

O 53: Graphene IV

Time: Wednesday 16:45–18:30

Location: MA 041

O 53.1 Wed 16:45 MA 041

Rotated / Scaled Overlayers and Moiré Patterns: a theoretical approach — ●KLAUS HERMANN — Abt. Theorie, Fritz-Haber-Institut, Berlin

Rotated and/or scaled overlayers at regular single crystal surfaces, such as graphene on Ru(0001) [1] or silver on Ni(100) substrate [2], are found to show long-range order expressed by approximate 2-dimensional surface periodicity with very large lattice constants. This phenomenon can be described geometrically analogous to interference effects resulting in periodic Moiré patterns which are characterized by 2-dimensional superlattices. Here we discuss in detail the mathematical formalism of determining such Moiré patterns based on concepts of coincidence lattices. The formalism provides simple relations that allow to calculate 2-dimensional Moiré lattices in their dependence on layer rotation angles α and scaling factors p for general Bravais lattices.

[1] D. Martoccia, P.R. Willmott, T. Brugger, M. Björck, S. Günther, C.M. Schlepütz, A. Cervellino, S.A. Pauli, B.D. Patterson, S. Marchini, J. Winterlin, W. Moritz, and T. Greber, Phys. Rev. Lett. 101 (2008) 126102.

[2] C. Chambon, J. Creuze, A. Coati, M. Sauvage-Simkin, and Y. Garreau, Phys. Rev. B 79 (2009) 125412.

O 53.2 Wed 17:00 MA 041

Graphene and hexagonal Boron Nitride 2D Super Structures Analysed by Scanning Probe Spectroscopy — ●THILO GLATZEL¹, SASCHA KOCH¹, SHIGEKI KAWAI¹, ERNST MEYER¹, SARA BARJA², and ENRICO GNECCO² — ¹Department of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — ²Instituto Madrileño de Estudios Avanzados en Nanociencia n (IMDEA Nanociencia), Cantoblanco, 28049 Madrid, Spain

By high temperature exposure of ethylene or borazine [(HBNH)₃] on transition metals between 500-1000°C under UHV conditions leads to the formation of graphene or a boron nitride monolayer, respectively. A lattice mismatch between the layers and the metal surfaces cause a hexagonal superstructure but while graphene is electrically conducting the boron nitride layer is insulating.

STM measurements showed various imaging contrasts arising from the complicated surface geometry and electronic properties. In our nc-AFM and KPFM experiments the complexity of the superstructures is also frequently observed in the topography as well as in the local contact potential difference. We thoroughgoing investigate the tip-sample interaction by 2D dynamic force spectroscopy at room temperature. From the variations in the resonance frequency of the probing tip in close proximity to the sample and the low dissipation accompanying the tip vibrations an elastic nature of the graphene and boron nitride elevations is concluded.

O 53.3 Wed 17:15 MA 041

Theory of graphene-boron nitride heterostructures — ●BURKHARD SACHS¹, TIM WEHLING¹, MIKHAIL KATSNELSON², and ALEXANDER LICHTENSTEIN¹ — ¹Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — ²Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

We report theoretical investigations of graphene-boron nitride heterostructures [1]. In detail, we investigate the adsorption of graphene sheets on hexagonal boron nitride substrates by means of first-principles calculations in the framework of adiabatic connection fluctuation-dissipation theory in the random-phase approximation. We obtain adhesion energies for different crystallographic stacking configurations and show that the interlayer bonding is due to long-range van der Waals forces. The interplay of elastic and adhesion energies is shown to lead to stacking disorder and moiré structures. Band-structure calculations reveal substrate induced mass terms in graphene, which change their sign with the stacking configuration. The dispersion, absolute band gaps, and the real-space shape of the low-energy electronic states in the moiré structures are discussed. We find that the absolute band gaps in the moiré structures are at least an order of magnitude smaller than the maximum local values of the mass term. Our results are in agreement with recent scanning tunneling microscopy experiments.

[1] B. Sachs, T. O. Wehling, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 84, 195414 (2011)

O 53.4 Wed 17:30 MA 041

Graphene on 3C-SiC(111): *Ab initio* study of structure and stability including van der Waals effects — ●LYDIA NEMEC, VOLKER BLUM, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

SiC is a widely used substrate for the growth of mono- and few-layer graphene. By Si sublimation, large ordered areas of graphene form on the Si side as $(6\sqrt{3} \times 6\sqrt{3})\text{-R}30^\circ$ (“ $6\sqrt{3}$ ”) commensurate periodic films [1]. In experiment, a first, partially covalently attached “buffer layer” (BL) $6\sqrt{3}$ carbon layer can be grown in a small temperature window, followed by a quasi-freestanding $6\sqrt{3}$ monolayer of graphene (GBL) at higher temperatures, and finally, few-layer graphene. What is not *a priori* clear is whether the BL and GBL phases are the result of some (narrow) *thermodynamic* equilibrium condition, and how the substrate affects the structure (monolayer graphene corrugation). Both are natural questions for theory, but a challenge for two reasons: (1) system size (up to ~ 2000 atoms in this work) and (2) van der Waals interactions, not accounted for by most standard density functionals. We show that the BL and GBL phases are in fact equilibrium phases within all-electron density functional theory (DFT) including van der Waals effects (PBE+vdW [2]). The equilibrium geometry emerges as a direct prediction, including the significant graphene layer corrugation. We also show that smaller-cell approximants may miss some geometric features, and could erroneously stabilize buffer layer defects due to artificially induced strain. [1] K. V. Emtsev *et al.*, Nature Materials 8, 203 (2009). [2] A. Tkatchenko, M. Scheffler, PRL 102, 073005 (2009).

O 53.5 Wed 17:45 MA 041

Graphene sublattice symmetry and isospin determined by ARPES using circularly polarized light — ISABELLA GIERZ¹, MATTI LINDROOS², HARTMUT HÖCHST³, ●CHRISTIAN R. AST¹, and KLAUS KERN¹ — ¹MPI für Festkörperforschung, Stuttgart — ²Tampere University of Technology, Tampere, Finland — ³Synchrotron Radiation Center, Stoughton, WI, USA

The origin of the Dirac-like electronic structure of graphene can be traced back to the symmetry properties of the honeycomb lattice characterized by the equivalence of the two carbon atoms within the unit cell (the sublattice symmetry) as well as their relative phase (the isospin). We determine these parameters using angle-resolved photoemission spectroscopy (ARPES) in combination with circularly polarized synchrotron radiation. We developed a simple theoretical model which shows that the photocurrent can be written as the product of a well known sublattice interference term containing the relevant information about the initial state and a — previously neglected — matrix element accounting for the influence of the geometry of the experimental setup as well as final state effects. We will show that for a photon energy of $h\nu = 52$ eV matrix element effects actually can be neglected which allows us to determine the sublattice symmetry parameter as well as the isospin with high accuracy.

O 53.6 Wed 18:00 MA 041

Nitrogen doped graphene on Ni(111) — ●ROLAND J. KOCH¹, MARTIN WESER², MARKUS OSTLER¹, JULIAN GEBHARDT³, FRANCESCO VINES³, WEI ZHAO⁴, CHRISTIAN PAPP⁴, ANDREAS GÖRLING³, HANSPETER STEINRÜCK⁴, KARSTEN HORN², and THOMAS SEYLLER¹ — ¹Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, 91058 Erlangen — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin — ³Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, 91058 Erlangen — ⁴Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen

We report on the N doping of CVD-grown graphene on Ni(111) using a N-containing precursor. After in-situ growth, the graphene film was investigated using ARPES to study the valence band structure, and XPS was used to determine the N content and bonding situation. The results from PES were supplemented by DFT calculations for various slab models that mimic different possible doping situations. The valence band spectra show a broadening of the photoemission features as well as a shift of the bands with respect to the Fermi level. In order to decouple the N doped graphene film from the strongly interacting

Ni substrate and to recover the Dirac cone, Au was intercalated. The XPS spectra show that the N doping is present in two different configurations. The majority of the N atoms are present in a pyridinic configuration, which involves a carbon vacancy. The minority of the N atoms is occupying a substitutional site. The observed variation of the electronic structure of N doped graphene compared to pristine graphene depends on the ratio of pyridinic to substitutional N.

O 53.7 Wed 18:15 MA 041

Phonons in single-layer and few-layer MoS₂ — •ALEJANDRO MOLINA-SANCHEZ and LUDGER WIRTZ — Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), Lille, France

In recent experiments, the single-layer dichalcogenide MoS₂ has exhibited a direct band-gap of 1.75 eV and a electron mobility close to that of graphene, becoming an appealing material in the area of optoelec-

tronic devices [1].

Recent Raman measurements have revealed unexpected trends in the vibrational properties of MoS₂ when the number of layers changes, as a frequency decreasing of the phonon mode E_{2g}^1 with increasing numbers of layers, that contradicts the expectation that the weak interlayer forces between neighbour layers should increase the effective restoring forces acting on atoms [2].

The purpose of our work is the clarification of this issue by a detailed *ab initio* study of the phonons, and comparing afterwards with experimental results. We explain this decrease by an enhancement of the dielectric screening of the long-range Coulomb interaction between the effective charges with a growing number of layers [3].

[1] B. Radisavljevic et. al., Nat. Nano. 6, 147 (2011). [2] C. Lee et. al., ACS Nano 4 2695 (2010). [3] A. Molina-Sanchez and L. Wirtz, Phys. Rev. 84, 155413 (2011).