O 81: 2D Materials 4: Heterostructures

Time: Friday 10:30–12:00 Location: S052

O 81.1 Fri 10:30 S052

Sub-angstrom non-invasive imaging of microstructures in 2D hybrid perovskites — •Shayan Edalatmanesh[1,3], Mykola Telychko[2], Kai Leng[2], Ibrahim Abdelwahab[2,4], Na Guo[5], Chun Zhang[5], Jesus Mendieta-Moreno[1], Matyáš Nachtigall[1], Jing Li[4], Kian Ping Loh[2], Pavel Jelínek[1,3], and Jiong Lu[2,4] — [1]Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic — [2]Department of Chemistry, NUS, Singapore — [3]RCPTM, Palacky University, Olomouc, Czech Republic — [4]CA2DM, NUS, Singapore — [5]Department of Physics, NUS, Singapore

Organic-inorganic hybrid two dimensional (2D) Ruddlesden-Popper perovskites (RPPs), made of soft insulating organic layers sandwiched between conducting inorganic frameworks, have recently gained a great deal of attention as candidates for the next generation of optoelectronic devices. To gain an understanding of the cooperative lattice relaxation governing the optoelectronic properties of 2D RPPs, we present sub-angstrom resolution imaging of both soft organic layers and inorganic framework in a prototypical 2D lead-halide RPP crystal using a tip-functionalized Scanning Tunneling Microscopy (STM), non-contact Atomic Force Microscope (ncAFM) and Kelvin Probe Force Microscopy (KPFM) corroborated by theoretical simulations, namely Density Functional Theory (DFT)[1]. We unveil the overall twin-domain composition of the RPP crystal, with alternating quasi-one-dimensional electron and hole-channels at neighboring twin-boundaries, possibly responsible for the long-distance exciton transport in RPPs. Reference: [1] https://arxiv.org/abs/2109.05878

O 81.2 Fri 10:45 S052

Electronic Structure of Quasi-Freestanding WS_2/MoS_2 Heterostructures — Borna Pielić[1], Dino Novko[1], Iva Šrut Rakić[1], Jiaqi Cai[2], Marin Petrović[1], Alice Bremerich[2], Robin Ohmann[2], Nataša Vujičić[1], Mario Basletić[3], Marko Kralj[1], and •Carsten Busse[2] — [1]Institute of Physics, Zagreb, Croatia — [2]Universität Siegen, Germany — [3]University of Zagreb, Croatia

Quasi-freestanding heterostructures of semiconductiong two-dimensional materials with sharp interfaces, large built-in electric field, and narrow depletion region widths are proper candidates for the future design of electronic and optoelectronic devices.

Here, we epitaxially grow lateral WS_2-MoS_2 and vertical WS_2/MoS_2 heterostructures on graphene under UHV conditions. By means of scanning tunneling spectroscopy (STS), we examine the electronic structure of monolayer MoS_2, WS_2, and WS_2/MoS_2 vertical heterostructure. Moreover, we investigate band bending in the vicinity of the narrow one-dimensional interface of the WS_2-MoS_2 lateral heterostructure. Density functional theory (DFT) is used for the calculation of the band structures, as well as for the density of states maps at the interfaces. For the WS_2-MoS_2 lateral heterostructure, we find type-II band alignment and determine the corresponding depletion regions, charge densities, and the electric field at the interface.

O 81.3 Fri 11:00 S052

Quantum spin Hall edge states and interlayer coupling in twisted bilayer WTe_2 — •Felix Lüpke[1], Dacen Waters[2], Anh Pham[3], Jiaqiang Yan[4], David G. Mandrus[5], Panchapakesan Ganesh[3], and Benjamin M. Hunt[6] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Physics, University of Washington — [3]Center for Nanophase Materials Sciences, Oak Ridge National Lab — [4]Materials Science and Technology Division, Oak Ridge National Lab — [5]Department of Materials Science and Engineering, University of Tennessee — [6]Physics, Carnegie Mellon University

The quantum spin Hall (QSH) effect, characterized by topologically protected spin-polarized edge states, was recently demonstrated in monolayers of the transition metal dichalcogenide (TMD) WTe_2. However, the robustness of this topological protection remains largely unexplored in van der Waals heterostructures containing one or more layers of a QSH insulator. In this work, we use scanning tunneling microscopy and spectroscopy (STM/STS), to study twisted bilayer (tBL) WTe_2 and compare it to topologically trivial natural bilayer. By comparing our experimental observations to first principles calculations, we conclude that the twisted bilayers are weakly coupled, preserving the QSH states and preventing back scattering.

O 81.4 Fri 11:15 S052

Real-time TD-DFTB simulations and modeling of Fano-induced transparency in molecular van der Waals Heterostructures — •Carlos R. Lien-Medrano[1], Franco P. Bonafé[2], Chi Yung Yam[3], Carlos-Andres Palma[4], Cristián G. Sánchez[5], and Thomas Frauenheim[1] — [1]BCCMS, Uni-Bremen, Germany — [2]MPSD, Hamburg, Germany — [3]CSAR, Shenzhen, P. R. China — [4]IOP, Beijing, P.R. China — [5]UNCuyo, Mendoza, Argentina

While gating and doping in two-dimensional (2D) materials is well-known, the physics of photosensitizing and advanced optical properties have not been fully investigated, especially in the context of molecular vdW heterostructures (MVHs), that is, regular monolayer stacks on 2D materials. In a recent work [1], we employed an adapted Gersten-Nitzan (two point dipoles) model and real time time-dependent density functional tight-binding to study the optoelectronics of self-assembled monolayers on graphene nanoribbons. We found Fano resonances that cause electromagnetic induced opacity and transparency and reveal an additional incoherent process leading to interlayer exciton formation with a characteristic charge transfer rate. These results showcase hybrid van der Waals heterostructures as paradigmatic 2D optoelectronic stacks, featuring tunable Fano optics and unconventional charge transfer channels. Our findings open a path for improved design of modular multilayer organic photovoltaic devices.

[1] Lien-Medrano, C. R., et al. Fano Resonance and Incoherent Interlayer Excitons in Molecular van der Waals Heterostructures. Nano Letters (2022), 22(3), 911-917.

O 81.5 Fri 11:30 S052

High-throughput stacking reveals emergent and switchable properties of 2D van der Waals bilayers — •Sahar Pakdel, Asbjørn Rasmussen, Mads Kruse, Alireza Taghizadeh, Thomas Olsen, and Kristian Sommer Thygesen — CAMD, Computational Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby Denmark

Stacking atomically thin two-dimensional monolayers into van der Waals (vdW) heterostuctures offer new opportunities to tune physical properties of 2D materials. Here we provide a systematic ab initio-based study of homo-bilayers created by stacking several hundreds of stable monolayers containing up to 10 atoms per unit cell. We investigate all configurations commensurate with the primitive cell and verify our approach by comparing our stacking orders with available bulk compounds. For the stable bilayers within a 3 meV/Å^2 binding energy distance from the most stable configuration, we calculate a range of electronic and magnetic properties. We explore switchable properties in bilayer pairs related with a slide vector. Our work is a step towards rational design of layered vdW materials and contributes to the systematisation of 2D materials. Our results will be available online and integrated with the Computational 2D Materials Database (C2DB) which allows for comparison between mono- and bilayer properties.

O 81.6 Fri 11:45 S052

1D p-n junction electronic and optoelectronic devices from transition metal dichalcogenide lateral heterostructures grown by one-pot chemical vapor deposition synthesis — •E. Najafidehaghani[1], Z. Gan[1], A. George[1], T. Lehnert[2], G. Q. Ngo[3], C. Neumann[1], T. Bucher[3], I. Staude[3], D. Kaiser[1], T. Vogl[3], U. Hübner[4], U. Kaiser[2], F. Eilenberger[3], and A. Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Germany — [2]Ulm University, Central Facility of Materials Science Electron Microscopy, Germany — [3]Friedrich Schiller University Jena, Institute of Applied Physics, Germany — [4]Leibniz Institute of Photonic Technology (IPHT), Germany

Lateral heterostructures (LH) of dissimilar monolayer transition metal dichalcogenides provide great opportunities to build 1D in-plane p-n junctions for sub-nanometer thin low-power electronic, optoelectronic, optical, and sensing devices. Electronic and optoelectronic applications of such p-n junction devices fabricated using a scalable chemical vapor deposition process yielding $MoSe_2$-WSe_2 LHs are reported here. Their growth is achieved by in situ controlling the partial pressures of the oxide precursors by a two-step heating protocol. The grown LHs are characterized structurally and optically using optical microscopy, Raman

spectroscopy, and photoluminescence spectroscopy. High-resolution transmission electron microscopy further confirms the high-quality 1D boundary between $MoSe_2$ and WSe_2 in the LH. p-n junction devices are fabricated from these LH and their applicability solar cells, photodetectors, and electroluminescent emitters are demonstrated.