

O 36: 2D materials beyond graphene: TMDCs, silicene and relatives I

Time: Tuesday 14:00–16:00

Location: MA 043

O 36.1 Tue 14:00 MA 043

Tuning the electronic and magnetic properties of monolayer phosphorene by doping and strain — ●JULIANA MORBEC¹, GUL RAHMAN², and PETER KRATZER¹ — ¹Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — ²Department of Physics, Quaid-i-Azam University, 45320 Islamabad, Pakistan

Phosphorene is an intriguing two-dimensional material with potential for a variety of applications. Its anisotropic optical and electronic properties combined with high carrier mobilities have attracted increasing attention in the past few years. Moreover, its superior mechanical flexibility has opened the possibility of tuning its electronic and magnetic properties by applying strain. Using first-principles calculations we investigate the interplay between defects, doping and strain on the electronic and magnetic properties of monolayer phosphorene. We find that (i) compressive strain can reduce the band gap of pristine phosphorene and induce a semiconductor-to-metal transition; and (ii) tensile strain can reduce the formation energy of magnetic single vacancies and lead to the stabilization of these defects. Our results also show that carbon-doping induces magnetism and a semiconductor-to-metallic transition; compressive biaxial strain has been found to suppress the magnetism whereas tensile strain opens the band gap and leads to an increase in the magnetic moment. Our findings suggest that doping and applying strain are important methods to tune the electronic and magnetic properties of monolayer phosphorene.

O 36.2 Tue 14:15 MA 043

An electrically controlled single atom magnetic switch on black phosphorus — ●BRIAN KIRALY, WERNER V. WEERDENBURG, ALEXANDER N. RUDENKO, MIKHAIL I. KATSNELSON, and ALEXANDER A. KHAJETOORIAN — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Single atoms at the surfaces of solids have demonstrated rich electronic, chemical, and magnetic properties. In this direction, we demonstrate that we can manipulate the orbital population of a single cobalt atom on a crystalline black phosphorus surface. Using the local electric field generated from an STM tip, individual cobalt atoms residing at the same hollow site can be reversibly switched between two stable states, which correspond to the different orbital configurations. The experimentally observed charge density of each configuration is corroborated with density functional theory calculations, which reveal the total magnetic moment and relaxation of the cobalt atom, as well as the electronic properties of the cobalt atom which locally dopes the black phosphorus. Utilizing tip-induced band bending, we further study the screening behavior of each Co atom configuration. We investigate the stability of each configuration, as well as compare the experimentally measured impurity states with DFT calculations. This system provides a new perspective on the horizon for fundamental properties of single atoms on surfaces.

O 36.3 Tue 14:30 MA 043

Characterisation of Defects in black phosphorus and phosphorene — ●JULIAN GABERLE¹, ALEXANDER SHLUGER¹, MARK WENTIK¹, TONY KENYON¹, and ALEXANDER SCHWARZ² — ¹University College London, WC1E 6BT London, UK — ²University of Hamburg, 20355 Hamburg, Germany

Interest in black phosphorus as a post graphene material has attracted considerable attention since 2014. Similar to graphene it consists of vdW bonded layers of covalently bonded phosphorus atoms. However, unlike graphene BP has a tunable direct bandgap, displays very high hole mobility and current switching ratios, which make it an interesting candidate for modern technologies. However, in order to make the transition from research labs to modern technologies the fundamental properties of BP and phosphorene need to be better understood. In particular point defects in the lattice and their effect on the electronic properties of BP are still not fully understood.

To characterise these defects, STM imaging was performed on black phosphorus and extended anisotropic defect states were observed. These defects have previously been attributed to phosphorus vacancies, but recently it has been suggested that Sn impurities are an alternative defect source. In order to better understand the nature of the defect, atomically resolved AFM imaging and XPS was performed. Combining state of the art experiments with ab initio DFT modelling

of vacancies and impurities, we were able to eliminate Sn impurities as a likely source of these defects and propose that these are indeed vacancies created in the cleavage process.

O 36.4 Tue 14:45 MA 043

Engineering Kondo State in Two-Dimensional Semiconducting Phosphorene — ●ROHIT BABAR¹ and MUKUL KABIR^{1,2} — ¹Department of Physics, Indian Institute of Science Education and Research, Pune, India — ²Center for Energy Science, Indian Institute of Science Education and Research, Pune, India

Correlated interaction between dilute localized electrons with the itinerant conduction electrons gives rise to Kondo effect below sufficiently low temperature. Beyond the conventional impurity in a metal systems, many artificial Kondo systems have been discovered in the last two decades. In sharp contrast to the artificial Kondo systems, we report an intrinsic, robust and high-temperature Kondo state in two-dimensional semiconducting phosphorene based on density functional theory calculations at different levels of approximations. While absorbed at a thermodynamically stable lattice defect, Cr impurity triggers an electronic phase transition in phosphorene to provide conduction electrons, which strongly interact with the localized moment generated at the Cr site. This manifests in an intrinsic Kondo state, where a multi-stage quenching of the impurity moment occurs in the temperature range 40-200 K. Further, along with a significantly small extension of Kondo cloud, the predicted Kondo state is shown to be robust under uniaxial strain and layer thickness, which greatly simplifies its future experimental realization. Our findings will broaden the current understanding of Kondo physics in two-dimensional materials.

O 36.5 Tue 15:00 MA 043

Investigating mechanical-high order elastic constants- and electronic properties of single layer borophene — MAHDI FAGHIHNASIRI¹, HOMAYOUN JAFARI², ●MOSTAFA SHABANI¹, and SINA MALAKPOUR ESTALAKI³ — ¹department of physics, shahrood university of technology, shahrood, iran — ²department of physics, iran university of science and technology, tehran, iran — ³department of aerospace and mechanical engineering, university of notre dame, Indiana, usa

Very recently two-dimensional layers of boron atoms, so-called borophene, have been successfully synthesized on the silver surfaces and attracts tremendous interest.

Borophene exhibits various structural polymorphs all of which are metallic. In this work, under in-plane uniaxial/biaxial strain/stress, we employ first-principles density functional theory calculations to investigate the electronic and mechanical properties of three single-layer borophene sheets ($\beta 12$, $\chi 3$, and striped borophene).

In the mechanical section, nonlinear in-plane elastic properties of borophene are calculated and we proposed a method to study high order elastic constants of the 2D rectangular structures. The continuum description of the elastic properties of monolayer borophene sheets is obtained using this method through ab initio density functional theory.

In electronic properties section by analyzing electronic band structure we observed an anisotropic behavior. Despite metallic character of borophene sheets, applying directional strain based on deformation matrices, create a band gap in some regions of Brillouin zones.

O 36.6 Tue 15:15 MA 043

Investigation of hexagonal boron-nitride (hBN) and graphene Gr-R0° on SiC(0001) — ●MARKUS FRANKE^{1,2}, SHAYAN PARHIZKAR^{1,2}, SERGUEI SOUBATCH^{1,2}, YOU-RON LIN^{1,2}, NAFISEH SAMISERESHT^{1,2}, MIRIAM RATHS^{1,2}, JANINA FELTER^{1,2}, FRANÇOIS C. BOCQUET^{1,2}, and CHRISTIAN KUMPF^{1,2} — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Among other 2D materials, hexagonal boron-nitride (hBN) seems to be a promising candidate for a new substrate material to achieve truly free-standing graphene layers. It forms a flat hexagonal lattice structure with a lattice parameter similar to that of graphene, but (in contrast to graphene) it is insulating (band gap > 5 eV). Here we report on the formation of hBN/SiC(0001) and on the subsequent preparation of graphene layers having the same orientation as the underlying SiC substrate (Gr-R0°). This orientation is unusual, typically epitaxial

graphene on SiC(0001) is rotated by 30° (Gr-R 30°).

We discuss the preparation of the layers performed by annealing SiC wafers in a borazine ($B_3N_3H_6$) atmosphere, and their properties based on results from core-level and angular resolved valence level electron spectroscopy (XPS and ARPES), as well as X-ray standing waves (XSW).

O 36.7 Tue 15:30 MA 043

Kelvin Probe Force Microscopy examination of defects of h-BN on Pt(111) — ●GINO GÜNZBURGER, ROLAND WIDMER, LIWEI LIU, and OLIVER GRÖNING — Nanotech@surfaces Laboratory, Empa - Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Epitaxial hexagonal boron nitride (h-BN) is an interesting material, which has attracted significant scientific interest for more than a decade. It has a hexagonal structure similar to the one of Graphene and it forms monolayers on many metals. The mono-layers have varying and interesting structures, such as a flat and even layers as on Ni(111), specific Moiré-patterns such as on Pt(111) and corrugated structures called "nanomesh" due to their mesh-like appearance (e.g on Rh(111)). The structure of the formed layer depends not only on the lattice mismatch between the h-BN and the substrate, but also on the strength of the interaction between the two [1]. We deposited an h-BN monolayer on Pt(111) by thermal decomposition of borazine (Cyclotriborazan, $(BHNH)_3$) on the hot substrate and subsequently examined it by STM and Kelvin Probe Force Microscopy (KPFM) using a Qplus STM/AFM in UHV at approximately 5K. On Pt(111) h-BN forms a Moiré pattern showing bright dots on a darker background when examined by STM at a high gap voltage. Defects in the h-BN appear as black spots in the STM image. They were located

by STM, examined by KPFM and identified as regions of higher work function.

[1] L. Camilli, E. Sutter and P. Sutter, 2D Materials 1, 025003 (2014)

O 36.8 Tue 15:45 MA 043

Corrugation in the weakly interacting h-BN/Cu(111) system — MARTIN SCHWARZ¹, ALEXANDER RISS¹, MANUELA GARNICA¹, JACOB DUCKE¹, PETER S DEIMEL², DAVID A DUNCAN², PARDEEP KUMAR THAKUR², TIEN-LIN LEE², ●ARI P SEITSONEN³, JOHANNES V BARTH¹, FRANCESCO ALLEGRETTI¹, and WILLI AUWÄRTER¹ — ¹Technical University of Munich, Department of Physics, Garching — ²Diamond Light Source, Harwell Science and Innovation Campus, Didcot — ³Département de Chimie, École Normale Supérieure, Paris

Atomically thin hexagonal boron nitride (h-BN) layers on metallic supports represent a promising platform for the selective adsorption of atoms, clusters, and molecular nanostructures. Here we employ complementary techniques including high-resolution noncontact atomic force microscopy, scanning tunnelling microscopy, low-energy electron diffraction, X-ray photoelectron spectroscopy, the X-ray standing wave method, and density functional theory to yield a comprehensive, quantitative structure determination including the adsorption height and the corrugation of the sp^2 -bonded h-BN layer on Cu(111) [1]. We compare the results to the adsorption structures of h-BN on other transition and coinage metal surfaces, in particular to h-BN/Ir(111) [2,3].

[1] Schwarz *et alia*, ACS Nano **11**, 9151-9161 (2017); DOI: 10.1021/acsnano.7b04022

[2] zum Hagen *et alia*, ACS Nano **10**, 11012-11026 (2016); DOI: 10.1021/acsnano.6b05819

[3] Seitsonen, Schulz and Liljeroth, in preparation