focus Session: Two-Dimensional Materials II (joint session DS, HL, TT, organized by HL)

Time: Monday 14:45–18:15

Location: POT 81

**Invited Talk** TT 9.1 Mon 14:45 POT 81  
**2D / 3D Heterostructures for Optoelectronics** — ●MAX LEMME  
 — University of Siegen, Germany

Broad spectral optical detection is of high interest for imaging, sensing, communication and spectroscopy. Two-dimensional (2D) materials are very promising for such applications due to their high optical absorption, potential wide detection range and material flexibility.

In this talk, graphene / silicon Schottky diodes made of chemical vapor deposited (CVD) graphene on n-type Si substrates will be discussed. Broad spectral response of 60 - 407 mA/W is measured from ultraviolet to near infrared light. In contrast to graphene, bulk molybdenum disulfide ( $MoS_2$ ) is an n-type semiconducting 2D material with an indirect band gap of 1.3 eV.  $MoS_2$ /Si hybrid diodes made with multilayer, CVD grown  $MoS_2$  yield a maximum spectral response of 8.6 mA/W.

Hybrid integration of large area CVD graphene as transparent conductive electrodes with amorphous silicon (a-Si) will be discussed for applications as multispectral photodetectors. A strong enhancement of the detectors' spectral response is observed in the ultraviolet region compared to reference devices with conventional aluminum doped zinc oxide electrodes. The maximum responsivity of these multispectral PDs can be tuned in their wavelength from 320 nm to 510 nm by external biasing, which allows single pixel detection of UV to visible light. The material combination of graphene and a-Si enables flexible diodes on polyimide substrates. Bilayer graphene boosts the maximum photoresponsivity of these flexible diodes up to 239 mA/W.

TT 9.2 Mon 15:15 POT 81  
**Optical properties of atomically thin MoS2 exposed to helium ions** — ●ANNA NOLINDER<sup>1</sup>, JULIAN KLEIN<sup>1,2</sup>, AGNIESZKA KUC<sup>4</sup>, MARCUS ALTZSCHNER<sup>1</sup>, JAKOB WIERZBOWSKI<sup>1</sup>, FLORIAN SIGGER<sup>1</sup>, FRANZ KREUPL<sup>3</sup>, THOMAS HEINE<sup>4</sup>, JONATHAN FINLEY<sup>1,2</sup>, URSULA WURSTBAUER<sup>1,2</sup>, ALEXANDER HOLLEITNER<sup>1,2</sup>, and MICHAEL KANIBER<sup>1</sup> — <sup>1</sup>Walter Schottky Institut und Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — <sup>2</sup>Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — <sup>3</sup>Department of Hybrid Electronic Systems, Technische Universität München, Arcisstr. 21, 80333 Munich, Germany — <sup>4</sup>Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

We present a spectroscopic study on atomically thin MoS2 exposed to helium ions. Distinct changes of the first-order Raman bands, additional defect luminescence and strong modification of the intrinsic valley spin relaxation properties are observed, shedding light on the effect of disorder on the optical properties and valley spin relaxation mechanisms. Moreover, our observations are in good qualitative agreement with Density Functional Theory calculations.

TT 9.3 Mon 15:30 POT 81  
**Coulomb Engineering of Excitonic Transitions in Transition Metal Dichalcogenides for New Non-Classical Light Sources** — ●SVEN BORGHARDT<sup>1</sup>, JIHI-SIAN TU<sup>1</sup>, TIM FLATTEN<sup>2</sup>, FRANK MATTHES<sup>2</sup>, DANIEL BÜRGLER<sup>2</sup>, DETLEV GRÜTZMACHER<sup>1</sup>, and BEATA KARDYNAL<sup>1</sup> — <sup>1</sup>Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>Peter Grünberg Institute 6 (PGI-6), Forschungszentrum Jülich, D-52425 Jülich, Germany

The spatial confinement of excitons is a key prerequisite for the creation of non-classical light sources. Since the dielectric environment of transition metal dichalcogenide monolayers (TMD-MLs) changes the screening of electrostatic fields and, thus, the interaction of charge carriers within the MLs, both the single particle band gap and the binding energy of exciton complexes in TMD-MLs can be tuned by modifying the dielectric properties of the environment.

In our experiments, we prepare TMD-MLs in different environments and apply optical spectroscopy methods in order to quantify the effects of the dielectric environment on the transition energies of exciton complexes. Furthermore, we correlate the results with single particle band gaps estimated from excited exciton states and single particle band gaps measured in scanning tunnelling spectroscopy experiments. This correlation gives access to the binding energy of exciton complexes.

In addition to TMD-MLs in laterally homogeneous environments, we

examine lateral heterostructures of TMD-MLs in environments with laterally changing dielectric properties, paving the way towards controllable confinement of excitons within TMD-MLs.

TT 9.4 Mon 15:45 POT 81  
**Exciton-trion competition and single photon emission in III-V- monolayer hybrid architectures** — ●OLIVER IFF<sup>1</sup>, YU-MING HE<sup>1</sup>, NILS LUNDT<sup>1</sup>, SEBASTIAN STOLL<sup>1</sup>, VASILIJ BAUMANN<sup>1</sup>, SVEN HOEFLING<sup>1,2</sup>, and CHRISTIAN SCHNEIDER<sup>1</sup> — <sup>1</sup>Technische Physik and Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Atomic monolayers represent a novel class of materials to study localized and free excitons in two dimensions and to engineer optoelectronic devices based on their significant optical features. Here, we investigate the role of epitaxially grown III-V substrates on the photoluminescence response from exfoliated MoSe2 and WSe2 monolayers in comparison to regular SiO2 substrates. In the case of MoSe2, we observe a significant qualitative modification of the emission spectrum, which is widely dominated by the trion resonance on InGaP substrates. Even more remarkably, in sheets of WSe2, we notice emission lines from localized excitons with linewidths down to 70  $\mu$ eV, only limited by our system resolution. Furthermore, these spectral signatures are identified as single photon or even photon pair emitters without any sign of spectral jitter or blinking. Overall, the results outline the enormous potential of hybrid III-V- monolayer architectures in obtaining high quality emission signals from atomic monolayers, enhancing their optical properties.

TT 9.5 Mon 16:00 POT 81  
**The Influence of the Substrate Material on the Optical Properties of Tungsten-Diselenide Monolayers** — SINA LIPPERT<sup>1</sup>, ●LORENZ SCHNEIDER<sup>1</sup>, DYLAN RENAUD<sup>1</sup>, KYUNG NAM KANG<sup>2</sup>, OBAFUNSO AJAYI<sup>3</sup>, MARC HALBICH<sup>1</sup>, ODAY ABDULMUNEM<sup>1</sup>, XING LIN<sup>1</sup>, JAN KUHNERT<sup>1</sup>, KHALEEL HASSOON<sup>1</sup>, SAIDEH EDALATI-BOOSTAN<sup>1</sup>, YOUNG DUCK KIM<sup>3</sup>, WOLFRAM HEIMBRODT<sup>1</sup>, EUI-HYEOK YANG<sup>2</sup>, JAMES HONE<sup>3</sup>, and ARASH RAHIMI-IMAN<sup>1</sup> — <sup>1</sup>Faculty of Physics, Philipps-Universität, Marburg 35032, Germany — <sup>2</sup>Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, New Jersey, 07030, USA — <sup>3</sup>Department of Mechanical Engineering, Columbia University, New York, New York, 10027, USA

In recent years 2D materials based on transition metal dichalcogenides (TMDs) have come up as an interesting material system mainly due to their remarkable properties in the monolayer regime after the successful exploration of graphene. While the main optical properties of these materials have been studied and understood well, the influence of the substrate material on the energy levels and the recombination dynamics are not yet sufficiently discussed. Here, we present a systematic comparison of the optical properties of monolayered WSe2 on different substrates including SiO2, sapphire, Si3N4-hBN and MgF2. In addition to the exfoliated monolayers, a CVD grown monolayer on sapphire is included. While similarities have been found for the Raman signal and PL of these samples, small differences regarding excitonic features, emission characteristics and decay dynamics have been observed in dependence on the substrate.

### Coffee Break

TT 9.6 Mon 16:45 POT 81  
**Excitons in colloidal 2D-CdSe nanocrystals** — ●ULRIKE WOGGON — Institut für Optik und Atomare Physik, TU Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

Two-dimensional II-VI semiconductor nanoplatelets (NPLs) gained increasing interest because of their unique electronic and optical properties, such as the Giant Oscillator Strength, strong electroabsorption response, low exciton-phonon interaction and high impact of dielectric confinement on exciton binding energies [1]. CdSe platelets are of special importance since they combine large particle volumes with ultra-strong confinement. We present a comprehensive study of the influence

of dimensionality, size and shape on excitons in CdSe NPLs. They are an attractive system allowing to control not only the exciton energy states by thickness (z-direction) but also with lateral size variation the LO-phonon coupling (x,y-direction) [2]. The larger the particles' aspect ratio, the greater is the confinement related electronic contribution to the increased two-photon absorption and CdSe NPLs are ideally suited for two-photon imaging and non-linear opto-electronics [3-5]. [1] A.W. Achtstein et al., Nano Letters 12, 3151 (2012); [2] A.W. Achtstein et al., Phys. Rev. Lett. 116, 116802 (2016); [3] A.W. Achtstein et al., J. Phys. Chem. C 119, 20156 (2015); [4] R. Scott et al., Nano Lett. 15, 4985 (2015); [5] A.W. Achtstein et al., ACS Nano 8, 7678 (2014)

TT 9.7 Mon 17:15 POT 81

**Controlled MoS<sub>2</sub> deposition by metal-organic vapour phase epitaxy** — MATTHIAS MARX<sup>1</sup>, DOMINIK ANDRZEJEWSKI<sup>2</sup>, ANNIKA GRUNDMANN<sup>1</sup>, YOU-RON LIN<sup>1,3</sup>, GERD BACHER<sup>2</sup>, HOLGER KALISCH<sup>1</sup>, ANDREI VESCAN<sup>1</sup>, and MICHAEL HEUKEN<sup>1,3</sup> — <sup>1</sup>GaN Device Technology, RWTH Aachen University — <sup>2</sup>WET, University Duisburg-Essen — <sup>3</sup>AIXTRON SE

Recently, layered transition metal dichalcogenides (TMDC) have attracted a lot of attention. Their thermodynamically stable 2D form and their unique electrical and optical properties are very promising for integration in future electronic devices. For systematic scientific studies and in particular for implementation in commercial devices, it will be necessary to achieve a reproducible, homogeneous and scalable deposition on wafer scale. A promising option to achieve this goal is to use metal-organic vapour phase epitaxy (MOVPE) processes employing MO precursors for the TMDC constituents. All deposition experiments reported here are carried out in an AIXTRON horizontal hot-wall reactor. Molybdenum hexacarbonyl (MCO) and Di-tert-butyl sulfide (DTBS) are used as Mo and S sources, respectively. The samples are characterized via Raman spectroscopy, photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) to investigate their optical and structural properties. To reduce and control the nucleation density and to promote a layer-by-layer growth mode, the growth parameters such as DTBS and MCO precursor flows are optimized and temperature treatment was adjusted.

TT 9.8 Mon 17:30 POT 81

**Ion implantation of 2D transition metal dichalcogenides monolayers** — JIHH-SIAN TU<sup>1</sup>, SVEN BORGHARDT<sup>1</sup>, HANS HOFSSASS<sup>2</sup>, URSEL BANGERT<sup>3</sup>, QUENTIN RAMASSE<sup>4</sup>, DETLEV GRÜTZMACHER<sup>1</sup>, and BEATA KARDYNAL<sup>1</sup> — <sup>1</sup>PGI 9, Forschungszentrum Jülich, Jülich, Germany — <sup>2</sup>II. Physikalisches Institut, Georg-August-University Göttingen, Göttingen, Germany — <sup>3</sup>Department of Physics, Univsity of Limerick, Limerick, Ireland — <sup>4</sup>SuperSTEM Laboratory, Daresbury, UK

Monolayer transition metal dichalcogenides (TMDs) have gained interest as material for optoelectronics. In order to realise the technological potential of the TMDs semiconductors, it is desirable to be able

to form heterostructures and introduce dopants in the monolayers. In this study, we examine the possibility to do so using ion implantation. We show that chalcogen atoms of the monolayer MoS<sub>2</sub> can be substituted using very low energy ion beams (<50 eV) as verified using Raman spectroscopy and scanning transmission electron microscopy. Implantation levels of a few percent are realised with no structural damage visible in Raman spectra. Significant changes of the photoluminescence compared with pristine MoS<sub>2</sub> monolayers are observed at cryogenic temperature. The technique under development is to be applied for forming lateral heterostructures of 2D TMDs.

TT 9.9 Mon 17:45 POT 81

**synthesis of bismuth/reduced graphene oxide composites and their electrochemical properties for Na-ion batteries** — BENRONG HAI<sup>1,2</sup>, YANG XU<sup>1</sup>, MIN ZHOU<sup>1</sup>, LIYING LIANG<sup>1</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>TU-ilmeneau, Ilmenau, Germany — <sup>2</sup>Northeastern University, Shenyang, P. R. China

Recently, Na-ion batteries have been considered as a desirable alternative to Li-ion batteries, because of the greater abundance and lower cost of sodium-containing precursors. Even though Na-ion batteries have attracted great attention, more research is needed to enhance their performance. Reduced graphene oxide sheets have extraordinary electronic transport properties, large surface area and mechanical flexibility. Therefore, reduced graphene oxide sheets have been considered as a matrix material to improve electrochemical performance of metal nanoparticles. Here, we demonstrate a facile strategy to prepare bismuth/reduced graphene oxide composites. Such composites exhibit high specific capacity and enhanced cycling performance as anode. Compared to pure bismuth nanoparticles, the enhancement of sodium storage could be attributed to the introduction of reduced graphene oxide sheets that not only buffer the large volume changes during the reaction of sodium and bismuth, but also provide a highly conductive network for rapid electron transport in electrochemical reaction.

TT 9.10 Mon 18:00 POT 81

**Optical properties of boron vacancies and boron vacancy complexes in hexagonal boron nitride** — MAŽENA MACKOIT and AUDRIUS ALKAUSKAS — Center for Physical Sciences and Technology, Vilnius, Lithuania

In this work we perform density functional theory calculations of boron vacancies and boron vacancy complexes with oxygen in hexagonal boron nitride. It is shown that interaction with oxygen significantly lowers the formation energy of boron vacancies. Therefore, when oxygen is present, complexes are more likely to occur than bare vacancies. We find that electronic defect states can be of both  $\sigma$  and  $\pi$  type. This gives rise to various possible configurations of ground and excited states. In particular, it is suggested that intra-defect luminescence can be polarized both in- and out-of-plane. We also provide estimates of intra-defect excitation energies and associated Franck-Condon shifts, making the connection with recent experimental observations of single photon emitters in this material.