

DS 3: Layer Properties: Electronic, Optical and Mechanical Properties

Time: Monday 9:30–12:45

Location: H39

DS 3.1 Mon 9:30 H39

Ab initio description of layered excitonic insulators — ●MALTE RÖSNER¹, GIACOMO MAZZA², HANNES HÜBENER³, SIMONE LATINI³, UMBERTO DE GIOVANNI³, ANGEL RUBIO³, and ANTOINE GEORGES¹ — ¹Center for Computational Quantum Physics, Flatiron Institute - Simons Foundation, New York, USA — ²Ecole polytechnique, CNRS, Université Paris Saclay, Paris, France — ³Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Although proposed more than half a century ago hints for excitonic ground states have been found in just a few materials so far. Among them, the layered van der Waals material Ta₂NiSe₅ is a prominent candidate for realizing such a ground state defined by spontaneous electron-hole pair condensation. Here, we show how the excitonic ground state can be described by means of ab initio calculations. From this we learn how this exotic condensate can be manipulated by its environment.

DS 3.2 Mon 9:45 H39

Effects of screening on the optoelectronic properties of 2D materials — ●ABDERREZAK TORCHE, JENS HÜHNERT, and GABRIEL BESTER — University of Hamburg, Germany

2D materials represent nowadays a promising route for new technologies due to their exceptional optical and electronic properties. These properties are highly dependent on the surrounding environment, consequently, one can modify a desired property such as the band gap or the doping simply by changing the environment. Despite the fact that 2D materials have been studied since the discovery of graphene in 2004, both at the experimental and the theoretical levels, the understanding of the effects of screening (e.g. substrate effects) is still not complete although some general rules are well established.

From a theoretical point of view, the study of screening in 2D materials is computationally heavy. Standard approaches to study the optical properties of materials, such as the BSE formalism, have several limitations because the inclusion of the environment hinders the calculation of quasi-particle energies in 2D.

The goal of our research is to go beyond these limitations and treat larger systems (i.e. thousands of atoms) which are more relevant from an experimental (and/or industrial) point of view. For that goal, we propose a hybrid approach combining density functional theory and configuration interaction methods to predict the binding energies of excitations in 2D materials (excitons, trions, ...) taking the effect of the environment into account via screening.

DS 3.3 Mon 10:00 H39

Interlayer excitons in stacked TMDC heterostructures — ●ROLAND GILLEN and JANINA MAULTZSC — Department Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91054 Erlangen

We computed the theoretical bandstructures and absorption spectra of bilayer MoSe₂-WSe₂ and MoS₂-WSe₂ heterostructures with different stacking orders by solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections [1] and inclusion of spin-orbit-coupling. We find two spin-orbit split Rydberg series of low oscillation strength below the absorption onset of the monolayer materials, which arise from spatially indirect excitations between the K points of the hexagonal Brillouin zones of the constituent materials with a binding energy on the order of 250-300 meV. Additionally, our calculations firmly establish that the fundamental band gap of MoSe₂-WSe₂ heterostructures is indirect and has a distinct interlayer nature, possibly giving rise to a momentum- and spatially indirect contribution [2]. These results confirm the recent experimental observation of a doublet nature of the interlayer photoluminescence. We further show that the local stacking order leads to small variations in the hybridization between the MoSe₂ and WSe₂ bands and has a decisive effect on the polarization dependence of the interlayer excitonic absorption [2]. Our results motivate detailed studies of electron-phonon coupling effects and exciton dynamics in TMDC heterostructures by time-resolved optical experiments and ab initio methods.

[1] Gillen et al., IEEE JSTQE 23, 1 (2017); arXiv:1605.01972 (2016)

[2] Gillen et al., Phys. Rev. B 97, 165306 (2018)

DS 3.4 Mon 10:15 H39

Flexible anode materials - 2D transition metal car-

bides — ●DOMINIK LEGUT¹, HANG ZHANG², ZHONGHENG FU², RUIFENG ZHANG², QIANFAN ZHANG², HONGZHEN TIAN², TIMOTH C. GERMANN³, YUANQI GUO², SHIYU DU⁴, and JOSEPH S. FRANCISCO⁵ — ¹IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — ²School of Mat. Sci. and Eng., Beihang University, Beijing, China — ³Theor. Div., Los Alamos National Laboratory, USA — ⁴Eng. Lab. and Nucl. Ene. Mater., Chinese Acad. Sciences, Zhejiang 31520, China — ⁵Dep. of Chem., Purdue University, USA

MXenes exhibit outstanding properties and therefore been considered as promising electrode material candidates. Taking 2D transition metal carbides (TMCs) as representatives, we systematically explored several influencing factors, including transition metal species, layer thickness, functional group, and strain on their mechanical properties (e.g., stiffness) and their electrochemical properties (e.g., ionic mobility). Considering potential charge-transfer polarization, we employed a charged electrode model to simulate ionic mobility and found that ionic mobility has a unique dependence on the surface atomic configuration influenced by bond length, valence electron number, functional groups, and strain. Under multiaxial loadings, electrical conductivity, high ionic mobility, low equilibrium voltage with good stability, excellent flexibility, and high theoretical capacity indicate that the bare 2D TMCs have potential to be ideal flexible anode materials, whereas the surface functionalization degrades the transport mobility and increases the voltage due to bonding between the nonmetals and Li.

DS 3.5 Mon 10:30 H39

Photo-induced anomalous Hall effect in the type-II Weyl-semimetal WTe₂ at room-temperature — PAUL SEIFERT¹, FLORIAN SIGGER^{1,2}, JONAS KIEMLE¹, KENJI WATANABE³, TAKASHI TANIGUCHI³, CHRISTOPH KASTL⁴, ●PHILIPP BOOTZ¹, URSULA WURSTBAUER^{1,2}, and ALEXANDER HOLLEITNER^{1,2} — ¹Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — ²Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — ³Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan — ⁴Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, 94720 Berkeley, California, United States

Using Hall photovoltage measurements, we demonstrate that an anomalous Hall (AH) voltage can be induced in few layer WTe₂ under circularly polarized light illumination. By applying a bias voltage along different crystal axes, we find that the photo-induced AH conductivity coincides with a particular crystal axis. Our results are consistent with the underlying Berry-curvature exhibiting a dipolar distribution due to the breaking of crystal inversion symmetry. We find that the decay time of the AH voltage exceeds the electron-phonon scattering time by orders of magnitude but is consistent with the comparatively long spin-lifetime of carriers in the momentum-indirect electron and hole pockets in WTe₂. Our observation suggests, that a helical modulation of an otherwise isotropic spin-current is the underlying mechanism of the AHE.

DS 3.6 Mon 10:45 H39

Local and correlated studies of humidity-mediated ferroelectric thin film surface charge dynamics — ●IAROSLAV GAPONENKO¹, NEUS DOMINGO², NICOLAS STUCKI³, ALBERT VERDAGUER², and PATRYCJA PARUCH¹ — ¹DQMP, University of Geneva, 1211 Geneva, Switzerland — ²ICN2, Campus UAB, 08193 Bellaterra, Spain — ³HES-SO/hepia, 1213 Geneva, Switzerland

Surface water is present on all materials exposed to ambient environmental conditions, modifying the ground state in fundamental studies as well as affecting the operation of bare-chip devices. Due to its polar nature, water strongly interacts with domains and domain walls in ferroelectric materials.

Here, we present a combined Kelvin probe force microscopy (KPFM) and near-ambient pressure x-ray photoelectron spectroscopy (AP-XPS) study of the relative humidity (RH) dependence of the formation and evolution of surface charges on oppositely polarised PZT thin films. AP-XPS measurements show chemical differences on surface adsorbates as well as significant changes in the bulk ionic distribution as a function of both the as-grown polarisation state and after switching. KPFM measurements tracking the dissipation of surface

charges confirm that both the initial state of the samples and their switching history have an influence on the electrochemistry and surface charge dynamics as a function of RH. Through these two approaches, we demonstrate the complexity of surface water mediated chemistry and electrochemistry on ferroelectric materials.

15 min. break

DS 3.7 Mon 11:15 H39

Impedance spectroscopy at tunnel junctions with adjacent solid-state electrolyte layer — RICHARD MARQUARDT¹, •JÜRGEN CARSTENSEN², GEORGE POPKIROV³, FINN ZAHARI¹, HERMANN KOHLSTEDT¹, and MARTIN ZIEGLER⁴ — ¹Chair of Nanoelectronics, Faculty of Engineering, Kiel University, Germany — ²Chair of Functional Nanomaterials, Faculty of Engineering, Kiel University, Germany — ³Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, Bulgarian — ⁴Micro- and Nanoelectronic Systems, Electrical Engineering and Information Technology, Ilmenau University of Technology, Germany

Memristive devices for neuromorphic networks and non-volatile memories are getting a rapidly increased amount of attention in the last couple of years for neuromorphic applications, one promising candidate is the double barrier Nb/Al/Al₂O₃/NbOx/Au memristive device. Recent studies showed evidence, that the memristive character is based on a filamentary-free, homogenous interfacial switching mechanism. Here, mobile oxygen ions confined within the 2.5 nm thin NbOx layer alter the Schottky barrier of the top NbOx/Au interface. Therefore lead to the resistance change in the order of two magnitudes at 0.7V together with a change in the threshold voltage by a factor of five. In order to proof this model Impedance spectroscopy was applied to correlate the inner electronic and ionic process with the observed I-V characteristics. Evidence has been found that the Schottky interface is the active interface, which is responsive for the resistive switching of the device. The Al₂O₃ tunneling barrier is modeled as a linear resistance.

DS 3.8 Mon 11:30 H39

Binding mechanism of fluorine-containing ketones on zinc oxide surfaces for thin film transistor passivation — •JONAS KÖHLING, NATALIYA KALINOVICH, GERD-VOLKER RÖSCHENTHALER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Solution processed metal-oxide thin film transistors are used in optical, mechanical and electrical applications. Oxygen and moisture induced surface traps cause instability and unreliability under electrical operation. For application purposes it is necessary to passivate surface traps. Tailored organic molecules can be effectively used for this task. For optimal functionality trap mechanisms and binding properties of these organic molecules have to be investigated.

In this work, the binding of fluorine-containing organic molecules on zinc oxide surfaces is monitored and the effect on electrical performance in thin film transistors was studied. Zinc oxide thin film transistors (12 nm thickness) were fabricated by aqueous spray pyrolysis. In order to overcome their instability against oxygen and moisture tailored organic fluorine-containing molecules with ketone groups as anchors sites were employed as passivation. Chemical binding of the molecules to hydroxide groups at the surface of zinc oxide is tracked by XPS and UV-Vis. The exact binding situation is elucidated by NMR. After passivation of the zinc oxide surface transistors exhibit almost vanished hysteresis, increased mobility and much better stability against electrical bias stress. Electrical results were correlated with the effective charge of the anchor atoms calculated by density functional theory.

DS 3.9 Mon 11:45 H39

Visualization of Engineered Catalytic Hydrogen Evolution Sites on Molybdenum Dichalcogenides under Reaction Conditions — •BEATRICE SALA², ELMAR MITTERREITER^{1,2}, YUNCHANG LIANG³, MATTHIAS GOLIBRZUCH², DAVID McLAUGHLIN³, CHRISTOPH CSOKLICH³, ALEXANDER HOLLEITNER^{1,2}, URSULA WURSTBAUER^{1,2}, and ALIAKSANDR S. BANDARENKA^{1,3,4} — ¹Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany — ²Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany —

³Physik-Department ECS, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ⁴Catalysis Research Center TUM, Ernst-Otto-Fischer-Straße 1, 85748 Garching, Germany

2D transition metal dichalcogenides are abundant and cost effective (co-)catalysts with tunable physical properties. In this respect, these materials are suitable for reactions related to energy provision, for instance hydrogen evolution reaction (HER). It is vital to understand which surface sites are highly active to improve the catalytic behavior of those materials. Here, we visualize catalytically active sites at the surface of molybdenum disulfide (MoS₂) with lateral resolution on the nanometer scale by means of electrochemical STM. The edges of single MoS₂ flakes show high catalytic activity, whereas their surfaces are inactive. Furthermore, we demonstrate that the inert basal plane of these materials can be activated towards the HER with the focused beam of a helium ion microscope. Thus, we show the possibility to generate active sites with a spatial resolution below a few nanometer.

DS 3.10 Mon 12:00 H39

High throughput investigation on the magnetic and electronic properties of out-of-plane ordered MXene — •XINRU LI and HONGBIN ZHANG — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Two-dimensional (2D) MXene systems which can be obtained by etching MAX phases are considered as a breakthrough in synthesizing 2D functional materials. In this work, based on our previous high throughput screening of 14 Al-based MAXs out of 1080 MAX systems, we investigated 80 corresponding MXenes with ordered out-of-plane TM substitutions (o-MXene) in an extensive way. The magnetic ground states were determined by considering ferromagnetic (FM), one collinear antiferromagnetic (cAFM), and one noncollinear antiferromagnetic (nocAFM) orderings. It is observed that 25 out of 41 cases are with the FM ground states, 9 out of 41 cases are cAFM, while the rest are with intriguing nocAFM configurations. Furthermore, for the nocAFM o-MXenes, it is observed that the in-plane magnetization direction can induce significant changes on the electronic properties.

DS 3.11 Mon 12:15 H39

Designing multifunctional i-MXene — •QIANG GAO, XINRU LI, and HONGBIN ZHANG — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

MXene which can be obtained by etching the bulk MAX phase has attracted intensive attention, as a class of two-dimensional (2D) materials for potential applications as electrode materials, thermoelectric materials, and topological insulators.[1] Recently, the in-plane ordered MAX (i-MAX) compounds (Cr_{2/3}M_{1/3})₂AlC (M = Sc and Y), (V_{2/3}Zr_{1/3})₂AlC, and (Mo_{2/3}Y_{1/3})₂AlC have been reported.[2,3] Motivated by this, we have performed high-throughput screening for novel i-MXene (as derived from the i-MAX phase) systems, focusing particularly on the transport properties of magnetic cases. It is observed that systems with intriguing properties can be realized, such as 2D spin-gapless semiconductors, topological insulators, and candidates for thermoelectric applications. [1] G.R. Bhimanapati, *et al.*, ACS Nano **9**, 11509 (2015). [2] J. Lu, A. Thore, R. Meshkian, Q. Tao, L. Hultman, and J. Rosen, Crystal Growth & Design **17**, 5704 (2017). [3] M. Dahlqvist, J. Lu, R. Meshkian, Q. Tao, L. Hultman, and J. Rosen, Sci. Adv. **3**, e1700642 (2017).

DS 3.12 Mon 12:30 H39

Superconductivity above 28 K in single unit cell FeSe films interfaced with GaO₂-δ layer on NdGaO₃(110) — •LILI WANG — Tsinghua University, Beijing, China

We prepared single unit cell FeSe films on GaO₂-δ terminated perovskite NdGaO₃(110) substrates and performed ex situ transport and scanning transmission electron microscopy measurements under protection of FeTe films. Our experimental measurements showed that the single unit cell FeSe films interfaced with GaO₂-δ layer get electron doped with interface charge transfer. Most importantly, this kind of heterostructure exhibits a superconducting transition with onset temperature of ~28 K, significantly enhanced compared to the value of 8 K for bulk FeSe. Our work indicates that FeSe/GaO₂-δ is another hetero-structure, after FeSe/TiO₂-δ, that hosts interface enhanced superconductivity, providing a new platform for investigating the mechanism of interface high temperature superconductivity.