DS 17: 2D Materials: Structure and Electronic Properties (Joint session of DS and O, organized by O)

Time: Tuesday 10:30–13:00 Location: H24

DS 17.1 Tue 10:30 H24

Structural and electronic properties of epitaxial multilayer *h*-BN on Ni(111) — Alexander Tonkikh[1], Elena Voloshina[2], Peter Werner[1], Horst Blumtritt[1], Boris Senkovskiy[3], Gernot Güntherodt[1,4], Stuart Parkin[1], and •Yuriy Dedkov[5,6] — [1]MPI Halle (Saale), Germany — [2]HU Belin, Germany — [3]TU Dresden, Germany — [4]RWTH Aachen, Germany — [5]SPECS GmbH, Germany — [6]IHP Frankfurt (Oder), Germany

Hexagonal boron nitride (*h*-BN) is a promising material for implementation in spintronics due to a large band gap, low spin-orbit coupling, and a small lattice mismatch to graphene and to close-packed surfaces of fcc-Ni(111) and hcp-Co(0001). Epitaxial deposition of *h*-BN on ferromagnetic metals is aimed at small interface scattering of charge and spin carriers. We report on the controlled growth of *h*-BN/Ni(111) by means of molecular beam epitaxy (MBE). Structural and electronic properties of this system are investigated using cross-section transmission electron microscopy (TEM) and electron spectroscopies which confirm good agreement with the properties of bulk *h*-BN. The latter are also corroborated by density functional theory (DFT) calculations, revealing that the first *h*-BN layer at the interface to Ni is metallic. Our investigations demonstrate that MBE is a promising, versatile alternative to both the exfoliation approach and chemical vapour deposition of *h*-BN.

DS 17.2 Tue 10:45 H24

Structural, thermodynamic and electronic properties of two-dimensional SiC, SiGe, and GeC alloys — Ivan Guilhon[1], Friedhelm Bechstedt[2], •Ronaldo Rodrigues Pela[1,3], Marcelo Marques[1], and Lara Kuhl Teles[1] — [1]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

We investigate structural, thermodynamic, electronic properties of 2D binary alloys made from graphene, silicene and germanene by means of density functional theory calculations and a statistical method that accounts for disorder and compositional effects. The GGA-1/2 method [1] is used in electronic properties calculations to approximately include quasiparticle corrections. $Si_{1-x}Ge_x$ is the only stable alloy at usual growth temperatures. In $Ge_{1-x}C_x$, strong distortions of the lattice lead to a pronounced tendency for phase separation. $Si_{1-x}C_x$ presents an ordered structure with composition $x = 0.5$ stable up to $T \approx 1000$ K. While $Si_{1-x}Ge_x$ and $Ge_{1-x}C_x$ are found to have vanishing band gaps, $Si_{1-x}C_x$ has, around $x = 0.5$, an appreciable band gap, which decreases exponentially with the growth temperature from ~ 2.2 eV at 300 K to ~ 1.2 eV at 900 K [2].
[1]: Phys. Rev. B 78, 125116 (2008); [2]: Phys. Rev. B 92, 075435 (2015).
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DS 17.3 Tue 11:00 H24

Unoccupied states in silicene nanoribbons on Ag(110) — •Nils Fabian Kleimeier, Luca Bignardi, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Unoccupied electronic states of silicene nanoribbons grown on Ag(110) were measured by inverse photoemission (IPE) in ultra-high vacuum conditions. The IPE setup consisted of a modified Erdmann-Zipf electron gun and an acetone filled Geiger-Müller tube with a CaF2 window acting as a bandpass filter. Three individual unoccupied states can be distinguished at 0.3, 0.9 and 1.4 eV above the Fermi level. To investigate occupied states of the nanoribbons, two-photon photoemission at a photon energy of $h\nu = 3.15$ eV was employed. Occupied states associated with the nanoribbons were only visible in spectra excited with p-polarized light. Electron dynamics of the lowest unoccupied state of the nanoribbons at $E - E_F = 0.3$ eV were measured by time-resolved three-photon photoemission at the same photon energy. The lifetime of the state was determined to $\tau = 20$ fs.

DS 17.4 Tue 11:15 H24

Absence of Dirac cones in monolayer silicene and multilayer Si films on Ag(111) — •Paolo Moras[1], Sanjoy K. Mahatha[1], Polina M. Sheverdyaeva[1], Valerio Bellini[1,2], Claudia Struzzi[3], Luca Petaccia[3], Tevfik O. Mentes[3], Andrea Locatelli[3], Roberto Flammini[4], Karsten Horn[5], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia - CNR, Trieste, Italy — [2]Istituto di Nanoscienze - CNR, Modena, Italy — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Istituto di Struttura della Materia - CNR, Roma, Italy — [5]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Monolayer silicene and multilayer silicon films on Ag(111) have been subject of many investigations within the last few years. For both systems, photoemission data have been interpreted in terms of linearly dispersing bands giving rise to the characteristic *Dirac cone* feature in the valence band. Here we show, on the basis of angle-resolved photoemission data and ab-initio calculations [1,2] that this assignment is not correct. In monolayer silicene the *Dirac cone* feature is caused by an Ag-derived interface state, while multilayer Si films exhibit a clear diamond-like structure and bulk-like Si bands. These results question the validity of the claim that graphene-like 2-D silicon and silicene multilayers are in fact formed on Ag(111).
[1] P. Moras et al., J. Phys.: Condens. Matter 26, 185001 (2014).
[2] S. K. Mahatha et al., Phys. Rev. B 89, 201416(R) (2014).

DS 17.5 Tue 11:30 H24

Low energy electron diffraction and angle resolved photoemission studies of Sn/Au(111) reconstructed surfaces — •Mahalingam Maniraj[1], Sebastian Emmerich[1], Dominik Jungkenn[1], Sebastian Jakobs[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], Stefan Mathias[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Recent experimental realization of Stanene, a two dimensional allotrope of Sn in a graphene-like structure, has motivated intense research on related Sn based ultrathin materials. We have investigated the growth of Sn on Au(111). Using low energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy, we found five surface reconstructions, each with a distinct band structure. Starting from a coverage of 0.3 monolayers, Sn forms a $(\sqrt{3} \times \sqrt{3})$R30° surface alloy which transforms into a complex superstructure for higher Sn coverages. An angle-resolved photoemission study shows inverted V-shaped bands which are symmetrically centered at the Gamma-point. Additionally, we observed states with parabolic dispersion showing a Rashba-type spin splitting. A direct comparison between our experimental results and band structure calculations will allow us to discuss the formation of Stanene-like band dispersions for these Sn/Au reconstructed surfaces.

DS 17.6 Tue 11:45 H24

Molecular interactions to control characteristics of transition metal dichalcogenide based atomically thin field effect devices — •Antony George[1], Sina Najmaei[2], Andreas Winter[1], Zian Tang[1], David Kaiser[1], Uwe Hübner[3], Pulickel Ajayan[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena — [2]Department of Materials Science and Nano Engineering, Rice University, Houston — [3]Leibniz Institute of Photonic Technology, 07702 Jena

Atomically thin field effect transistors (FET) based on monolayer transition metal dichalcogenides have been attracted an immense research interest recently due to their application potential in ultrathin, lightweight transparent device technology. Here we discuss the possibility to tailor the characteristics of monolayer molybdenum disulphide (MoS2) based FET devices using molecular interactions. We have used self-assembled monolayers (SAMs) to control the surface chemistry of the interface between the semiconducting channel and the gate oxide [1]. Therewith such device parameters like mobility, threshold voltage, carrier density can be tuned. We further extend this concept to the development of FETs, which can be tuned by optically switchable

molecules. To this end, we fabricated van der Waals heterostructures using MoS2 and carbon nanomembrane (CNM) [2] functionalized with optically switchable molecules. These devices can have different operational modes depending on the type of molecular switching which is triggered by external optical stimulation. [1] Nano Letters 14, 1354 (2014) [2] Prog. Surf. Sci. 87, 108 (2012)

DS 17.7 Tue 12:00 H24

Spatial conductivity mapping of unprotected and capped black phosphorus using microwave microscopy — Pieter J. de Visser[1,2], Rebekah Chua[1,3], Joshua O. Island[1], Matvey Finkel[1,4], Allard J. Katan[1], •Holger Thierschmann[1], Herre S.J. van der Zant[1], and Teun M. Klapwijk[1,4] — [1]Kavli Insitute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, The Netherlands — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Department of Physics, National University of Singapore, Singapore — [4]Physics Department, Moscow State Pedagogical University, Russia

Within the family of 2D materials thin flakes of black Phosphorus (bP) play a special role due to their tuneable direct bandgap and high carrier mobilities. Under ambient conditions, however, degradation changes the electronic properties of bP dramatically within hours [1]. Hence, applying protection measures is essential. We compare different protecting layers by measuring the local conductivity of bP flakes over time with scanning microwave impedance microscopy (sMIM). This novel AFM-based technique [2] probes the local sheet resistance with high spatial resolution and even for buried layers. For a bare bP flake we observe drastic changes in conductivity within 24 h. Coverage with 10 nm of HfOx delays degradation. The bP flake is stable for more than a week. Boron Nitride flakes appear to be less effective as a protection. sMIM reveals that here degradation starts at the edges and evolves over days, indicating a diffusive process. [1] Island J O, et al. 2DMat 2, 011002 (2015). [2] K. Lai, et al. Rev Sci Inst 79, 063703 (2008).

DS 17.8 Tue 12:15 H24

Coulomb interaction in transition metal dichalcogenides: effects on many-body instabilities — •Gunnar Schönhoff[1,2], Malte Rösner[1,2], Stephan Haas[3], and Tim Oliver Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

We develop a material realistic, microscopic model to describe the Coulomb interaction in a TMDC monolayer, focussing on molybdenum disulfide under electron doping. Starting from ab initio Coulomb interaction for the undoped system, we calculate values for the screened matrix elements in real space and see how the interaction becomes more localized with doping. Additionally, we obtain the doping dependend electron-phonon matrix elements and observe a Charge Density Wave instability at high doping.

To quantify the influence of the Coulomb interaction on the superconducting phase, we calculate the Morel-Anderson coefficient μ^*. In contrast to the frequent use of μ^* as a fit parameter or a constant, this leads to a decrease of μ^* with electron doping from 0.25 to 0.1. The influence of the Coulomb interaction turns out to be most important at the boundary between the metallic and the superconducting phase where it delays the phase transition. We argue that the character of the superconducting phase in MoS_2 is phononic.

DS 17.9 Tue 12:30 H24

The electronic structure of a 2D MoS_2-WSe_2 heterojunction investigated with photoemission spectroscopy — •Mathias Gehlmann[1], Markus Eschbach[1], Pika Gospodaric[1], Ewa Mlynczak[1], Sven Döring[1], Philipp Nagler[2], Tobias Korn[2], Christian Schüller[2], Slavomír Nemšák[1], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Department of Physics, University of Regensburg, D-93040 Regensburg, Germany

Heterostructures built from van der Waals materials are considered excellent candidates for next generation electronic devices that could overcome the restrictions of classical, Si-based electronics. The weak interlayer interaction in such heterostructures leaves the electronic properties of their building blocks largely intact. Nevertheless, by combining the two different transition metal dichalcogenides (TMDCs) MoS_2 and WSe_2, we produced a two-dimensional p-n junction, with drastically different optical and transport properties compared to the isolated TMDC monolayers and studied the influence of the interlayer coupling on the electronic structure in this novel, two-dimensional heterojunction.

By using photoemission spectroscopy we investigated the band alignment in the two materials. In order to directly observe the electronic band dispersion from micrometer-size flakes we performed k-space microscopy employing a photoemission microscope in angular resolved mode.

DS 17.10 Tue 12:45 H24

Superconductivity in the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ — •Corinna Grosse[1], Matti B. Alemayehu[2], Matthias Falmbigl[2], Olivio Chiatti[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

The ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ are artificially layered materials consisting of n $NbSe_2$ single-layers stacked alternately with atomic double layers of PbSe. $NbSe_2$ is a transition metal dichalcogenide with interesting electrical properties such as superconductivity and charge density waves. The influence of turbostratic disorder, a random rotation between the $NbSe_2$ and PbSe layers, on the superconducting transition temperature has been unknown so far.

We investigate the structural and temperature-dependent electrical properties of the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ by means of scanning transmission electron microscopy, X-ray diffraction, in-plane resistivity and Hall measurements and compare them to those of analogous non-disordered misfit layer compound (MLC) polymorphs. We observe a superconducting transition in the resistivity of the ferecrystals. The transition temperatures are reduced by up to 55 % with respect to the analogous MLC polymorphs. This indicates that turbostratic disorder substantially weakens the electron-phonon coupling in $(PbSe)_{1.14}(NbSe_2)_n$. We discuss the results of the structural and electrical properties of the ferecrystals with respect to their MLC analogues and also with respect to ultra-thin $NbSe_2$ layers.