O 78: Poster Session VI: 2D Materials: Electronic structure, excitations, etc. II

Time: Wednesday 13:30–15:30 Location: P

O 78.1 Wed 13:30 P

Transitional metal doped $Bi_{2-n}X_nO_2Se$ - novel 2D magnetic semiconductor — •Dominik Legut[1], Xiaopeng Liu[2], Ruifeng Zhang[2], Zhongheng Fu[2], Tinshuai Wang[2], Yanchen Fan[2], and Qianfan Zhang[2] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — [2]School of Mat. Sci. and Eng., Beihang University, Beijing, China

For the spintronic applications like large data storages (high capacity HDD) the industry searches for ferromagnetic insulators at nanoscale size. Recently the discovery of Bi_2O_2Se/Te phases that exist as 2D material and still are semiconducting attract attention. Here we investigate $Bi_{2-n}X_nO_2Se$ by transitional metal doping to introduce a magnetic spin order. We explore the electronic and magnetic properties of various ferromagnetic (e.g. Fe) or antiferromagnetic (e.g. Mn) transitional metals doped Bi_2O_2Se phases within the framework of density functional theory based electronic structure calculations. We start with the magnetic order of the bulk phase in which the magnetic atoms form interlayer coupling that vary with the type and concentration of doped atoms and go towards the nanoscale dimension, i.e. 2D materials. As a result of the competitions of magnetic interactions the magnetic anisotropy energy is a crucial quantity. In combinations with Monte Carlo simulations we are able to solve the exchange interaction constants for the Heisenberg model and therefore evaluate the Curie temperature to see if these types of materials are suitable to become novel dilute magnetic semiconductors for spintronic applications at room and above temperatures.

O 78.2 Wed 13:30 P

Analysis of interlayer excitons in the case of MoS_2 on GaSe. — •Christian Wagner, Mahfujur Rahaman, Dietrich R.T. Zahn, and Sibylle Gemming — Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

We study the formation of *interlayer* excitons in GaSe | MoS_2 heterostacks as a function of layer composition from first principles in order to specifically tailor photon absorption in layered heterostacks.

The electronic interaction in semiconducting 2D layered material heterostacks is often reasonably described by a perturbation of the physical effects of the isolated homostacks. But their optical properties go beyond this picture of weak layer interaction: moiré potentials influence exciton dynamics and bound *interlayer* excitons may emerge. Interlayer excitons are composed of electron and hole states from different layers. These mixed states are measured experimentally by photoluminescence and photocurrents and predicted by theory, e.g. in MoS_2 on GaSe [1].

The composition of all interlayer excitons are thoroughly analyzed by solving the Bethe-Salpeter equation for the heterobilayer of MoS_2 on GaSe. The exciton Hamiltonian is diagonalized and the exciton wave functions are projected onto layers as a function of k-space. By means of density functional theory and optical selection rules, these optical interlayer transitions are extrapolated for larger heterostacks and compared directly with experiments.

[1] M. Rahaman, C. Wagner et al., J. Phys.: Condens. Matter 31, 114001 (2019).

O 78.3 Wed 13:30 P

Spin-polarized VLEED from single-layer MoS_2/Au(111): Investigation of spin-orbit-induced effects — •Christoph Angrick[1], Annika Henriksen[1], Nicole Mutzke[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

The influence of spin-orbit interaction on low-energy electron reflection from single-layer MoS_2 on Au(111) was studied by VLEED (very-low-energy electron diffraction) [1,2]. The spin-dependent electron reflection was investigated for a wide range of electron incidence angles and kinetic energies. Since the adlayer coverage is about 30%, we studied the Au(111) substrate and a MoS_2 bulk sample for comparison. This approach enabled us to distinguish between adlayer and substrate signals.

For MoS_2/Au(111), we detected a spin asymmetry of the reflected intensities, which shows a characteristic feature with alternating sign in the energy region of a VLEED fine structure [1]. The Au(111) substrate, in contrast, shows qualitatively different spin-asymmetry features, partially with reversed sign compared with MoS_2/Au(111). The results of bulk MoS_2 confirm that the characteristic feature in the single-layer data originates from MoS_2. The influence of the adlayer-substrate interaction on the results will be discussed.

[1] Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)
[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020)

O 78.4 Wed 13:30 P

Four- and twelve-band low-energy symmetric Hamiltonians and Hubbard parameters for twisted bilayer graphene using ab-initio input — •Arkadiy Davydov, Kenny Choo, Mark H. Fischer, and Arkadiy Davydov — Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich (Switzerland)

A computationally efficient workflow for obtaining low-energy tight-binding Hamiltonians for twisted bilayer graphene, obeying both crystal and time-reversal symmetries, is presented in this work. The Hamiltonians at the first magic angle are generated using the Slater-Koster approach with parameters obtained by a fit to ab-initio data at larger angles. Low-energy symmetric four-band and twelve-band Hamiltonians are constructed using the Wannier90 software. The advantage of our scheme is that the low-energy Hamiltonians are purely real and are obtained with the maximum-localization procedure to reduce the spread of the basis functions. Finally, we compute extended Hubbard parameters for both models within the constrained random phase approximation (cRPA) for screening, which again respect the symmetries. The relevant data and results of this work are freely available via an online repository. The workflow is straightforwardly transferable to other twisted multi-layer materials.

O 78.5 Wed 13:30 P

Optoelectronic properties of point defects in hBN — •Alexander Kirchhoff, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

While pristine hexagonal boron nitride (hBN) is a wide-gap insulator, its point defects are discussed as light emitters in the visible optical spectrum. In this study, we examine two substitutional carbon impurities, C_N and C_B, the nitrogen vacancy V_N, the divacancy V_{NB} and a carbon substitution with a nitrogen vacancy adjacent to it, C_BV_N, in a hBN monolayer from an *ab initio* approach, via the GW/BSE approximation. Our results show deep defect states and defect-related excitations with energies in the visible regime. We present a detailed analysis of their spatial structure and energetic composition.

O 78.6 Wed 13:30 P

Proroper ab-initio dielectric function of 2D materials and their polarizable thickness — •Lorenzo Sponza and François Ducastelle — Université Paris-Saclay, ONERA, CNRS, Laboratoire d'étude des microstructures, 92322, Châtillon, France

We derive a formalism allowing us to separate inter-layer contributions to the polarizability of a periodic array of 2D materials from intra-layer ones. To this aim, effective profile functions are introduced. They constitute a tight-binding-like layer-localized basis involving two lengths, the effective thickness d characteristic of the 2D material and the inter-layer separation L. The method permits, within the same formalism, either to compute the single-layer dielectric function from an ab-initio periodic calculation (ab-initio exfoliation) or to stack several 2D materials to generate a finite-thickness van der Waals heterostructure (ab-initio stacking).

O 78.7 Wed 13:30 P

Electronic and vibrational properties of TMDs heterogeneous bilayers, nontwisted bilayers silicene/TMDs heterostructures and photovoltaic heterojunctions of fullerenes with TMDs monolayers — •Mohamed Barhoumi[1] and Moncef Said[2] — [1]Monastir university, Monastir, Tunisia — [2]Monastir university, Monastir, Tunisia

In the recent years, many studies have been showed that bilayer and heterobilayer transition metal dichalco- genides might offer properties superior to those of monolayer. Nevertheless, only very few have been

synthe- sized. Using first-principles calculations, we study the structural, electronic and vibrational properties of new transition metal dichalcogenides heterogenous bilayers (i.e., MX2/MX2 with M, M = Pd, Pt, W; X, X = S, Se). Also, we investigate the structural, vibrational and electronic properties of silicene/TMDs and C60/TMDs. Our results show that the predicted geometry can well reproduce the structural parameters, where very well agreement was obtained between the calculated and previous studies for the monolayers. Our calculations show that all the heterobilayers are indirect band-gap semiconductors with the exception of the WS2/PdSe2 and WSe 2/PdSe2 heterobilayers, which are metallic systems. In the case of the heterostructures bilayers (silicene/MX2), the bandgap is decreased when Pd is changed to Pt, and when the atomic number of X increases, the band-gap increases. Also, by analyzing the electronic band structures and the electron density, it appeared that C60/MX2 is a promising system for photovoltaic applications.

O 78.8 Wed 13:30 P

Decoupled Strain Response of Ferroic Properties in Multiferroic $VOCl_2$ Monolayer — •Akshay Mahajan and Somnath Bhowmick — Department of Materials Science and Engineering, Indian Institute of Technology, Kanpur, Kanpur 208016, India

Two-dimensional (2D) magnetoelectric multiferroic materials are a special class of 2D materials that holds promising applications in the miniaturization of logic and memory devices, along with the possibility to realize new low-dimensional device architectures. In this work, we have reported a strain-engineering-based study for a 2D multiferroic material, $VOCl_2$ monolayer, that shows independent control of magnetic and ferroelectric properties via applying strain along the different in-plane crystallographic directions. An in-plane strain of around 4% along the non-polar axis was found to cause a transition from an antiferromagnetic (AFM) ground state with an out-of-plane magnetization to a ferromagnetic (FM) ground state with in-plane magnetization. Additionally, the tensile strain along the polar axis enhances the ferroelectric polarization. An increase in the ferroelectric switching energy barriers and the magnitude of the magnetic exchange coupling parameter suggest enhancing ferroelectric and ferromagnetic stability with tensile strain. The work reveals the $VOCl_2$ monolayer as a strain-tuneable multiferroic material holding great promises for future generation nanoelectronic devices.

O 78.9 Wed 13:30 P

Band structure and image potential states of hBN/Cu(111) — •Jan Beckord, Matthias Hengsberger, and Jürg Osterwalder — Physik-Institut, Universität Zürich, Schweiz

We present a study on the band structure and the image potential states of a hexagonal boron nitride (hBN) monolayer on the Cu(111) surface. The orientation of the bare copper surface was measured by XPD and ARPES. The hBN layer was then grown by chemical vapour deposition from borazine. XPS spectra confirm the presence of a full monolayer with the correct stoichiometry, and ARPES band structure measurements with He IIa radiation along the high symmetry directions $\overline{\Gamma K}$ and $\overline{\Gamma M}$ are in excellent agreement with literature values for other metal substrates. The work function is significantly reduced from 4.9 eV to 4.1 eV, which agrees with the reported work function in valleys of the corrugated surface measured by STM. We then measured the unoccupied electronic states with two-photon photoelectron spectroscopy on the bare copper as well as on the hBN covered surface. Varying the photon energy allowed us to separate the first two image potential states n=1 at 0.83 eV and n=2 at 0.16 eV below the vacuum level from the Shockley surface state at a binding energy of 0.27 eV. The valence band maximum in normal emission direction appeared at a binding energy of 2.21 eV.

O 78.10 Wed 13:30 P

Gate-Tunable Curvature-Induced Charge Localization in Two-Dimensional Semiconducting Monolayers — •bong gyu shin[1], jz-yuan juo[1], soon jung jung[1], and klaus kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale deLausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization in monolayer MoS_2 on SiO_2/Si using a gate-tunable home-built scanning tunneling microscope at ∼4.9K. A MoS_2 monolayer follows surface roughness of the substrate, exhibiting random distribution of bending strain with band gap reduction at a local region, acting like a potential well leading to charge localization. At higher electron doping levels, the tunneling-barrier-height over high curvature regions is reduced since localized electron charges lower the local work function. Moreover, we observed the spatial flattening of the conduction (valence) band edge over the band gap fluctuation at electron- (hole-) doping of $\sim 10^{13}$ cm^{-2}. In our theoretical calculations, the trends of local work function and spatial flattening of band edges by doping levels were confirmed in various thin 2D semiconductors, providing the general mechanism of charge localization via curvature effects.

O 78.11 Wed 13:30 P

Spin and orbital nature of electronic structure in transition metal dichalcogenides — •Jakub Schusser[1,2,3], Mauro Fanciulli[1], Samuel Beaulieu[4], Maria C. Richter[2], Olivier Heckmann[2], Zakariae El Youbi[2,5], Cephise Cacho[5], Ralph Ernsthofer[4], Karol Hricovini[1], Jan Minar[2], and Friedel Reinert[3] — [1]LPMS, CY Cergy-Paris University, Neuville-sur-Oise, France — [2]NTC, University of West-Bohemia, Pilsen, Czech Republic — [3]EP VII and Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [4]DPC, Fritz-Haber-Institute, Berlin, Germany — [5]DLS, Harwell Campus, Didcot, UK

Our work is concerned with the polarization of electrons and orbital texture in non-magnetic materials. We studied stationary and dynamic electron states by photoemission and spin-polarized relativistic Korringa-Kohn-Rostoker calculations on three bulk transition metal dichalcogenide samples. On bulk WTe2, a Weyl type-II semimetal candidate, we performed spin-, time- and angle-resolved photoemission spectroscopy experiments at different pump-probe time delays to reveal the mechanism behind the relaxation process of spin-polarized electrons above the Fermi level in the supposed Weyl points region. On bulk 2H-WSe2, using different crystal orientations that are mathematically equivalent to time-reversal operation, we introduce a new observable called "time-reversal dichroism" which contains information about the hidden orbital texture of the electronic states. For 1T-HfTe2 as a model system with both inversion and time-reversal symmetries in the bulk, we performed an analysis of the spin-polarized photocurrent.

O 78.12 Wed 13:30 P

Strain control of the competition between metallic and semiconducting states in single-layers of $TaSe_3$ — •Jose Angel Silva-Guillen[1] and Enric Canadell[2] — [1]School of Physics and Technology, Wuhan University, Wuhan 430072, China — [2]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus Bellaterra, 08193 Bellaterra, Spain

Recently, layered group IV transition-metal trichalcogenides have been the object of much attention because they provide a convenient platform as single- or few-layers flakes for applications in devices. Interestingly, group V transition metal chalcogenides have not yet been thoroughly studied as single-layers or few-layer flakes. One of them, TaSe3, is a semi-metal and superconductor in the bulk and a charge density wave has been claimed to occur in mesowires. Since in the bulk there are noticeable interlayer Se–Se interactions it is challenging to see how suppression of interlayer interactions can modify the electronic structure and physical properties of this material. We report a DFT study of the electronic structure of $TaSe_3$ single-layers and its evolution under different types of strain. We find that the pristine TaSe3 single-layer exhibits a metallic state which can be modified in different ways under the application of biaxial strain or uniaxial strain along either the short or long directions of the layer. Electronic instabilities related to both electron and hole pockets as well as the stabilization of a semiconducting state are shown to be possible. These single-layers are thus predicted to be versatile materials where different states compete as a function of relatively small differences in strain.

O 78.13 Wed 13:30 P

Ab Initio study of the structural and electronic properties of Niobium Sulfide (NbS2) and Lithium Niobium Sulfide (LiNbS2) bulk and (001) surfaces — •Jorge D. Vega and Henry P. Pinto — Universidad Yachay Tech, Urcuqui, Ecuador

In the context of the discovery of new materials, intercalation of Lithium (Li) atoms among layers of NbS2 can be performed. However, few experimental works deal with this material. Recently, Voiry et al. performed some experiments with LiNbS2 providing some insights about the properties of this system. Hence, we describe this material

with state of the art non-empirical density functionals in the framework of density-functional theory (DFT). Specifically, we describe various insights regarding the electronic and atomic structure, lattice parameters, scanning tunnelling microscopy images and phonons of the bulk and surfaces of LiNbS2. We perform the computations with the meta-GGA SCAN functional and some variations of the hybrid HSE as implemented in VASP. We found out that SCAN+rVV10 performs very well in the description of certain properties of LiNbS2 and NbS2. Besides, we tested the hybrid HSE12 and HSE12s and compared with the customary HSE06. The performance of the hybrids is discussed too. Interestingly, we found that the intercalation of Li on NbS2 produces a considerable band-gap, making the material a semiconductor and providing promising technological applications.

O 78.14 Wed 13:30 P

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistor — •Aleksandar Matković[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[3], Markus Kratzer[1], Esther Karner-Petritz[2], Alexander Fian[2], Herbert Gold[2], Michael Gärtner[4], Andreas Terfort[4], Christian Teichert[1], Egbert Zojer[3], Karin Zojer[3], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Joanneum Research MATERIALS, Weiz, Austria — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Germany

This study aims at direct imaging of contact resistance in MoS_2-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS_2 have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both carrier injection and extraction points, we demonstrate asymmetry of contact resistances in MoS_2-based TFTs, as well as their non-linear and bias-dependent behavior [10.1002/aelm.202000110].