

## O 94: 2D Materials V: Novel Systems

Time: Friday 10:30–12:30

Location: H9

O 94.1 Fri 10:30 H9

**Orbital texture in the band structure of a new binary honeycomb lattice AgTe** — ●MAXIMILIAN ÜNZELMANN<sup>1</sup>, HENDRIK BENTMANN<sup>1</sup>, TILMAN KISSLINGER<sup>2</sup>, LUTZ HAMMER<sup>2</sup>, M. ALEXANDER SCHNEIDER<sup>2</sup>, THOMAS FAUSTER<sup>2</sup>, PHILIPP ECK<sup>3</sup>, DOMENICO DI SANTE<sup>3</sup>, GIORGIO SANGIOVANNI<sup>3</sup>, and FRIEDRICH REINERT<sup>1</sup> — <sup>1</sup>Experimentelle Physik 7, Universität Würzburg — <sup>2</sup>Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg — <sup>3</sup>Theoretische Physik 1, Universität Würzburg

In recent years two-dimensional (2D) materials like honeycomb-structured thin films or transition metal dichalcogenides attracted a lot of attention in solid state physics. Lattice symmetry as well as strong spin-orbit coupling leads to phenomena like non-trivial band topology [1,2]. Therefore it is important to gain knowledge about the orbital character of the involved valence-state wave functions.

Here we will present a new binary honeycomb lattice namely AgTe, whose structure is realized on a Ag(111)-substrate. Using angle-resolved photoemission we will determine the 2D band structure of the AgTe layer. By means of light-polarization dependent measurements, anisotropies in the band dispersion and linear dichroism we analyze the orbital character of the valence bands. Based on the determined orbital symmetry we discuss a possible topological band inversion in AgTe.

(1) F. Reis et al., Science 357, 287 (2017)

(2) S. Tang et al., Nature Physics 13, 683 (2017)

O 94.2 Fri 10:45 H9

**Stabilizing Plumbene on Fe/Ir(111): a combined experimental and theoretical study** — ●GUSTAV BIHLMAYER<sup>1</sup>, JONAS SASSMANNSHAUSEN<sup>2</sup>, ANDRÉ KUBETZKA<sup>2</sup>, KIRSTEN VON BERGMANN<sup>2</sup>, ROLAND WIESENDANGER<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — <sup>2</sup>Department of Physics, University of Hamburg, D-20355 Hamburg, Germany

As a heavy analog of graphene, plumbene is a two-dimensional material with strong spin-orbit effects. Although not a topological insulator, in external fields plumbene can realize a promising platform for topological phenomena [1]. Therefore, the synthesis of Pb monolayers with honeycomb structure is of substantial interest. On hexagonal substrates like Ir(111) a c(2x4) structure is found like in the graphene intercalated films on Ir [2]. In contrast, scanning tunneling microscopy images show that on a Fe covered Ir(111) surface Pb forms a honeycomb lattice. We use density functional theory calculations to rationalize these findings and analyse the impact of the hybridization on the plumbene band structure. In the unoccupied states the splitting of the Dirac cone by spin-orbit interaction is clearly observed and the influence of the iron's exchange field as function of magnetization direction is studied. In the occupied states of the freestanding plumbene we find a band inversion that leads to a topologically non-trivial gap, which undergoes strong hybridization with the substrate states.

[1] X.-L. Yu et al., Phys. Rev. B **95**, 125113 (2017).[2] F. Calleja et al., Nature Phys. **11**, 43 (2015).

O 94.3 Fri 11:00 H9

**Atomic buckling, structure and defects in silicene determined by atomic force microscopy** — ●PAWLAK RÉMY<sup>1</sup>, CARL DRECHSEL<sup>1</sup>, PHILIPP D'ASTOLFO<sup>1</sup>, ERNST MEYER<sup>1</sup>, and JORGE IRIBA CERDA<sup>2</sup> — <sup>1</sup>Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056 — <sup>2</sup>Theory of Surfaces, Interfaces and Nanostructures Group, Department Nanostructures and Surfaces, Instituto de Ciencia de Materiales de Madrid, Sor Juana Inés de la Cruz, 3 28049 Madrid, Spain

The atomic buckling in two-dimensional "X-enes" [1] (such as graphene and silicene) can foster a plethora of exotic electronic properties such a quantum spin hall effect, that could be readily engineered by external strain. Quantifying buckling with sub-Å precision is however challenging, since epitaxially grown 2D-layers exhibits complex restructuring and coexist at surfaces. Here, we accurately characterize the structure, defects and atomic buckling within 0.1 Å precision of all silicene phases grown on Ag(111) using low temperature atomic force microscopy (AFM) with CO-terminated tips assisted by density func-

tional theory (DFT). While no sign of Dirac cones is found due to the strong Ag-Si hybridization, the intrinsic buckling, varying from 0.8 to 1.1 Å, yields to slight differences in the silicene electronic properties. We think that our method pave the way for future atomic scale analysis of the interplay between structural and electronic properties in other emerging 2D-Xenes.

[1] Molle, A. et al. Nature Mat. 16, 163-169 (2017).

O 94.4 Fri 11:15 H9

**Investigation of two-dimensional germanium on Ag(110) by means of XPS** — ●LUKAS KESPER<sup>1,2</sup>, PETER ROESE<sup>1,2</sup>, KARIM SHAMOUT<sup>1,2</sup>, ULF BERGES<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Straße 4a, D-44221 Dortmund — <sup>2</sup>DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44221 Dortmund

Since the discovery of graphene in 2004 the new field of two-dimensional materials in solid state physics expanded massively. Apart from graphene other Dirac materials, like silicene and germanene, for instance, provide similar properties in a two dimensional structure [1]. Because of their strong spin-orbit coupling and tunable band gap they are predestined for realising topological field effect transistor [2]. After the report of the first synthesis of silicene [3], one dimensional silicon nano-ribbons [4] on different substrates, we present two-dimensional germanium, epitaxially grown on a Ag(110) surface. The stronger buckling and spin-orbit coupling of germanene may allow to observe the quantum spin Hall effect [2, 5]. The structural investigation of the system Ge/Ag(110) was done by using Low Energy Electron Diffraction and X-Ray Photoelectron Spectroscopy at the U55 beamline 11 at DELTA.

[1] M. Ezawa et al., Riv. Nuovo Cimento 41, 175 (2018). [2] A. Molle et al., Nature Mat. 16, 163 (2017). [3] P. Vogt et al., PRL 108, 155501 (2012). [4] C. Léandri et al., Surf. Sci. 574, L9 (2005). [5] C.-C. Liu et al., PRL 107, 076802 (2011).

O 94.5 Fri 11:30 H9

**Band Renormalization of Blue Phosphorus on Au(111)** — ●EVANGELOS GOLIAS<sup>1,2</sup>, MAXIM KRIVENKOV<sup>1</sup>, ANDREI VARYKHALOV<sup>1</sup>, JAIME SÁNCHEZ-BARRIGA<sup>1</sup>, and OLIVER RADER<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein Straße 15, 12489 Berlin, Germany — <sup>2</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Most recently, theoretical calculations predicted the stability of a two-dimensional honeycomb lattice of phosphorus atoms named blue phosphorus. We report on the successful growth of blue phosphorus on Au(111) surface using molecular beam epitaxy. We studied in detail the structural properties of blue phosphorus using low-energy electron diffraction, scanning tunneling microscopy and density functional theory calculations. Furthermore, by employing angle-resolved photoemission spectroscopy measurements we mapped the electronic structure of this novel two-dimensional allotrope of phosphorus. We find that the substrate breaks the sublattice symmetry of blue phosphorus leading to an orbital-dependent band renormalization upon the formation of a (4 × 4) superstructure on Au(111). Most importantly, the semiconducting two-dimensional phosphorus realizes its valence band maximum at 0.9 eV binding energy, however, shifted in momentum space due to the substrate-blue phosphorus interaction.

O 94.6 Fri 11:45 H9

**Electrostatic Screening at the Surface of Black Phosphorus** — ●BRIAN KIRALY, ELZE KNOL, DANIEL WEGNER, and ALEXANDER KHAJETOORIANS — Radboud University, The Netherlands

Under applied electric fields, black phosphorus theoretically demonstrates an electronic phase transition from insulating to metallic [1]. Using chemical dopants with very small electronegativity, bulk black phosphorus can be doped into such a transition [2]; however, atomic-scale insight into the local screening and surface charge inhomogeneity is missing. Here, we probe the spatial distribution of deposited potassium adatoms on the surface of black phosphorus, with low temperature scanning tunneling microscopy, as a function of temperature and coverage. We relate the spatial distribution of adatoms to the underlying screened electrostatic potential, utilizing thermodynamic formal-

ism, and extract the 2D vector mean potential. The data reveal the presence of extremely anisotropic, long-range interactions with strong oscillations along the zig-zag direction. The data is discussed within the context of screened Coulomb interactions, free carrier mediated Friedel-like oscillations, and strong electrostatic confinement.

[1] Q. Liu, X. Zhang, L. B. Abdalla, A. Fazzio, A. Zunger. *Nano Lett.* 15 (2), 2015. [2] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B. G. Park, J. Denlinger, Y. Yi, H. J. Choi, K. S. Kim. *Science* 349 (6249), 2015.

O 94.7 Fri 12:00 H9

**Calculating critical temperatures for magnetic order in 2D materials. Renormalized spin-waves vs Monte Carlo simulations** — DANIELE TORELLI and •THOMAS OLSEN — Technical University of Denmark, Copenhagen, Denmark

Magnetic order in two-dimensional (2D) materials is intimately coupled to magnetic anisotropy (MA) since the Mermin-Wagner theorem implies that rotational symmetry cannot be spontaneously broken at finite temperatures in 2D. Large MA thus comprises a key ingredient in the search for magnetic 2D materials that retains the magnetic order above room temperature. Magnetic interactions are typically modeled in terms of Heisenberg models and the temperature dependence on magnetic properties can be obtained with the Random Phase Approximation (RPA), which treats magnon interactions at the mean-field level. In the present work we show that large MA gives rise to strong magnon-magnon interactions that leads to a drastic failure of the RPA. We then demonstrate that classical Monte Carlo (MC) simulations correctly describe the critical temperatures in the large MA limit and agree with RPA when the MA becomes small. A fit of the MC results leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants, which significantly simplifies the theoretical search for new 2D magnetic materials with

high critical temperatures. The expression is tested on a monolayer of  $\text{CrI}_3$ , which were recently observed to exhibit ferromagnetic order below 45 K and we find excellent agreement with the experimental value.

O 94.8 Fri 12:15 H9

**Theoretical investigation on the magnetic properties of atomically-thin  $\text{NiPS}_3$**  — •TAE YUN KIM and CHEOL-HWAN PARK — Department of Physics, Seoul National University, Seoul 08826, Korea

Since the discovery of ferromagnetism in atomically-thin crystals [1, 2], the so-called magnetic van der Waals (vdW) materials have attracted much attention from the community of condensed-matter scientists [3]. Transition metal phosphorus trisulfide ( $\text{TMPS}_3$ ) family is a group of antiferromagnetic vdW materials with very interesting characters. A recent Raman experiment on  $\text{FePS}_3$  showed the existence of (Ising-type) antiferromagnetic order in a real two-dimensional crystal [4]. In this presentation, we will focus on  $\text{NiPS}_3$ , which exhibits quite different magnetic properties compared to  $\text{FePS}_3$ . We discuss the magnetic properties of atomically-thin  $\text{NiPS}_3$  based on our recent first-principles density-functional-theory calculations on the electronic and vibrational properties and compare our results with recent experiments.

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, *Nature* 546, 270-273 (2017) [2] C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, *Nature* 546, 265-269 (2017) [3] K. S. Burch, D. Mandrus, and J.-G. Park, *Nature* 563, 47-52 (2018) [4] J.-U. Lee, S. Lee, J. H. Ryoo, S. Kang, T. Y. Kim, P. Kim, C.-H. Park, J.-G. Park, and H. Cheong, *Nano Lett.*, 16 7433-7438 (2016)