O 18: Poster: 2D Materials I

Time: Monday 18:00–20:00 Location: P2/EG

O 18.1 Mon 18:00 P2/EG

CVD growth of 2D transition metal dichalcogenides for electronics and optoelectronics — •Seung Heon Han[1], Ziyang Gan[1], Emad Najafidehaghani[1], Julian Picker[1], Christof Neumann[1], Uwe Hübner[2], Antony George[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [2]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany

Two-dimensional (2D) transition metal dichalcogenides (TMDs) are of great interest for fundamental science and technology due to their exceptional electronic and photonic properties. Chemical vapor deposition (CVD) is a viable method for scalable growth of high-quality monolayer TMDs on various substrates and with tailored properties. Here, we present some of our recent research results on the CVD growth of 2D TMDs including monolayer single-crystal TMDs, atomically sharp TMD1-TMD2 lateral heterostructure, and TMD1-TMD2 lateral heterostructure alloys. Moreover, we demonstrate various exciting applications of these monolayers in field-effect transistors, high-performance photodetectors and memtransistors.

O 18.2 Mon 18:00 P2/EG

Assembly of van der Waals heterostructures with ultra-clean surfaces for surface science techniques — Keda Jin[1], Tobias Wichmann[1], Felix Lüpke[1], Tomáš Samuely[2], Oleksander Onufriienko[2], F. Stefan Tautz[1], Markus Ternes[1], and •Jose Martinez-Castro[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia

Van der Waals heterostructures have become an excellent platform to study emerging physical phenomena that are the result of synergistic proximity effects. Until recently, surface science techniques such as ARPES or STM have been excluded from the study of such heterostructures because of their high sensitivity to surface contamination and the fact that they are sensitive to the top-most layer and thus, not being able to use, boron nitride as the encapsulating layer. Here, we report a novel technique for the assembly of van der Waals heterostructures that do not require encapsulation nor melting of polymers, allowing the study of air-sensitive materials surface. By performing low temperature STM, we demonstrate no surface degradation, achieving atomic resolution as well as detecting a perfectly formed superconducting gap in NbSe2.

O 18.3 Mon 18:00 P2/EG

Chemical vapor deposition of $MoSe_2$-WSe_2 lateral heterostructures with atomically sharp one-dimensional interfaces — •Ziyang Gan[1], Dorian Beret[2], Ioannis Paradisanos[2], Hassan Lamsaadi[2], Emad Najafidehaghani[1], Christof Neumann[1], Tibor Lehnert[4], Johannes Biskupek[4], Ute Kaiser[4], Laurent Lombez[2], Jean-Marie Poumirol[3], Bernhard Urbaszek[2,5], Antony George[1], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany — [2]Université de Toulouse, INSA-CNRS-UPS, Toulouse, France — [3]Université de Toulouse, CEMES-CNRS, Toulouse, France — [4]Ulm University, Central Facility of Electron Microscopy, Ulm, Germany — [5]Technische Universität Darmstadt, IPKM, Darmstadt, Germany

Chemical vapor deposition (CVD) enables the epitaxial growth of transition metal dichalcogenide (TMD) lateral heterostructures with one-dimensional interfaces. The growth is achieved by in situ controlling the precursor partial pressures by a two-step heating protocol. Here we characterize the lateral heterostructures of $MoSe_2$-WSe_2 by optical microscopy, Raman spectroscopy, and photoluminescence spectroscopy. Scanning transmission electron microscopy (STEM) demonstrates the high-quality 1D boundary between $MoSe_2$ and WSe_2 with a width of around 3nm. Furthermore, tip-enhanced photoluminescence (TEPL) enables to demonstrate that the heterojunction acts as an excitonic diode resulting in unidirectional exciton transfer from WSe_2 to $MoSe_2$. npj 2D Mater. Appl. 6 (2022) 84

O 18.4 Mon 18:00 P2/EG

Growth and characterization of transition metal dichalcogenides on Au(111) grown by chemical vapor deposition — •Julian Picker[1], Felix Otto[2], Ziyang Gan[1], Maximilian-Schaal[2], Marco Gruenewald[2], Christof Neumann[1], Antony George[1], Roman Forker[2], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Lessingstraße 10, 07743 Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Transition metal dichalcogenides (TMDs) are layered two-dimensional (2D) materials which have attracted significant attention in recent years. Especially, the exciting properties of their monolayers such as the strong, direct bandgap photoluminescence make them promising for novel electronic and optoelectronic applications. Here, we demonstrate the *ex-vacuo* growth of different TMD monolayers on Au(111) by chemical vapor deposition (CVD). Afterwards, the samples were analyzed in ultra-high vacuum (UHV) with the help of surface sensitive methods, including (low-temperature) scanning tunneling microscopy and spectroscopy (STM/STS), low-energy electron diffraction (LEED), as well as X-ray and angle-resolved ultraviolet photoelectron spectroscopy (XPS/ARPES). While we confirm the formation of high-quality TMDs, we also accessed the structural and electronic properties of these samples down to the atomic scale. In particular, the focus is on the interaction of the TMDs and Au(111) as Au is the most widely used electrical contact material for TMD devices.

O 18.5 Mon 18:00 P2/EG

Unoccupied electronic states of the CDW material 1T-$TiSe_2$ — •Patrick Geers, Marcel Holtmann, and Markus Donath — Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present angle-resolved inverse-photoemission (IPE) measurements of the unoccupied electronic structure of the transition metal dichalcogenide 1T-$TiSe_2$. The spectra along the $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ high symmetry directions are dominated by the Ti-3d bands with rather flat $E(\mathbf{k}_\parallel)$ dispersion. The two energetically separated subgroups e_g and t_{2g} are clearly resolved in the spectra. We observe two e_g bands as expected, while the spectral features of the t_{2g} group are too broad to identify the three predicted states individually. In addition, an image-potential surface state with its free-electron-like dispersion is observed below the vacuum energy. We compare our experimental $E(\mathbf{k}_\parallel)$ results with a theoretical 3D bandstructure by estimating the $\mathbf{k}_\perp$-component of the electron wavevector within the nearly-free-electron approximation. Furthermore, we observe temperature-dependent changes in our IPE data that are attributed to the charge density wave phase transition. Interestingly, only bands of t_{2g} symmetry show energy shifts, proving the orbital selectivity of bands involved in the phase transition [1].

[1] Watson *et al.*, Phys. Rev. Lett. **122**, 076404 (2019).

O 18.6 Mon 18:00 P2/EG

Electronic structure of benzene on MoS2 — •Jan-Phillip Topmöller and Michael Rohlfing — Institute of solid state theory, Münster, Germany

TMDCs show great potential in terms of their applicability in optical electronics. Due to their large surface, molecules can easily bind to the TMDC, which might affect its electronic properties. We investigate benzene as such a molecule because it is a small, prototypical one.

We use DFT (LDA, GGA) and DFT-D3 to determine the most stable adsorption position of benzene on MoS2. Subsequently, we use many body perturbation theory to calculate the electronic structure of the adsorbate system and its individual components (MoS2 and the benzene molecule). For example, we find that the HOMO-LUMO of the benzene molecule decreases from 10.5eV by 2.07eV when considering the screening of the monolayer.

O 18.7 Mon 18:00 P2/EG

Evolution of Band structure in 2D transition metal dichalcogenides alloy $Mo_xW_{1-x}Se_2$ — •Sarath Sasi[1], Laurent Nicolaï[1], Lucie Nedvědová[1], Rostislav Medlín[1], Michal Procházka[1], Marie Netrvalová[1], Sunil Wilfred Dsouza[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia,

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Among two-dimensional (2D) materials that emerged in the research scenario after the discovery of graphene, transition metal dichalcogenides (TMDCs) with the general formula MX_2 (M=Mo, W; X=S, Se, Te) attract huge interest as a potential candidate for electronic and optoelectronic applications. There are many artificial methods to engineer the bandgap and spin-polarized bands, such as chemical doping, external electric field etc. Here we are studying the band structure of $Mo_xW_{1-x}Se_2$ single crystals alloy with various stoichiometric ratio x in comparison with WSe_2. The structural characterisation of samples was analysed using Low energy electron diffraction, Raman Spectroscopy and Scanning Electron Microscopy with Energy Dispersive X-Ray Analysis, X-ray photoemission spectroscopy(XPS). Angle-Resolved Photoemission Spectroscopy (ARPES) was used to investigate the electronic band structure of the samples. We evaluated the band dispersion and observed the bands' splitting at the K point. Thus we are evaluating a potential way for band engineering in TMDCs.

O 18.8 Mon 18:00 P2/EG

Tuning the electronic structure of MoS2: how self-intercalation affects screening, interactions and strain — •Borna Pielic[1,2], Matko Muzevic[3], Dino Novko[2], Jiaqi Cai[1], Alice Bremerich[1], Robin Ohmann[1], Marko Kralj[2], Iva Srut Rakic[2], and Carsten Busse[1] — [1]Department Physik, Universitat Siegen, Siegen, Germany — [2]Institute of Physics, Zagreb, Croatia — [3]Department of Physics, Josip Juraj Strossmayer University of Osijek, Osijek, Croatia

Growth of quasi-freestanding 2D materials on van der Waals (vdW) typed substrates can be accompanied by intercalation in order to modify their intrinsic properties. In this work, we epitaxially grow MoS2 monolayer islands on graphene on Ir(111) using two different procedures: (i) two-step molecular beam epitaxy (MBE) growth which results in S intercalation between graphene and Ir(111), and (ii) single-step MBE growth resulting in Mo intercalation. Scanning tunneling microscopy (STM) measurements reveal significant difference in MoS2 islands morphology, and suggests that S intercalation weakens the interaction in the MoS2/graphene stack, while Mo intercalation strengthens it. More importantly, our scanning tunneling spectroscopy (STS) measurements show notable non-rigid shifts of electronic states. The numerical calculations reveal a strong correlation between substrate screening, strain and binding energy, that are in line with experiment. We suggest that this elegant and non-invasive technique could in general be used for altering vdW, electron-electron and electron-phonon interactions in 2D materials.

O 18.9 Mon 18:00 P2/EG

Designing a symmetry-correct minimal model for *2H*-WSe_2 — •Max Xylander[1,2], Philipp Eck[1,2], Simon Moser[2,3], Lukasz Plucinski[4], and Giorgio Sangiovanni[1,2] — [1]ITPA, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence, ct.qmat — [3]EP4, Universität Würzburg, Germany — [4]PGI-6, Peter Grünberg Institut Jülich, Germany

Transition metal dichalcogenides (TMDCs) have been studied for their structure-dependent valley physics. Due to inversion symmetry breaking in combination with strong SOC originating from the transition metal *d*-shell, these materials posess momentum-dependent spin splitting. Recently, the interest in TMDCs has been further stimulated by twisted moiré lattices, where the emerging flat bands have been associated to chiral representations in twisted bilayer graphene.

Here we present a study on the chiral wavefunctions in *2H*-WSe_2 based on *ab initio* calculations and minimal modeling. Especially, we will focus on an analysis of the irreducible representations, which allow us to design a minimal *d*-orbital tight-binding Hamiltonian with SOC and inversion symmetry breaking terms. For the validation of the model, we plan further experimental studies with circularly polarized light angle-resolved photoemission.