O 98: Graphene VI

Time: Friday 11:15–13:15   Location: WIL A317

O 98.1   Fri 11:15   WIL A317

Tuning the Kohn Anomaly in the Phonon Dispersion of Graphene by Interaction with the Substrate — •Ludger Wirtz and Adrien Allard — Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), CNRS, Lille, France

The phonon dispersion of graphene displays two strong Kohn Anomalies (kinks) in the highest optical branch (HOB) at the high-symmetry points G and K. The slope of the HOB around K is a measure of the electron-phonon coupling (EPC) and determines the dispersion of the Raman D and 2D lines as a function of the laser energy [1]. We show that the EPC can be strongly modified both due to interaction with the substrate [2] (in particular, if the substrate is metallic) and due to doping [3]. For graphene grown on a Ni(111) surface, a total suppression of the Kohn anomaly occurs: the HOB around K becomes completely flat. This is due to the strong hybridization of the graphene pi-bands with the Nickel d-bands which lifts the linear crossing of the pi-bands at K. For other metallic substrates, where the distance between the graphene sheet and the substrate is larger, hybridization is much less pronounced and the Kohn anomaly is only weakly perturbed. From experimental phonon dispersions one can therefore draw conclusions about the interaction strength between graphene and its different substrates .

[1] S. Piscanec, M. Lazzeri, F. Mauri, A.C. Ferrari, and J. Robertson, PRL 93, 185503 (2004). [2] C. Attaccalite, L. Wirtz, M. Lazzeri, F. Mauri, and A. Rubio, Nano Lett. 10, 1172 (2010). [3] A. Allard and L. Wirtz, Nano Lett. 10, 4335 (2010)

O 98.2   Fri 11:30   WIL A317

Electronic and magnetic properties of the graphene/Fe/Ni(111) system: A theoretical study — •Elena Voloshina[1], Martin Weser[2], Karsten Horn[2], and Yuriy Dedkov[2] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Fritz-Haber Institut der Max-Planck Gesellschaft, 14195 Berlin, Germany

Layers of graphene on ferromagnetic (FM) surfaces may provide an ideal spin filtering effect in FM/graphene/FM sandwich-like structures [1]. Prior to being able to implement graphene/FM system in any kind of spintronic unit, its electronic, magnetic, and interfacial properties have to be investigated. Related DFT studies of the graphene/Fe/Ni(111) trilayer system have been performed. We observed noticeable modifications of the graphene and substrate band structures in the system. Intercalation of iron underneath of graphene layer changes drastically the magnetic response from the graphene layer that is explained by the formation of the highly spin-polarized 3d quantum-well state in thin iron layer. Obtained results are compared with experimental data.

[1] V. M. Karpan et al., Phys. Rev. Lett. **99**, 176602 (2007).

O 98.3   Fri 11:45   WIL A317

Accurate adsorption energies of graphene/Ni(111) — •Florian Mittendorfer — TU Vienna, Vienna, Austria

Due to the exceptional transport properties of graphene, graphene-based materials offer a promising route for spintronics. Yet even a prototypical system for a spin-filtering device, the interface between a ferromagnetic surface and a graphene sheet, cannot be described consistently on the basis of density functional theory (DFT) calculations. Even advanced functionals, such as the van der Waals density functional (vdW-DF), vastly overestimate the metal-graphene distance for graphene/Ni(111) [1], and hence fail to predict the experimentally observed opening of a band gap at the Dirac point.

In a recent publication, we could demonstrate that the description of adsorption energies can be significantly improved using a many-electron approach, the random phase approximation (RPA) [2]. In this contribution, we present RPA calculations for the adsorption of graphene on Ni(111). Using this approach, we could not only predict the correct adsorption site and electronic structure of the adsorbed graphene, but also determine the adsorption energy of the system accurately. The RPA calculations allow to evaluate the non-local (van der Waals) contributions and consequently to assess the quality of computationally cheaper approaches.

[1] M. Vanin, J. J. Mortensen, A. K. Kelkkanen, et al., Phys. Rev. B 81, 081408(R) (2010)

[2] L. Schimka, J. Harl, A. Stroppa, et al., Nature Materials 9, 741 (2010)

O 98.4   Fri 12:00   WIL A317

Graphene on lattice-mismatched metal surfaces: STM and ARPES studies — •Hendrik Vita[1], Alexander Generalov[1], Martin Weser[1], Yuriy S Dedkov[1], Karsten Horn[1], Muriel Sicot[2], Philipp Leicht[2], Andreas Zusan[2], and Mikhail Fonin[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]Universität Konstanz, Department of Physics, Universitätsstraße 10, D-78464 Konstanz

Since metal contacts to graphene are mandatory for potential electronic device applications of graphene, an investigation of graphene/metal interfaces is important. Here we study the electronic structure of graphene in a strongly bonded situation on Rh(111) and compare it to weakly bonded graphene/Ir(111). Angle-resolved photoemission maps of graphene/Ir(111), along the Γ-M-K-Γ direction, exhibit all features attributed to almost free-standing graphene (a Dirac cone with a linear dispersion of the π-band, weak p-doping). The graphene/Rh(111) system, on the other hand demonstrates strong hybridization between graphene band and the Rh 4d valence bands. This leads to pronounced corrugation of the graphene layer as revealed by STM, and a disappearance of the specific electronic band features of graphene. The deposition of thin ferromagnetic metal films on graphene/Ir(111) is also discussed.

O 98.5   Fri 12:15   WIL A317

Edge state on graphene probed by scanning tunneling spectroscopy — •Dinesh Subramaniam[1], Christian Pauly[1], Viktor Geringer[1], Rafael Reiter[2], Marco Pratzer[1], Marcus Liebmann[1], Yan Li[4], Carsten Busse[3], Riccardo Mazzarello[4], Florian Libisch[2], Thomas Michely[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Institut für theoretische Physik, Technische Universität Wien, Austria — [3]II. Physikalisches Institut, Universität zu Köln, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany

Epitaxial graphene islands are prepared by ethylene deposition on Ir(111) at room temperature and subsequent annealing to 1050°C. The lateral dimension of the islands varies from 5 nm to 40 nm always showing zigzag edges. Atomic resolution STM images show singly saturated zigzag edges which are predicted to feature a spinpolarized state. Scanning tunneling spectroscopy (STS) measurements at the graphene edge partly show a pronounced peak at the Fermi level. Reference STS measurements on the iridium surface reveal a similar peak with lower intensity at the Fermi level, which could be identified as an iridium surface state. This suggests that the increase in intensity at the edge of the graphene is due to a coupling of the edge state to the iridium surface state which enhanced strongly the intensity of the peak. Recent DFT band structure calculation support this assumption. Spin-polarized STS has been performed using a bulk chrome tip in order to analyze the magnetic character of the edge state.

O 98.6   Fri 12:30   WIL A317

Scanning tunneling spectroscopy of confined states within graphene nanoislands — •Christian Pauly[1], Dinesh Subramaniam[1], Viktor Geringer[1], Rafael Reiter[2], Marco Pratzer[1], Marcus Liebmann[1], Carsten Busse[3], Florian Libisch[2], Thomas Michely[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Institut für theoretische Physik, Technische Universität Wien, Austria — [3]II. Physikalisches Institut, Universität zu Köln, Germany

Epitaxial graphene islands are prepared by ethylene deposition on Ir(111) at room temperature and subsequent annealing to 1050°C. The lateral dimension of the islands varies from 5 nm to 40 nm. Using scanning tunneling spectroscopy we were able to visualize confined states within the islands. The state energies and corresponding local density of states patterns are in good agreement with third nearest neighbor tight-binding calculations for graphene. However, we had to include the potential of the moiré structure as well as a strongly absorbing character of the edge states. The width of the confined state energy

peaks has been used to determine the lifetime of the Dirac electrons, which is inversely proportional to energy.

O 98.7 Fri 12:45 WIL A317

Scanning Tunneling Microscopy of Graphene on a Boron Nitride Substrate — •RÉGIS DECKER[1,2], YANG WANG[1], VICTOR BRAR[1,2], WILLIAM REGAN[1], HSIN-ZON TSAI[1], QIONG WU[1], ALEX ZETTL[1,2], and MICHAEL CROMMIE[1,2] — [1]University of California, Berkeley, 366 Le Conte Hall, Berkeley CA 94720 — [2]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley CA 94720

Graphene placed on a boron nitride (BN) substrate has been shown to result in increased mobility and improved Quantum Hall measurements. It is therefore of great interest to understand how BN substrates differently influence graphene compared to more standard Silicon oxide substrates. I will present new scanning tunneling microscopy measurements of graphene placed on a BN substrate. Differences in the local behavior of graphene on a BN substrate versus a Silicon oxide substrate will be discussed.

O 98.8 Fri 13:00 WIL A317

Adhesion of graphene on hexagonal boron nitride substrates: First-principles investigation within the random phase approximation — •BURKHARD SACHS[1], TIM WEHLING[1], MIKHAIL KATSNELSON[2], and ALEXANDER LICHTENSTEIN[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

Hexagonal boron nitride (h-BN) substrates in graphene devices promise enhanced electron mobilities and low carrier inhomogeneities [1]. The stability of such compounds originates from weak adhesive long-range forces. By applying the random phase approximation (RPA) within the adiabatic connection fluctuation-dissipation theory (ACFDT), we investigate the adsorption of graphene sheets on h-BN substrates from first-principles. In detail, we obtain adhesion energies for different crystallographic stacking configurations and compare the results to experiments. Analyzing the elastic properties of graphene and h-BN, we discuss possible mechanisms leading to stacking disorder.

[1] C.R. Dean et al., Nature Nanotechnology 5, 722-726 (2010)