

CPP 40: 2D Materials V: Growth, Structure and Substrate Interaction (joint session O/CPP)

Time: Wednesday 15:00–17:30

Location: GER 37

CPP 40.1 Wed 15:00 GER 37

Te on Pt(111): Structure and Growth of Surface Tellurides and Pt_xTe_y Films — TILMAN KISSLINGER, ALEXANDRA SCHEWSKI, ANDREAS RAABGRUND, HANNAH LOH, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

By LEED-IV, STM and DFT we investigated the tellurization of Pt(111) in UHV. For Te coverages $\Theta < 0.5$ ML surface tellurides are formed. In this coverage regime and after thermal annealing, we find only two well ordered surface telluride structures with (3×3) and (10×10) periodicity, the former was mistaken for a defective $PtTe_2$ film [1]. Our LEED-IV structure analyses determine the atomic structure and show that the Pt(111) surface undergoes massive reconstructions upon reaction with Te.

For $\Theta > 0.5$ ML, compact islands develop which eventually coalesce to a complete platinum telluride layer. Again by LEED-IV analyses we find that the first layer is a Pt_2Te_2 layer on which as second layer a $PtTe_2$ film can be grown. Both form an overlayer where 7×7 film unit cells lie on 10×10 Pt(111) unit cells. Furthermore, we find that the interface to the Pt(111) bulk still contains the ≈ 0.5 ML Te originally bound in the (10×10) superstructure. Electronic properties of the films determined by STS and implications for the MBE growth of transition metal dichalcogenides by surface tellurization will be discussed.

[1] L. Liu, D. Zemlyanov, and Y.P. Chen, 2D Mater. **8**, 045033 (2021)

CPP 40.2 Wed 15:15 GER 37

Electronic, chemical and structural properties of ultrathin Ta_2NiSe_5 flakes — KATHRIN KÜSTER¹, YUANSHAN ZHANG¹, DENNIS HUANG¹, ULRICH STARKE¹, and HIDENORI TAKAGI^{1,2,3} — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — ²Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70569 Stuttgart, Germany — ³Department of Physics, University of Tokyo, 113-0033 Tokyo, Japan

The excitonic insulator is a theoretically proposed state of matter wherein a macroscopic condensate of electron-hole pairs, i.e., excitons, spontaneously forms below a transition temperature. The 2D-layered chalcogenide Ta_2NiSe_5 has arisen as a leading candidate of an excitonic insulator in a bulk crystal. Here we prepared ultrathin films (down to 2 nm) of Ta_2NiSe_5 and analyzed their structural, electronic and chemical properties with a NanoESCA (Scienta Omicron) on a local scale. Angle-resolved photoelectron spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS), together with photoelectron emission microscopy (PEEM) and imaging XPS give detailed insight into the thickness dependent properties of the flakes. By exposure to UV-light we observe a contrast change in the PEEM images which is caused by a strong modification of the work function of the flakes, which we tentatively relate to a phase transition of the Ta_2NiSe_5 flakes.

CPP 40.3 Wed 15:30 GER 37

Transition from fractal-dendritic to compact islands for the 2D-ferroelectric SnSe on graphene/Ir(111) — PAULUS ALEKSA, SAMMER IQBAL, MUHAMMAD ALI MARTUZA, JIAQI CAI, THAIS CHAGAS, ROBIN OHMANN, and CARSTEN BUSSE — Universität Siegen, Germany

Monolayer islands of the 2D-ferroelectric SnSe have been grown by MBE under UHV conditions using inert and weakly interacting graphene on Ir(111) as the substrate. After deposition at room temperature, fractal-dendritic islands are observed in STM. The preferential growth directions are aligned with high-symmetry directions of the substrate. Upon annealing the islands become more compact. At 560 K they exhibit their equilibrium shape, higher temperatures lead to desorption. The equilibrium shape cannot be simply explained by minimization of the number of unsaturated bonds around the perimeter of an island with given area. The model has to be extended to incorporate the polar character of SnSe, leading to island edges that are charged in dependence of their orientation.

CPP 40.4 Wed 15:45 GER 37

Reaction of submonolayer amounts of Ti and Te on Au(111) — ANDREAS RAABGRUND, TILMAN KISSLINGER, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — Universität Erlangen-Nürnberg, 91058

Erlangen, Germany

Titanium ditelluride ($TiTe_2$) belongs to the family of layered 2D transition metal dichalcogenides. It achieved a lot of attention due to the emergence of a charge density wave in the single layer limit. Thicker films, however, do not show this transition [1]. Aiming the MBE growth of $TiTe_2$ we investigated the initial growth of titanium telluride structures on Au(111) both structurally and electronically by STM, STS, LEED-IV structural analysis, and DFT. For a Te coverage of 0.4 ML and a Ti coverage of 0.2 ML on Au(111) a chain-like $(5 \times \sqrt{3})_{\text{rect}}$ superstructure is formed. Our LEED-IV best-fit structure with a Pendry R factor of 0.11 (redundancy $\rho = 9.6$) reveals incorporated Ti atoms each of which forms bonds to two Te atoms residing in approximately hollow positions. Our findings regarding the $(5 \times \sqrt{3})_{\text{rect}}$ superstructure disprove the proposed $TiTe_2$ monolayer on Au(111) [2]. STS shows an approximately 0.5 eV (FWHM) wide peak at +1 V which we can correlate to the density of Ti d-states as obtained from DFT.

[1] P. Chen et al., Nat. Commun. **8**, 516 (2017)

[2] Z. Song et al., Chin. Phys. B **102**, 056801 (2019)

CPP 40.5 Wed 16:00 GER 37

Monolayers of $CoCl_2$ and $CoBr_2$ on Au(111) - Chemical, magnetic and structural investigation — SAMUEL KERSCHBAUMER¹, SEBASTIEN HADJADJ², ANDREA AGUIRRE BAÑOS³, DANILO LONGO³, WOLFGANG KUCH², JOSÉ IGNACIO PASCUAL³, CELIA ROGERO¹, and MAXIM ILYN¹ — ¹Centro de Fisica de Materiales (CSIC/UPV-EHU), 20018 Donostia-San Sebastian, Spain — ²Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany — ³CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain

Magnetic 2D materials have gained increasing interest, due to their potential applications. But while many theoretical calculations predict magnetic order in various 2D materials [1], only few have been experimentally measured [2]. A very promising classes of materials are transition metal halides (TMHs), as many of them crystallise in Van der Waals layered structures, making them easily cleavable, while their partially filled d orbitals generate the perfect foundation for magnetic order, further increasing their attractiveness for future nanotechnologies. In this talk chemical, magnetic and structural properties of single-layer $CoCl_2$ and $CoBr_2$ on Au(111) by scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and X-ray absorption spectroscopy (XAS/XMCD) will be presented.

[1] Michael A. McGuire, Crystals, 7(5), 121, (2017)

[2] Djuro Bikaljevic et al., ACS Nano, 15, 14985 (2021)

CPP 40.6 Wed 16:15 GER 37

Structure determination of mono- and few-layers of the 2D-ferroelectric SnSe on graphene on Ir(111) — DINA WILKS¹, PAULUS ALEKSA¹, SIMON CHUNG², PETER MODREGGER¹, DMITRI V. NOVIKOV³, VEDRAN VONK², ANDREAS STIERLE^{2,4}, and CARSTEN BUSSE¹ — ¹Physics Department, University of Siegen, Germany — ²Nanolabor Centre for X-ray and Nano Science CXNS, Germany — ³Deutsches Elektronen-Synchrotron DESY, Germany — ⁴Physics Department, University of Hamburg, Germany

For conventional ferroelectrics the critical temperature T_c quickly falls below technically feasible values for very thin films. This is not the case for two-dimensional materials. Theory predicts strong ferroelectricity for group-IV monochalcogenides, where individual layers are puckered sheets with a phosphorene-like structure. For SnSe, stable ferroelectricity of monolayers at room temperature has been shown by controlled microscopic manipulation. Here, we provide the missing structure determination of these monolayers.

We use surface X-ray diffraction to determine the structure of SnSe mono- and few-layers, the influence of the substrate, and the difference in stacking between a few-layered system and the bulk. SnSe films are prepared by MBE using graphene on Ir(111) as an inert and weakly interacting substrate. We observe one phase with three different orientations of monolayer SnSe islands with respect to graphene, while for the few-layered system two phases are found, each with three different orientations. A change in structure with rising temperature for both systems is seen, which hints towards T_c .

CPP 40.7 Wed 16:30 GER 37

Electronic properties of epitaxially grown monolayer and bilayer VS₂ on Au(111) — ●MIKHAIL FONIN¹, SABINA SIMON¹, FELIX FÖRSCHNER¹, JANNIK DORNSEIFF¹, JULIA TESCH¹, ELENA VOLOSHINA², and YURIY S. DEDKOV² — ¹Department of Physics, University of Konstanz, 78457 Konstanz, Germany — ²Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

Electronic properties of metallic two-dimensional materials can be strongly influenced by the supporting substrates, upon charge transfer or hybridization effects. In this context, suppression of many-body states in metallic transition metal dichalcogenides epitaxially grown on metallic substrates was recently reported [1]. By combination of scanning tunneling microscopy and first principle calculations we study monolayers and bilayers of VS₂ epitaxially grown on Au(111). We investigate the electronic properties of the monolayer and observe a metallic state with the presence of the incommensurate charge density wave state. Going from monolayer to bilayer VS₂, we observe an evolution from the metallic state to an insulating state.

[1] C. E. Enders *et al.*, Phys. Rev. B 94, 081404(R) 2016.

CPP 40.8 Wed 16:45 GER 37

Vanadium sulphides on graphene on Ir(111): polymorphs, charge density waves, layer dependency — ●CAMIEL VAN EFFEREN¹, JOSHUA HALL¹, VIRGÍNIA BOIX², TOBIAS WEKKING¹, NIKOLAY VINOGRADOV³, ALEXEI PREOBRAJENSKI³, JAN KNUDSEN², JEISON FISCHER¹, WOUTER JOLIE¹, and THOMAS MICHELY¹ — ¹Universität zu Köln — ²Lund University — ³MAX IV Laboratory

Among 2D materials, vanadium based compounds like VS₂ have attracted substantial research interest due to their predicted electronically correlated and magnetic ground states. However, the charge density wave (CDW) in monolayer (ML) VS₂ and VS₂ competes with predicted magnetic ground states. This has led to new research directions attempting to unlock the magnetic moment of the V atoms, e.g. via defect creation, alloying or the intercalation of atoms between VS₂ layers.

Here, we present a comprehensive X-ray photoemission spectroscopy and scanning tunneling microscopy study of few-layer, quasi-freestanding V₄S₇ and V₅S₈ on Gr/Ir(111), which are created via annealing of stoichiometric VS₂. Annealing ML VS₂ without background S pressure removes S atoms from the top layer of VS₂, creating the striped compound V₄S₇. In contrast, annealing ML VS₂ in a S atmosphere forms V₅S₈, where V atoms have self-intercalated between the VS₂ layers in a 2 × 2 pattern. Surprisingly, we find that V₅S₈ has a layer-dependent CDW at low temperature, with bilayer V₅S₈ exhibiting a $\sqrt{3} \times \sqrt{3}$ CDW, while the trilayer hosts a striped CDW phase akin to that of ML VS₂.

CPP 40.9 Wed 17:00 GER 37

Nucleation stage for the oriented growth of tantalum sulfide monolayers on Au(111) — ●THAIS CHAGAS¹, KAI MEHLICH¹, ABDUS SAMAD², CATHERINE GROVER¹, DANIELA DOMBROWSKI^{1,3}, JIAQI CAI¹, UDO SCHWINGENSCHLÖGL², and CARSTEN BUSSE¹ — ¹Department Physik, Universität Siegen, Siegen, Germany — ²Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — ³Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

We study the nucleation stage in the epitaxial growth of monolayer TaS₂ as a model system for monolayer transition metal sulfides. The growth was done under ultra-high vacuum conditions with Au(111) as a substrate on which the metal atoms are evaporated, and the sulfur is provided from a background of H₂S. Using scanning tunneling microscopy (STM), we find small trimers with a well-defined triangular shape that act as nuclei for the further growth of extended tantalum sulfide monolayers. We identify these trimers as TaS₃ using density functional theory (DFT). We propose that the unique orientation of the trimers is the cause of the well-defined orientation of a complete TaS₂ layer found under favorable growth conditions.

CPP 40.10 Wed 17:15 GER 37

Growth and structure of two-dimensional single-layer HfS₂ on Au(111) — ●MONIKA SCHIED, PAOLO LACOVIG, and SILVANO LIZZIT — Elettra-Sincrotrone Trieste

HfS₂ is a promising 2D material for low-power semiconductor devices due to its predicted high electron mobility and low contact resistance for n-type carrier transport. For actual applications, layers with excellent structural and electronic properties are needed. However, films with the necessary quality are only available from exfoliation, which is neither scalable nor very reproducible and only few experimental studies on a single-layer (SL) of HfS₂ have been performed so far. In analogy to the growth of high-quality SL transition metal dichalcogenides (TMDCs) such as MoS₂ and WS₂ [1,2] we have epitaxially grown an ordered layer of HfS₂ on Au(111) by chemical vapour deposition (CVD). Monitoring the S 2p and Hf 4f core levels in real time by fast X-ray photoelectron spectroscopy (XPS) allows the fine-tuning of the relevant parameters – such as the dosing rate and temperature – during the growth. The characterization by X-ray photoelectron diffraction (XPD) and low-energy electron diffraction (LEED) gives insight into the crystal structure of the film grown in this way.

[1] Bana, H., *et al.*, 2D Mater. 5 035012 (2018)

[2] Bignardi, L. *et al.*, Phys. Rev. Mat. 3, 014003, (2019)