TT 106: Graphene: Interaction with the Substrate (organized by HL)

Time: Friday 11:15–13:00 Location: POT 081

TT 106.1 Fri 11:15 POT 081

Phonons of graphene on metallic and semiconductor surfaces, an ab-inito approach — •Alejandro Molina-Sanchez and Ludger Wirtz — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC (i.e., the buffer layer). We use ab-initio methods to obtain the phonon modes, the density of states, and the strength of the electron-phonon coupling. When we deal with large supercells, we use an unfolding scheme to visualize the phonon bands in the primitive unit cell. Thus, we can distinguish clearly the changes in the phonon dispersion of perturbed-graphene with respect to the one of pristine graphene. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation as due to a weakening of the electron-phonon interaction via screening of electron-electron correlation by the dielectric substrate. Graphene on iridium, also displays weak interaction but the underlying material is a metal. This leads to an even more pronounced screening of the electron-electron interaction in graphene. In the last case, we study the buffer layer of graphene on silicon carbide. The hybridization of graphene with silicon carbide changes the electronic structure of graphene and the phonon bands.

TT 106.2 Fri 11:30 POT 081

The (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction: Surface phase equilibria near the graphene formation regime on 3C-SiC($\bar{1}\bar{1}\bar{1}$) — •Lydia Nemec[1], Florian Lazarevic[2], Patrick Rinke[1], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]AQcomputare GmbH, Chemnitz — [3]MEMS Department, Duke University, Durham, NC, USA

To refine the growth quality of epitaxial graphene on the C-side of SiC and improve the resulting electronic character of these films, it is important to understand the atomic- and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases, as well as of the SiC-graphene interface, is unknown.

We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron, numeric, atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range.

The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. In comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which could explain the observed phase mixture.

TT 106.3 Fri 11:45 POT 081

Reststrahl band assisted photocurrents in epitaxial graphene layers — •P. Olbrich[1], C. Drexler[1], L.E. Golub[2], S.N. Danilov[1], V.A. Shalygin[3], V.A. Shalygin[3], R. Yakimova[4], S. Lara-Avila[5], S. Kubatkin[5], B. Redlich[6], R. Huber[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]State Polytechnic University, St. Petersburg, Russia — [4]Linköping University, Linköping, Sweden — [5]Chalmers University of Technology, Göteborg, Sweden — [6]FOM Institute for Plasma Physics, Nieuwegein, The Netherlands

We report on the observation of reststrahl band assisted photocurrents in epitaxial graphene on SiC. The samples were excited by the infrared radiation from the tunable free electron laser "FELIX" and a CO_2 gas laser [1]. We show that the photoresponse due to linearly (circularly) polarized mid-infrared light is strongly enhanced (suppressed) in the vicinity of the reststrahl band of SiC. Our data, in particular a complex spectral behavior, are well described by the developed theory taking into account photon drag and photogalvanic effects affected by an enhanced light-matter interaction in the range of substrate's negative dielectric function in its reststrahl band. Moreover, our work demonstrates that substrate phonons strongly influence the transport properties of the carriers in graphene.

[1] P. Olbrich *et al.*, arXiv:1308.0123

TT 106.4 Fri 12:00 POT 081

Towards superlattices: Lateral bipolar multibarriers in graphene — •Martin Drienovsky[1], Franz-Xaver Schrettenbrunner[1], Andreas Sandner[1], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg — [2]Institut für Theoretische Physik Universität Regensburg

We report on transport properties of monolayer-graphene (MLG) with a laterally modulated charge carrier density profile. For that we employed a planar back gate and striped top gate electrodes of 25 nm width and a spacing of 100 nm up to 200 nm, separated from the MLG by an Al_2O_3 dielectric. Tuning of top and back gate voltages gives rise to multiple potential barriers and wells, enabling the investigation of resistance either in the unipolar or the bipolar transport regime. In the latter pronounced single- and multibarrier Fabry-Pérot (FP) resonances are observed. The experimental data of different devices with alternating numbers of top gate stripes and pitch, taken at different temperatures, is consistent with a ballistic transport calculation, employing a realistic potential profile, extracted from classical electrostatic simulation combined with the quantum capacitance model. The origin of resistance oscillations in our multibarrier graphene system can be explained in the FP-picture, without resorting to an artificial band structure.

TT 106.5 Fri 12:15 POT 081

Scanning Tunnelling Spectroscopy of Moiré Patterns on Graphene/Rh(111) — •Anne Holtsch, Tobias Euwens, Hussein Schanak, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

The lattices of graphene and Rh(111) provide a difference of approximately 9% between the two lattice constants. This mismatch results in the formation of a Moiré pattern with a lattice constant of 2.9 nm. Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. The locations of the minima in the dI/dV curves are identical for the different symmetry regions. Beyond the minimum, the symmetry points show differences in the dI/dV curves according to the C-Rh interaction strength.

[1] M. Iannuzzi and J. Hutter, Surf. Sci. 605, 1360 (2011).

TT 106.6 Fri 12:30 POT 081

Varied Moiré patterns of graphene/Rh(111) measured by scanning tunnelling microscopy — •Tobias Euwens, Anne Holtsch, Hussein Schanak, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate the superstructures that originate from the different lattice parameters of the graphene and the substrate. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. Their origin lies in either the surface inhomogenities of the Rh(111) substrate or in the form of folds and steps in the graphene itself. Knowing the properties of the growth of graphene on the rhodium surface is important for the construction of more complex graphene-based electronics. Understanding the specific structure of the Moiré patterns can help in that regard as it relays information about the angle between the carbon and the rhodium lattice and potential reasons for the twisting between the two lattices.

TT 106.7 Fri 12:45 POT 081

Impact of the substrate on the electronic properties of graphene — •Hussein Shanak, Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Electronic properties of graphene grown on different substrates such as Rh, Cu and SiO2 were investigated using scanning tunnelling microscopy and spectroscopy. The different kinds of substrates result in different types of superstructures due to the mismatch between graphene and substrate. Comparison of the electronic properties obtained for graphene on the different substrates leads to a better understanding of the graphene doping behaviour. Additionally, the existence of different superstructures leads to different growing properties of the materials on top of graphene itself.