HL 18: 2D Materials and Heterostructures: Emerging Materials and Phenomena

Time: Tuesday 9:30–13:00 Location: EW 201

HL 18.1 Tue 9:30 EW 201

Quantum transport in monolayer and multilayer Black Phosphorene — Jouda J. Khabthani[1], Khouloud Chika[1], Ghassen Jemaï[1], Didier Mayou[2], and •Guy Trambly de Laissardière[3] — [1]Lab. de Physique de la Matière Condensée, Faculté des Sciences de Tunis, University El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS / Univ. Grenoble Alpes, Grenoble, France — [3]Lab. de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, Cergy-Pontoise, France

The electronic properties of Phosphorene are very sensitive to local defects such as fonctionalization which may be covalent (resonant) or non-covalent (non-resonant). Here, we present numerical studies on the electronic structure and quantum transport in monolayer Black Phosphorus (BP), few-layer BP, and bulk BP, with a relatively high concentration of defects (a few %). In contrast to the usual Boltzmann approach for electronic transport calculations, our real space method [1,2] takes into account all the effects of defects on the electronic structure itself and the impacts of multiple scattering on conductivity. Our study shows that resonant and non-resonant scatterers have different consequences on the gap and conductivity, sometimes leading to metal-insulator transitions by varying the defect concentration.

[1] F. Triozon *et al.*, Phys. Rev. B **65**, 220202, (2002).

[2] G. Trambly de Laissardière, D. Mayou, Phys. Rev. Lett. **111**, 146601 (2013).

HL 18.2 Tue 9:45 EW 201

Influence of highly charged ion irradiation on the electrical and memory properties of black phosphorus field-effect transistors — •Stephan Sleziona, Osamah Kharsah, Lucia Skopinski, Leon Daniel, Jennifer Schmeink, and Marika Schleberger — Fakultät für Physik und CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47057 Duisburg, Germany

Black phosphorus (bP) is one of the more recently discovered layered materials. In particular its high hole mobility and finite, thickness dependent, direct bandgap may pave its way to new applications as optoelectronic devices. Utilizing the hysteresis in the transfer characteristics of bP field-effect transistors (FETs), several approaches to realize non-volatile memory devices have been successfully put forward. This hysteresis is commonly attributed to charge trapping and detrapping in defects and impurities either in the underlying substrate, or in the bP itself. In this work we deliberately introduce additional defects into bP FETs by irradiating the devices with highly charged Xe^{30+} at a kinetic energy of 180 keV to manipulate the electrical and memory properties of the devices. We find an increase of conductivity and p-doping with increasing ion fluence, while other device parameters, like i.e. charge carrier mobility, degrade for the higher irradiation fluences. Most importantly, we find an increase in the width of the hysteresis and the memory window due to the irradiation. By controlling the kinetic energy of the ions, we can demonstrate, that this increase is caused by additional defects in the underlying SiO_2 substrate and not in the bP itself.

HL 18.3 Tue 10:00 EW 201

On-site Coulomb energy in TMDC compounds — •Yashasvi Mehra[1,2,3], Samuel Bealieu[4], Mauro Fanciulli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Marcin Rosmos[5], Natalia Olszowska[5], Aki Ismo Olavi Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Université de Bordeaux, CNRS, CEA, CELIA, UMR5107, Talence, France — [5]SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland

The Coulomb interaction U, serves as a pivotal parameter influencing electron behavior, particularly accentuated within low-dimensional materials. Transition Metal Dichalcogenides, quasi-2-D systems, exhibit diverse electronic traits like CDW order, co-existing CDW with superconductivity, and topologically non-trivial phases. Their 2D nature intensifies electron-coulomb interaction, leading to phenomena like Mott-Hubbard transitions. We aim to determine the on-site Coulomb interaction for each element within two series of TMDC materials (MX2, where X = S, Se, Te, M = Nb, Ta) by resonant ARPES.

HL 18.4 Tue 10:15 EW 201

Tuning properties of 2D Janus MoSSe — •Jennifer Schmeink, Jens Osterfeld, Osamah Kharsah, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Two-dimensional (2D) Janus materials such as MoSSe are defined by their asymmetrical structure, where the transition metal atoms, specifically molybdenum (Mo), are sandwiched between opposing sites of different species of chalcogen atoms, notably selenium (Se) and sulfur (S). This uniquely structured material allows a new way for tuning existing properties of 2D transition metal dichalcogenide (TMDC) materials and new characteristics emerge from the loss of inversion symmetry in the structure.

The method for synthesizing such Janus materials involves utilizing a base TMDC, e.g. molybdenum diselenide ($MoSe_2$). The process involves the creation of vacancies in the top layer of chalcogen atoms, subsequently filling these vacancies with an additional species [1]. Depending on the process details, this results in Janus MoSSe or in Janus-like $MoS_{2(1-x)}Se_{2x}$ alloys, where $0 > x > 1$ and $x \neq 0.5$. The latter is characterized by the coexistence of Janus MoSSe and $MoSe_2$ or MoS_2 phases. This constitutes yet another tunable platform for tailoring material properties.

This talk will present studies of the (opto-)electronic properties of Janus MoSSe and its Janus-like alloys. Furthermore, the influence of Se-vacancies in $MoSe_2$ and the Janus-like alloys will be highlighted and defect related findings discussed.

[1] J. Schmeink *et al.*, Nanoscale (2023), **15**, 10834-10841

HL 18.5 Tue 10:30 EW 201

$PtSe_2$ vdW single-crystal surfaces studied at the atomic scale with ncAFM — •Igor Sokolović[1,2], Saeed Rasouli[2], Bing Wu[3], Zdeněk Sofer[3], Aleksandar Matković[4], Michael Schmid[2], Ulrike Diebold[2], and Tibor Grasser[1] — [1]Institute of Microelectronics, TU Wien, Vienna, Austria — [2]Institute of Applied Physics, TU Wien, Vienna, Austria — [3]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague, Czech Republic — [4]Chair of Physics, Montanuniversität Leoben, Leoben, Austria

Surfaces of van-der-Waals-bonded (vdW) single-crystal $PtSe_2$ cleaved in ultrahigh vacuum (UHV) were studied with noncontact atomic force microscopy (ncAFM) at the atomic level. Typical ionic and electronic defects were characterized with single-atom precision: the identification of surface and subsurface defects was achieved by observing the atomic and electronic structure in parallel. The metallic single crystals exhibit a proclivity of the PtSe2 toward different defect types compared to the synthesized trilayer thin films of semiconducting $PtSe_2$ and other Pt-based TMDs. Cleaved surfaces are representative of the commonly exfoliated flakes so further experiments with *in situ* deliberate stoichiometry adjustments and the adsorption of gasses will be presented. Additionally, the growth of a CaF_2 dielectric on these surfaces will be demonstrated.

HL 18.6 Tue 10:45 EW 201

Nanoscale Charge Transport Characterization of Novel Type 2D MOFs and COFs — •Jonas Pöhls[1], Zhiyong Wang[2,3], Laura Frey[4], Renhao Dong[2], Dana Medina[4], Xinliang Feng[2,3], and Thomas Weitz[1] — [1]1st Institute of Physics, University of Goettingen, Goettingen, Germany — [2]Chair of Molecular Functional Materials, TU Dresden, Germany — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Chemistry Department, LMU Munich, Germany

In recent years, Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have emerged as fascinating and promising materials classes, owing to their exceptional structural versatility and tunable properties, which make them interesting for a wide range of technological applications. At the same time, the study of 2D van der Waals materials has become the probably most relevant and dynamic area in solid state research at present, offering numerous opportunities to uncover novel physical phenomena and engineer advanced nanoscale devices. With recent advances in the synthesis of two-dimensional MOFs and COFs, these material classes have also entered the field of

van der Waals materials [1]. We will characterize the charge transport in novel type 2D coordination network materials like Cu-BHT, considering also the influence of properties like structure or defects. By that, we will demonstrate why they are promising candidates for implementation into van der Waals heterostructures.

15 min. break

HL 18.7 Tue 11:15 EW 201

Srain control of exciton and trion spin-valley dynamics in monolayer transition metal dichalcogenides — Zhao An[1], Pedro Soubelet[2], Yaroslav Zhumagulov[3], Michael Zopf[1], •Alex Delhomme[2], Chenjiang Qian[2], Paulo Faria Junior[3], Jaroslav Fabian[3], Xin Cao[1], Jingzhong Yang[1], Andreas Stier[2], Fei Ding[1], and Jonathan Finley[2] — [1]Institute of Solid State Physics, Leibniz Universitat Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Walter Schottky Institut and TUM School of Natural Sciences, Technische Universitat Munchen, Am Coulombwall 4, 85748 Garching, Germany — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany.

The electron-hole exchange interaction is a fundamental mechanism that drives valley depolarization via intervalley exciton hopping in semiconductor multivalley systems. Here, we report polarization-resolved photoluminescence spectroscopy of neutral excitons and negatively charged trions in monolayer MoSe2 and WSe2 under biaxial strain. We observe a marked enhancement (reduction) on the WSe2 triplet trion valley polarization with compressive (tensile) strain while the trion in MoSe2 is unaffected. The origin of this effect is shown to be a strain-dependent tuning of the electron-hole exchange interaction. A combined analysis of the strain-dependent polarization degree using ab initio calculations and rate equations shows that strain affects intervalley scattering beyond what is expected from strain-dependent band-gap modulations. The results evidence how strain can be used to tune valley physics in energetically degenerate multivalley systems.

HL 18.8 Tue 11:30 EW 201

Strain fingerprinting of exciton valley character in 2D semiconductors — •Abhijeet Kumar[1], Denis Yagodkin[1], Roberto Rosati[2], Douglas J. Bock[1], Christoph Schattauer[3], Sarah Tobisch[3], Joakim Hagel[4], Bianca Höfer[1], Jan N. Kirchhof[1], Pablo H. López[5], Kenneth Burfeindt[1], Sebastian Heeg[5], Cornelius Gahl[1], Florian Libisch[3], Ermin Malic[2], and Kirill I. Bolotin[1] — [1]Free Universität Berlin, Germany — [2]Philipps-Universität Marburg, Germany — [3]TU Wien, Austria — [4]Chalmers University of Technology, Sweden — [5]Humboldt-Universität Berlin, Germany

Momentum-indirect excitons define optoelectronic properties of many 2D semiconductors, but are challenging to detect due to their weak coupling to light. The identification of the excitons' valley character is further limited by complexities associated with momentum-selective probes. Here, we study the photoluminescence of controllably strained 2D materials at cryogenic temperatures and find that indirect excitons i) exhibit valley-specific energy shifts, enabling their valley fingerprinting, and ii) hybridize with bright excitons, becoming directly accessible to optical spectroscopy methods. This approach allows us to identify multiple previously inaccessible excitons with wavefunctions residing in K, Γ, or Q valleys in the momentum space, as well as various types of defect-related excitons. Overall, our approach is well-suited to unravel and tune intervalley excitons in various 2D systems.

HL 18.9 Tue 11:45 EW 201

Strain control of hybridization between dark and localized excitons in a 2D semiconductor — •Pablo Hernández López[1], Sebastian Heeg[1], Christoph Schattauer[2], Sviatoslav Kovalchuk[3], Abhijeet Kumar[3], Douglas J. Bock[3], Jan N. Kirchhof[3], Bianca Höfer[3], Kyrylo Greben[3], Denis Yagodkin[3], Lukas Linhart[2], and Florian Libisch[2] — [1]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Vienna University of Technology, Vienna, Austria — [3]Physics Department, Freie Universität Berlin, Berlin

Mechanical strain is a powerful tuning knob for excitons, Coulomb-bound electron-hole complexes dominating optical properties of two-dimensional semiconductors. While the strain response of bright free excitons is broadly understood, the behaviour of dark free excitons (long-lived excitations that couple weakly with light due to conservation laws) or localized excitons related to defects remains mostly unexplored. Here, we study the strain behaviour of these fragile many-body states on pristine suspended WSe2 kept at cryogenic temperatures. We find that upon straining, dark and localized excitons in monolayer WSe2 are brought into energetic resonance, forming a new hybrid state that inherits the properties of the constituent species. The characteristics of the hybridized state, including an order-of-magnitude enhanced light/matter coupling, avoided-crossing energy shifts, and strain tunability of many body interactions, are all supported by first-principles calculations. The hybridized exciton reported here may play a critical role in the operation of single quantum emitters based on WSe2.

HL 18.10 Tue 12:00 EW 201

Electronic effects on wrinkled 2D TMDCs — •Mohammadreza Daqiqshirazi and Thomas Brumme — Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstraße 66c, 01069 Dresden, Germany

Strain can be used to change the electronic properties of 2D materials considerably especially since they can undergo strong deformations before breaking. It has been shown that there are various techniques to create wrinkles or folds in 2D materials. The wrinkles exert an inhomogeneous strain field on the 2D material that goes beyond the conventional uniaxial and biaxial strain effects. It is very important to understand these effects as wrinkles and bubbles can also occur during the synthesis or due to the transfer process. Unfortunately, these inhomogeneous strains are rarely studied using fundamental methods because the size of the systems is enormous. Here we investigate the effect of an inhomogeneous strain field in the form of wrinkles in 2D WSe2 monolayers, bilayers and heterostructures of WSe2-MoSe2. We use density functional theory and include spin-orbit coupling in our calculations. We find that spin-orbit coupling and symmetry breaking in monolayers lead to a strong Rashba-like splitting. Furthermore, from the band structures, we can explain the localization of the excitons in certain regions of the systems due to strain fields.

HL 18.11 Tue 12:15 EW 201

Extended suspension of transition metal dichalcogenide monolayers — •Leonard Geilen[1,3], Lukas Schleicher[2,3], Eva Weig[2,3], and Alexander Holleitner[1,3] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Chair of Nano and Quantum Sensors, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Suspended 2D materials offer great possibilities in the realm of investigating the fundamentals of nano- and micromechanical systems as well as chip-based sensors. So far, 2D materials have been suspended on the order of tens of micrometers in the case of few-layer materials and up to ten for monolayers. We demonstrate how a dry-transfer allows fabricating suspended monolayers of transition metal dichalcogenides with diameters larger than ten micrometers and a reduced impact of fabrication residues.

HL 18.12 Tue 12:30 EW 201

Impact of atomic layer deposition growth rate on the properties of MoS_2 and WS_2 — •Christian Tessarek, Tim Grieb, Florian F. Krause, Christian Petersen, Alexander Karg, Alexander Hinz, Niels Osterloh, Christian Habben, Stephan Figge, Andreas Rosenauer, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

The direct band gap of monolayer MoS_2 and WS_2 enables the use of these layers in optoelectronic applications. To overcome the limited and random size of exfoliated flakes from bulk material, chemical vapor deposition (CVD) techniques are necessary to grow homogeneous layers on large substrates.

Atomic layer deposition, a modified CVD method using an alternating precursor supply at lower process temperature, was used to grow MoS_2 and WS_2 on SiO_2/Si substrates. The growth rate is identified as a major parameter that influences the optical and structural properties. Raman spectroscopy investigations were carried out to characterize the 2D layers. Monolayers only form applying a slow growth rate. For a fast growth rate multilayers with minor structural properties directly develop in the initial phase. The optical activity was demonstrated by photoluminescence measurements which show typical A and B excitonic emission for MoS_2 and WS_2 monolayers. Further studies by X-ray photoelectron spectroscopy and transmission electron microscopy were carried out to reveal the stoichiometry and crystalline quality of the layers.

HL 18.13 Tue 12:45 EW 201

Oxidative chemical vapor deposition of highly conductive and transparent polymer layers for contact fabrication in 2D-MoS_2-based FET structures — •Jinmei Zhu[1,3], Florian Meierhofer[1], Marius Eckert[1,2], Stefan Wundrack[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology (IHT), TU Braunschweig, Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [3]Shijiazhuang College of Applied Technology, Shijiazhuang, China

For 2D MoS_2 field-effect transistors (FETs), contact fabrication easily results in damaging the MoS_2 channel due to the fragility of the atomically thin structure, making it difficult to reliably achieve high-performance devices. To overcome this challenge, the deposition of highly conductive and transparent polymer layers from the gas phase (oxidative chemical vapor deposition (oCVD)), is a promising approach that can lead to low-defect Ohmic contacts. In this work, we fabricated 2D MoS_2 bottom-gated FETs with poly (3, 4- ethylenedioxythiophene) (PEDOT) electrodes. PEDOT is a conductive polymer widely used as a transparent electrode material. We developed two contacting strategies to achieve a low-defect interface: in-situ oCVD electrode growth and electrode transfer method. By these means, we could pattern PEDOT layers and contact them onto MoS_2 channels without aggressive chemical and physical treatments. This allowed us to achieve low-defect MoS_2 channels with a clean and smooth interface of the PEDOT electrodes, significantly decreasing the charged impurity and interface-roughness scattering processes.