

O 58: 2D materials beyond graphene: TMDCs, silicene and relatives II

Time: Wednesday 10:30–13:00

Location: MA 043

O 58.1 Wed 10:30 MA 043

Fabrication of germanane from Ge(111) single-crystal wafers — ●KORNELIA HUBA¹, ULRICH HAGEMANN², and HERMANN NIENHAUS¹ — ¹Faculty of Physics, CENIDE, University of Duisburg-Essen, Duisburg — ²Interdisciplinary Center for Analytics on the Nanoscale (ICAN), CENIDE, Duisburg

Germanane is a layered semiconducting material composed of single two-dimensional Ge sheets with dangling bonds saturated with hydrogen atoms. It is fabricated in a two-step procedure from clean Ge(111) wafers. First, a Zintl phase of CaGe_2 is formed under ultrahigh vacuum conditions by evaporating Ca atoms onto Ge at 810°C. Second, the sample is transferred under atmosphere to the wet-chemical treatment where it is etched in concentrated hydrochloric acid (HCl) at low temperatures for several hours. This leads to deintercalation of Ca and forming layered germanane flakes on top of the Ge(111) substrate. The flakes are exfoliated and transferred to other substrates, e.g., Si wafers for characterisation. The lateral extension of the germanane flakes ranges between 30 and 150 μm . X-ray photoelectron spectroscopy for chemical analysis detects Ge, no Ca and slight oxygen contaminations. From a 20% attenuation of the Si substrate line intensities a germanane layer thickness in the nm range is extracted demonstrating that single layer preparation is feasible. Currently, transmission electron microscope studies and micro-Raman spectroscopy are performed to elucidate morphology and structure of the germanane material.

O 58.2 Wed 10:45 MA 043

On the adatom doping of 2-Dimensional siligene (SiGe) with alkali metals — ●AMRETASHIS SENGUPTA — BCCMS, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany — Indian Institute of Engineering Science and Technology, Shibpur, Howrah - 711 103, India

An interesting hybrid 2D material, siligene has received attention for its possible applications in nanoelectronics and thermoelectrics. In this work we study the effect of adatom doping of 2D SiGe with alkali metal atoms (Li, Na and K), with density functional theory (DFT) simulations using generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof(PBE) functionals. The simulations showed a moderate adsorption energy of 0.75, 0.62 and 0.87eV for Li, Na and K atoms respectively, with possible doping concentrations upto $\text{M}_{0.88}\text{SiGe}$ (M=Li,Na,K). For ion-battery applications, the specific capacities are evaluated as 223, 196 and 175 mAhg⁻¹ for Li,Na and K storage respectively. Nudged elastic band (NEB) simulations showed a diffusion barrier of 0.71, 0.49 and 0.32eV for Li, Na and K atoms. In all cases a significant modulation in the Fermi energy (E_f) could be seen for varying degrees of doping. While Li adatom can dope the system from slight p-type to n-type ($\delta E_f = -0.05$ to $+0.5$), the Na and K atoms dope the system from moderate to strongly n-type ($\delta E_f = +0.3$ to $+1.4$ for Na and $+0.6$ to $+1.86$ for K) depending upon coverage. The results show possibilities concerning applications of 2D SiGe in ion-batteries, sensors and nanoscale devices.

O 58.3 Wed 11:00 MA 043

Unoccupied band structure of Si nanoribbons on Ag(110) — ●NILS FABIAN KLEIMEIER^{1,2}, GABI WENZEL¹, ADRIAN JOE URBAN¹, JÜRGEN BRAUN³, HUBERT EBERT³, ELENA VOLOSHINA⁴, YURIY DEDKOV⁴, and HELMUT ZACHARIAS^{1,2} — ¹Physikalisches Institut, Westfälische Wilhelms-Universität Münster — ²Center for Soft Nanoscience (SoN), Westfälische Wilhelms-Universität Münster — ³Department Chemie, Ludwig-Maximilians-Universität München — ⁴International Centre for Quantum and Molecular Structures, Shanghai University

Adsorption of Si atoms on the Ag(110) surface leads to the formation of monolayer silicon nanoribbons along the $[\bar{1}10]$ direction. Depending on the surface temperature during adsorption, nanoribbons with widths of either 0.8 nm or 1.6 nm, as determined by STM, are formed, leading to a (3×2) or (5×2) reconstruction, respectively. Employing k-resolved inverse photoemission spectroscopy (KRIPES), the unoccupied band structure of both reconstructions has been determined and is compared to measured and calculated KRIPES spectra of the bare Ag(110) surface. The experimental results for the band structures of both nanoribbon types are compared to DFT calculations for different pentagonal as well as hexagonal silicon nanoribbon models on Ag(110)

found in the literature. As expected for one-dimensional materials, all states associated with the nanoribbons show no dispersion in the $\bar{\Gamma}\bar{Y}$ direction (across the nanoribbons), but disperse in $\bar{\Gamma}\bar{X}$ direction (along the nanoribbons).

O 58.4 Wed 11:15 MA 043

STM Study of Current-Induced Forces in Graphene Nanoribbons on Au(111) — ●TOBIAS PREIS¹, SASHA VRBICA², NEMANJA KOCIC¹, ULRIKE PAAP¹, JONATHAN EROMS¹, DIETER WEISS¹, JAN VAN RUITENBEEK², and JASCHA REPP¹ — ¹Universität Regensburg, Institut für Experimentelle und Angewandte Physik - Regensburg, Germany — ²Leiden University, Huygens-Kamerlingh Onnes Laboratorium - Leiden, Netherlands

In electromigration, an electrical current flowing through a material exerts a force on atoms in the material or on its surface eventually leading to a displacement of these atoms. Although this phenomenon is technologically relevant for device reliability and has been addressed both theoretically [1] and experimentally [2] it is not fully understood yet. Electromigration of single gold atoms on a Ni(111) surface was reported based on scanning tunneling microscopy (STM) experiments [3].

Here, we address this issue with a very similar approach as in [3] but for single cobalt atoms adsorbed on narrow graphene nanoribbons adsorbed on a metal surface. By approaching the ribbons with an STM tip and injecting current pulses we observe motion of the adatoms predominantly along the ribbons. We could not observe a preferential direction with respect to a motion towards versus away from the tip.

[1] P. J. Rous et al., Phys. Rev. B 62, 8478-8486 (2000)

[2] B. C. Regan et al., Nature 428, 924-927 (2004)

[3] K.-F. Braun et al., Appl. Phys. Lett. 90, 023118 (2007)

O 58.5 Wed 11:30 MA 043

Thermal transport in 2D transition metal dichalcogenides within the relaxon picture — ●MICHELE SIMONCELLI¹, ANDREA CEPPELLOTTI^{2,3}, and NICOLA MARZARI¹ — ¹Theory and Simulations of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Station 12, CH-1015 Lausanne, Switzerland. — ²Department of Physics, University of California at Berkeley, California 94720, USA — ³Materials Science Division, Lawrence Berkeley National Laboratory, California 94720, USA

In electronics, the contemporary quest for device miniaturization has stimulated the search for 2D semiconducting materials with direct band-gap and favorable mechanical properties. Moreover, electronic devices are subject to Joule heating, which can result in a temperature increase up to values that cause chip damages or even melting. It is therefore desirable to find materials featuring a high thermal conductivity to ease the heat removal. In this study we focus on the thermal transport in 2D transition metal dichalcogenides (TMDCs), which are promising materials for their electronic and mechanical properties.

It has been shown recently [Cepellotti and Marzari, PRX, 2016] that the microscopic mechanism underlying heat conduction in crystals can be explained in terms of a gas of collective phonon excitations, called relaxons and defined as the eigenvectors of the scattering matrix appearing in the phonon Boltzmann equation. We used this theoretical framework to predict the thermal properties of the TMDCs of type MX_2 , where M=Mo, W and X=S, Se, Te.

O 58.6 Wed 11:45 MA 043

The Role of Substrate Symmetry on the Structural Properties of 2D Materials — ●ANTONIO J. MARTÍNEZ-GALERA and JOSÉ M. GÓMEZ-RODRÍGUEZ — Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

Predicting the properties that graphene and h-BN monolayers will exhibit after their growth on a certain substrate is a major challenge. While the influence on these properties of the electron configuration of the atoms comprising the underlying surface is well-known, the effects of substrate geometry still remain unclear. Herein, the structural properties of h-BN and of graphene monolayers grown on the rectangularly-packed Rh(110) surface are characterized and compared to those that both materials exhibit on substrates with different crys-

tallographic orientations. The STM apparent corrugation of the quasi-one-dimensional moiré patterns found in both systems is unexpectedly small, compared to the values previously reported for a number of lattice-mismatched interfaces with hexagonal supports of 4d metals, in which, as in the case of Rh, the d band is half-filled and, as a result, a strong interaction of the 2D material layer with the substrate is expected. This discrepancy is explained by the differences in the possible binding landscapes at the interface for differently oriented substrates. In consequence, a rule is derived to predict how the corrugation at the interface, as well as the existence and the extent of sub-regions, within the moiré supercell, containing favorable sites for orbital mixing between h-BN or graphene and their supports depend on the substrate symmetry.

O 58.7 Wed 12:00 MA 043

Damage Mechanisms in Two-Dimensional Materials — SILVAN KRETSCHMER¹ and ●ARKADY V. KRASHENINNIKOV^{1,2} — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Department of Applied Physics, Aalto University School of Science, Aalto, Finland

As the influence of defects on material properties heavily depends on the dimensionality, understanding defect production mechanisms in detail plays a major role for two-dimensional (2D) materials. The defect production under irradiation e.g. in the transmission electron microscope (TEM) can be subdivided into three mechanisms, namely knock-on damage, ionization damage and chemical etching. Surprisingly, as shown for transition metal dichalcogenides, in TEM defects are produced far below the knock-on threshold [1]. Here we investigate ionization and excitation damage mechanisms for Graphene, MoS₂ and hexagonal BN using first-principles simulation techniques.

[1] Y.Lin, T.Björkman, H.Komsa et al. *Nature Communications* 6 (2015), 6736.

O 58.8 Wed 12:15 MA 043

Observing structural information of TMDCs with FM-AFM in ambient and UHV — ●KORBINIAN PÜRCKHAUER, DOMINIK KIRPAL, LEO WALDHAUSER, ALFRED J. WEYMOUTH, and FRANZ GIESSIBL — University of Regensburg, Regensburg, Germany

The development in nanoelectronics demands reducing the size of its elements which led to an increase of interest in TMDCs. These show a range of interesting properties like a band gap in the range of Si and GaAs and allow high on/off switching ratios for FETs.

We studied bulk MoS₂, WS₂, MoSe₂ and WSe₂ cleaved in air with a qPlus AFM. The high stiffness ($k > 1$ kN) of the qPlus sensor allows us to operate in the frequency-modulation mode with sub-Angstrom amplitudes. On all surfaces we were able to observe atomic resolution in ambient conditions. The spacing between steps on MoS₂ and WS₂ were very large (at least hundreds of nm). In contrast, the MoSe₂ and WSe₂ surfaces appeared to be contaminated directly after cleavage. Both surfaces were covered with particles that were approximately 10 nm high. These particles were not observed on the MoS₂ and WS₂ surfaces. Transferring MoSe₂ into vacuum and annealing at 700°C resulted in a cleaner surface. This suggests that TMDCs with Sulfur

as a chalcogen atom are more suitable for devices made in ambient conditions.

O 58.9 Wed 12:30 MA 043

Lateral heterostructures of two-dimensional materials by electron-beam induced stitching — ●ANDREAS WINTER¹, ANTONY GEORGE¹, CHRISTOF NEUMANN¹, ZIAN TANG¹, MICHAEL MOHN², JOHANNES BISKUPEK², NIRUL MASURKAR³, ARAVA REDDY³, THOMAS WEIMANN⁴, UWE HÜBNER⁵, UTE KAISER², and ANDREY TURCHANIN¹ — ¹Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — ²Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm — ³Department of Mechanical Engineering, Wayne State University, 48202 Detroit, USA — ⁴Physikalisch-Technische Bundesanstalt, 38116 Braunschweig — ⁵Leibniz Institute of Photonic Technology, 07745 Jena

We present novel two-dimensional (2D) lateral heterostructures of graphene and MoS₂ sheets with molecular carbon nanomembranes (CNMs), synthesized by electron beam induced stitching. Graphene and MoS₂ were transferred onto gold substrates and lithographically patterned. Self-assembled monolayers (SAMs) of aromatic thiols were grown in the areas between the 2D materials. Irradiation with an electron beam converts the SAMs into CNMs and simultaneously stitches the CNM to graphene or MoS₂, forming a heterogeneous film of two different materials. These heterostructures are mechanically stable, enabling their preparation as freestanding sheets. We characterized them by means of Raman spectroscopy, atomic force microscopy (AFM), helium ion microscopy (HIM), X-ray photoelectron spectroscopy (XPS) and high resolution transmission electron microscopy (HRTEM) and find that they possess molecularly sharp boundaries.

O 58.10 Wed 12:45 MA 043

Low energy electron induced crosslinking of aromatic SAMs — ●CHRISTOF NEUMANN¹, RICHARD A. WILHELM^{2,3}, MARIA KÜLLMER¹, ANDREAS WINTER¹, and ANDREY TURCHANIN¹ — ¹Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — ²Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — ³Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany

Aromatic self-assembled monolayers (SAMs) can be converted into carbon nanomembranes (CNMs) via low energy electron irradiation [1]. Due to their mechanical and thermal stability as well as tunable chemical functionalization, CNMs are a 2D material with a large potential for application. Nevertheless, the conversion process is not yet understood in detail on the molecular level. In order to study the crosslinking we subsequently irradiated 4'-nitro-4-biphenylthiol SAMs on gold/mica substrates with different electron energies (5-50 eV) in UHV. Here we present the results obtained under in-situ conditions using X-ray photoelectron spectroscopy (XPS), Low Energy Electron Diffraction (LEED) and Low Energy Electron Microscopy (LEEM). To show the successful conversion process the samples were transferred onto TEM grids and Si wafers with 300 nm of thermal oxide and analyzed using optical, scanning electron (SEM) and atomic force microscopy (AFM). [1] A. Turchanin and A. Götzhäuser, Adv. Mater. 28, 5075 (2016)