O 66: Poster Session V: 2D Materials: Electronic structure, excitations, etc. I

Time: Wednesday 10:30–12:30 Location: P

O 66.1 Wed 10:30 P

Selective Oxygen Functionalization of the h-BN/Rh(111) Nanomesh — •Eva Marie Freiberger, Florian Späth, Fabian Düll, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität, Erlangen, Germany

2D materials such as the graphene analogue hexagonal boron nitride (h-BN) are interesting due to their unique structural, chemical and electronic properties. The morphology of a supported h-BN layer strongly depends on the underlying crystal surface. In the case of Rh(111) as substrate, a Moiré with pore and wire regions evolves, also known as nanomesh. Chemical modification, e.g. covalent functionalization with hydrogen and oxygen, of Ni(111) supported h-BN has already been reported. In the case of the h-BN nanomesh on Rh(111), such functionalization is especially interesting since the pores and wires may show different reactivity towards functionalization enabling spatially defined modification of h-BN.

Herein, we present detailed studies on the adsorption of molecular oxygen on the h-BN nanomesh on Rh(111). Using synchrotron radiation-based in situ high-resolution X-ray photoelectron spectroscopy we are able to provide a deep insight in this system regarding the adsorption behavior and the thermal stability of the covalent functionalization. Oxygen functionalization is performed via a supersonic molecular beam and is found to be an activated process occurring selectively in the pores of h-BN. The adsorbed oxygen is proposed to bind molecularly to two boron atoms in the pores of the Moiré. It is stable up to about 650 K.

O 66.2 Wed 10:30 P

Unconventional superconductivity mediated by spin fluctuations in single-layer NbSe2 — Wen Wan, Paul Dreher, Rishav Harsh, Francisco Guinea, and •Miguel M. Ugeda — Donostia International Physics Center (DIPC), Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain.

Van der Waals materials provide an ideal platform to explore superconductivity in the presence of strong electronic correlations, which are detrimental of the conventional phonon-mediated Cooper pairing in the BCS-Eliashberg theory and, simultaneously, promote magnetic fluctuations. Despite recent progress in understanding superconductivity in layered materials, the glue pairing mechanism remains largely unexplored in the single-layer limit, where electron-electron interactions are dramatically enhanced. Here we report experimental evidence of unconventional Cooper pairing mediated by magnetic excitations in single-layer NbSe2, a model strongly correlated 2D material. Our high-resolution spectroscopic measurements reveal a characteristic spin resonance excitation in the density of states that emerges from the QP coupling to a collective bosonic mode. This resonance, observed along with higher harmonics, gradually vanishes by increasing the temperature and upon applying a magnetic field up to the critical values, which sets an unambiguous link to the superconducting state. Furthermore, we find clear anticorrelation between the energy of the spin resonance and its harmonics and the local superconducting gap, which invokes a pairing of electronic origin associated with spin fluctuations.

O 66.3 Wed 10:30 P

A full gap above the Fermi level: the charge density wave of monolayer VS2 — •Camiel van Efferen[1], Jan Berges[2], Joshua Hall[1], Erik van Loon[2], Stefan Kraus[1], Arne Schobert[2], Tobias Wekking[1], Felix Huttmann[1], Eline Plaar[1], Nico Rothenbach[3], Katharina Ollefs[3], Lucas Machado Arruda[4], Nick Brookes[5], Gunnar Schönhoff[2], Kurt Kummer[5], Heiko Wende[3], Tim Wehling[2], and Thomas Michely[1] — [1]UzK, Köln, Germany — [2]UB, Bremen, Germany — [3]UDE, Duisburg, Germany — [4]FUB, Berlin, Germany — [5]ESRF, Grenoble, France

We present experimental evidence, via scanning tunneling microscopy and spectroscopy, of a 2/3ΓK charge density wave (CDW) in monolayer VS2. The CDW is shown to be stable at room temperature, and causes a full CDW gap in the unoccupied states of VS2. Unlike conventional CDWs, which undergo a metal-insulator transition, creating a gap at the Fermi level, the CDW in VS2 induces a topological metal-metal Lifshitz transition. Our ab initio calculations show anharmonic coupling of transverse and longitudinal phonons to be essential for the formation of the CDW and the full gap above the Fermi level. Additionally, x-ray magnetic circular dichroism reveals the absence of net magnetization in this phase, pointing to a coupled CDW-antiferromagnetic ground state.

O 66.4 Wed 10:30 P

Charge Transfer of Twist-Angle-Dependent Phosphorene-Graphene Heterobilayers. — •el-abed Haidar — The University of Sydney, Sydney, Australia

Twistronics is the study of the changes to the electronic properties of two-dimensional material bilayers due to rotational stacking, or twisting. In this work we explore the impact of twisting on the vertical charge transfer in a graphene-phosphorene bilayer using density-functional theory. We examine different twist angles and find significant drop in charge transfer when the twist changes from zero to greater than zero degrees. Such interesting feature can have major impacts in enriching two dimensional twistronics concepts especially their electronic properties.

O 66.5 Wed 10:30 P

Electronic structure and charge density wave in monolayer NbS_2 — •Timo Knispel[1], Jeison A. Fischer[1], Daniela Mohrenstecher[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], and Thomas Michely[1] — [1]Institute of Physics II, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institute of Theoretical Physics, Bremen Center for Computational Materials Science, University Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

We investigated monolayer 1H-NbS_2 grown in-situ on Gr/Ir(111) by high resolution scanning tunneling microscopy and spectroscopy at temperatures down to 0.4K. The characteristic 3x3 CDW pattern is present only in the monolayer, but absent in the bilayer. We analyze the CDW gap, contrast inversion in the dI/dV maps towards both sides of the gap and the suppression of the CDW pattern in the gap. Furthermore, quasiparticle interference is observed at island edges and defects and enables us to measure the dispersion of the hole-like pocket around the Γ-point. Density of states, dispersion around the Γ-point and the properties of the CDW are compared to density functional theory calculations.

Support from the Deutsche Forschungsgemeinschaft, SFB 1238 (project number 277146847, subprojects A01 and B06) is gratefully acknowledged.

O 66.6 Wed 10:30 P

Metal-to-insulator transition in MoS_2 by contactless chemical gating — •Wouter Jolie[1,2], Clifford Murray[1], Camiel van Efferen[1], Jeison A. Fischer[1], Carsten Busse[2], Hannu-Pekka Komsa[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Microelectronics Research Unit, University of Oulu, Finland

We present an effective way to gate semiconducting transition metal dichalcogenides without changing their direct chemical environment. The principle is demonstrated for MoS_2 on graphene on Ir(111). Intercalation of oxygen (europium) between graphene and Ir(111) removes (adds) charge in graphene, leading to a strong gating effect in MoS_2. Using scanning tunneling microscopy, we show that removing charge with oxygen leads to a 450 meV shift of the MoS_2 band gap with respect to the Fermi level. Adding charge with europium shifts the conduction band below the Fermi energy, accompanied by a band gap reduction of 700 meV due to renormalization. In addition, we find that gating also shifts the one-dimensional band present in MoS_2 mirror twin boundaries, which can be used as gating sensors.

O 66.7 Wed 10:30 P

Surface and interface effects in oxygen deficient $SrMnO_3$ thin films grown on $SrTiO_3$ — •Moloud Kaviani and Ulrich Aschauer — Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland

Complex oxide functionality, such as ferroelectricity, magnetism or superconductivity, is often achieved in epitaxial thin-film geometries. Oxygen vacancies tend to be the dominant type of defect in these

materials but a fundamental understanding of their stability and electronic structure has so far only been established in the bulk or strained bulk, neglecting interfaces and surfaces present in the thin-film geometry. We investigate here by first-principles calculations, oxygen vacancies in the model system of a $SrMnO_3$ (SMO) thin-film atop a $SrTiO_3$ (STO) (001) substrate. We establish structural and electronic differences compared to bulk SMO that, in addition to misfit strain result also from under-coordination at the film surface. We then study the stability and electronic structure of oxygen vacancies in both the thin-film and the substrate, showing that electrostatics render oxygen vacancies more stable towards the film surface. As opposed to bulk SMO, we observe only partial reduction of Mn^{4+} to Mn^{3+} and for oxygen vacancies in SrO layers, a reduction of Mn only in the layer below the vacancy. We relate this to crystal field changes at the surface, that strongly alter the defect chemistry in the film. Our results show that surface and interface effects lead to significant differences in stability and electronic structure of oxygen vacancies in thin-film geometries compared to the (strained) bulk.

O 66.8 Wed 10:30 P

Mechanism of Self-Intercalation in Niobium Disulphide Monolayers on Gr/Ir(111) — •Daniela Mohrenstecher[1], Timo Knispel[1], Carsten Speckmann[2], Jeison Fischer[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Physics of Nanostructured Materials, University of Vienna, 1090 Wien, Austria

For 2D layered TMDCs the intercalation of native metal atoms into the van-der-Waals gap under metal excess conditions is a well-known phenomenon [1] and may result in covalently bonded materials that may exhibit phenomena like ferromagnetic order or spin-frustrated Kagome lattices [2]. Here we report self-intercalation for in-situ grown NbS_2 monolayers on Gr/Ir(111) .The process utilizes Nb atoms that are already present in the material and traverse from the pristine material into the van-der-Waals gap between NbS_2 and graphene during post-growth annealing.
Our quantitative coverage analysis based on scanning tunneling microscopy images indicates a conversion of Nb from the pristine material into the intercalated phase containing a stoichiometry of $Nb_{5/3}S_2$, featuring a $\sqrt{3} \times \sqrt{3}$ R30° superstructure. Moreover, self-intercalation suppresses the charge density wave of the NbS_2 monolayer. Using tunneling spectroscopy dramatic changes are found in the electronic structure self-intercalated compared to pristine non-intercalated layers.
[1] Jellinek et al. Nature 185, 376 - 377 (1960)
[2] Zhao et al. Nature 581 171-177 (2020)

O 66.9 Wed 10:30 P

The role of surface termination in the electronic, magnetic and catalytic properties of hematene: a computational study — •Mahdi Ghorbani-Asl, Yidan Wei, and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

Very recently, a new class of non-van der Waals 2D materials including hematene have been successfully exfoliated from their non-layered crystal counterparts.[1] Using density functional calculations, we have systematically studied the stability, electronic and magnetic properties of 2D α-Fe_2O_3 nanosheets and their functionalized derivatives.[2] Our results show that not only that different surface passivation with hydrogen on hydroxyl groups may exist but also passivation with the former group significantly facilitates the stability of material under ambient conditions. The hydrogenated sheets are found to be a half-metal, whereas the fully hydroxylated sheets are antiferromagnetic semiconductors. We show that the reduced dimensionality and defects on the hematene surface can also enhance the catalytic activity of the material for the oxygen evolution reaction.[3]

[1] A. Puthirath Balan, S. Radhakrishnan, C. F. Woellner, et al. Nat. Nanotechnol. 13, 602 (2018).
[2] Y. Wei, M. Ghorbani-Asl, and A. V. Krasheninnikov, J. Phys. Chem. C 124, 22784 (2020).
[3] B. Mohanty, Y. Wei, M. Ghorbani-Asl, A.V. Krasheninnikov, et. al, J. Mater. Chem. A 8, 6709 (2020).

O 66.10 Wed 10:30 P

Electronic properties of metal (Fe, Co, Ni, V) / $MoSe_2$ 2D-heterostructures. — •Lyes Mesbahi[1], Omar Messaoudi[1], Hamid Bouzar[1], and Samir Lounis[2] — [1]Laboratoire de Physique et Chimie Quantique (LPCQ), Mouloud Mammeri University, BP 17 RP, 15000 Tizi-Ouzou, Algeria — [2]Peter Grunberg Institut and Institute for Advanced Simulation, Forschungszentrum Julich & JARA, D-52425 Julich, Germany

We present a comparative first principles investigation of the electronic properties of 2D systems consisting of a $MoSe_2$ monolayer with a transition metal overlayer : Fe, Co, Ni and V. Our calculations show that Fe-$MoSe_2$ and Co-$MoSe_2$ are half-metallic ferromagnets with bandgaps of 0.94 eV and 0.74 eV, respectively, for one of the spin channels. Moreover, Ni-$MoSe_2$ converges into a semi-conductor with an indirect bandgap of 0.68 eV. Interestingly, V-$MoSe_2$ turns out to be an anti-ferromagnetic material with a gapless dirac-cone located 0.20 eV below the Fermi level. The combined effect of time-reversal symmetry breaking and the effect of spin-orbit coupling induced by Mo, lead to non-degenerate K and K′ valleys, which renders these heterostructures good candidates for diverse spintronic applications.

O 66.11 Wed 10:30 P

Atomic-scale characterization of few-layer Cr5Se8 — •Paul Dreher[1], Wen Wan[1], Carmen Gonzalez Orellana[2], Max Ilyn[2], Javier Herrero-Martin[3], Pierluigi Gargiani[3], Marco Gobbi[4], Santiago Blanco-Canosa[4], and Miguel Ugeda[1] — [1]Donostia International Physics Center, Donostia - San Sebastián, Spain — [2]Centro de Física de Materiales (CSIC-UPV/EHU) — [3]ALBA Synchrotron Light Source — [4]CIC Nanogune

The realization of magnetic order at the two-dimensional limit is currently a priority for Materials Science. In this arena, transition metal chalcogenides have emerged as candidate magnetic 2D materials with unprecedented robust chemical stability, which could enable their integration in durable, flexible magnetic devices. Here we perform combined atomic-scale structural and electronic characterization of few layer Cr5Se8 with its mesoscopic magnetic characterization. We have studied the atomic, electronic and magnetic structure of MBE-grown few-layer Cr5Se8 on graphene substrates (BLG/SiC(0001) and HOPG) by means of 4.2K-STM/STS and XMCD measurements. STM imaging reveals that Cr5Se8 present both Se- and Cr-terminations, the latter showing a 2x2 periodicity in the Cr plane stable up to room temperature. Both terminations exhibit a semiconducting behavior with an accused layer-dependent gap value maximized at 1.2 eV for three layers. Lastly, our XMCD measurements are compatible with a weak ferromagnetic ground state down to 2K.

O 66.12 Wed 10:30 P

Elelctronic structure and bonding of h-BN on Pt(110) — •Marco Thaler[1], Dominik Steiner[1], Alexander Menzel[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Institute of Applied Physics and Center for Computational Materials Science, University of Technology, Vienna, Austria

The electronic properties and substrate interaction of single domain hexagonal boron nitride (h-BN) grown on structurally incommensurable Pt(110) were investigated by density functional theory (DFT), angle-resolved photoemission spectroscopy (ARPES), and work function measurements. DFT calculations show that the h-BN-substrate interaction is dominated by nonlocal van der Waals forces. However, locally, a covalent bond forms between on-top N and Pt atoms, forcing the Pt(110)-surface to adapt to the adlayer in the form of a (1xn)-m.r. reconstruction. In addition, the covalent bond gives rise to a peak in the local density-of-states at the Fermi level within the h-BN band gap and generally to hybridization of h-BN and substrate bands in the calculated band structure. In contrast, the experimental band dispersion coincides well with band structure calculations for a free-standing h-BN monolayer. We attribute the difference to correlation effects, i.e. the confinement of the photo-hole within the h-BN monolayer. Considerable correlation is also indicated by the appearance of a flat band in the σ manifold. The Moiré structure causes the appearance of umklapp bands in the ARPES data, differing in nature from Moiré-induced replica bands observed in e.g. Ru(0001) or Rh(111).

O 66.13 Wed 10:30 P

Highly ordered metallic phase of Indium on SiC(0001) — •Jonas Erhardt, Maximilian Bauernfeind, Simon Moser, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg D-97074, Germany

Indium thin films attract attention due to diverse electronic properties,

which feature for instance a two-dimensional electron gas (2DEG) [1] and superconductivity [2] in the 2D limit or Dirac-electrons in a triangular lattice [3]. Here, we present a combined angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling microscopy (STM) study of ultrathin (~ 2 monolayers) epitaxial indium films on silicon carbide (SiC). STM reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm assigned as a $(4\sqrt{3} \times 4\sqrt{3})$R30° reconstruction. Additionally, ARPES as well as scanning tunneling spectroscopy (STS) show a metallic band structure with a pronounced electron pocket, indicative of a 2DEG. Interestingly, STS further reveals negative differential conductance, which is in contrast to the canonical interpretation of the dI/dV signal as local density of states and is possibly related to substrate effects.

[1] E. Rotenberg *et al.*, Phys. Rev. Lett. **91**, 246404 (2003).
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010).
[3] M. Bauernfeind *et al.*, (unpublished)