O 43: Graphene I

Time: Wednesday 10:30–12:45 Location: H31

O 43.1 Wed 10:30 H31

Mechanical characterization of graphenoid nanomembranes from self-assembled monolayers — •Xianghui Zhang, Christoph T. Nottbohm, André Beyer, Andrey Turchanin, and Armin Gölzhäuser — Fäkultät für Physik, Universität Bielefeld, Postfach 10 01 31, 33501, Germany

We report on the fabrication and mechanical characterization of novel graphenoid nanomembranes with a thickness of approximately 1 nm. The nanomembranes are prepared from electron cross-linked aromatic self-assembled monolayers (SAMs). After etching the support, the nanomembranes are transferred to window-structured substrates for mechanical characterization. Bulge testing within an atomic force microscope (AFM) is utilized to investigate their mechanical properties. A series of biphenyl-based molecules with different types of terminal groups and/or anchor groups were used to prepare the nanomembranes, such as carbonitrile-biphenyl-trimethoxysilyl (CBPS), biphenylthiol (BPT), nitro-biphenyl-thiol (NBPT) and biphenyl-propanethiol (BP3). Biphenyl-based nanomembranes display elastic moduli ranging from 6 to 12 GPa. Annealing of the cross-linked nanomembranes in ultra high vacuum (UHV) gives rise to a systematic increase of the Young's moduli from 10 GPa to ~45 GPa for an annealing temperature of ~1000 K. Strain relaxation lowers the residual strain from 0.9 % to ~0.35 % for temperatures of 800 K and above. This indicates that the relevant structural transformation is completed at that temperature.

O 43.2 Wed 10:45 H31

Collective Excitations of Graphene in a Strong Magnetic Field — Andrea Fischer[1], Alexander Dzyubenko[2,3], and •Rudolf Römer[1] — [1]University of Warwick, Coventry, UK — [2]California State University, Bakersfield, US — [3]Russian Academy of Science, Moscow, Russia

Graphene, a two-dimensional form of carbon, has become famous for its wide range of unusual properties, both fundamental and applicable. Both theory and experiment indicate the relevance of many body interactions to the magneto-optical response of graphene. Neutral collective excitations of pristine graphene in a strong perpendicular magnetic field have already been studied theoretically. In this work, we consider graphene with a low impurity density and determine the neutral magnetoplasmons, which become localised on an impurity. Two impurity types are considered: a screened Coulomb impurity and a δ-function scatterer due, e.g., to a neutral foreign atom on one of the lattice sites. We assume Zeeman and valley splitting of Landau levels (LLs) n=0 and $n = \pm 1$, so that these LLs have four sublevels; we consider various integer fillings of the zeroth LL. For both impurity types, we predict the existence of optically active bound states above and below the magnetoplasmon continuum for high enough impurity strengths [1]. Our results indicate that polarisation-resolved magneto-optical spectroscopy can be an effective tool for discriminating between different types of impurities in graphene. [1] A. M. Fischer, A. B. Dzyubenko, and R. A. Römer, PRB **80**, 165410 (2009)

O 43.3 Wed 11:00 H31

Absolute Raman Cross Section of Graphene — •Philipp Klar[1], Robert Panknin[1], Elefterios Lidorikis[2], Andrea Carlo Ferrari[3], Stephanie Reich[1], and Cinzia Casiraghi[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Engineering Department, University of Ioannina, Greece — [3]Engineering department, Cambridge University, UK

Raman spectroscopy in graphitic systems is extremely interesting because it involves resonant conditions, defect-induced processes and because of strong electron-phonon coupling effects [1-3]. However, measurements of the absolute scattering cross section of graphite are rather scarce [4-5]. Here we measured the first- and second-order Raman spectrum of graphene and graphite using excitation energies covering the visible range, from 1.96 eV to 2.7 eV. By using the substitutional method, we have found that the G peak Raman cross section is $\sim 2 \times 10^{-5} m^{-1} Sr^{-1}$ at 2.41 eV for both graphene and graphite, in agreement with Ref. 5. The 2D peak Raman cross section of graphene is $\sim 3 \times 10^{-5} m^{-1} Sr^{-1}$ at 2.41 eV, well comparable with the one of the first order G peak. This confirms the resonant nature of the 2D peak [1-2].

1. C. Thomsen, S. Reich, PRL 85, 5214 (2000)
2. D. M. Basko, PRB, 78, 125418 (2008)
3. S. Piscanec et al, PRL 93, 185503 (2004)
4. K. Sinha, J. Menendez, PRB 41, 10845 (1990)
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O 43.4 Wed 11:15 H31

Electronic bound and scattering states in an integrable graphene quantum dot — •George Pal, Walter Apel, and Ludwig Schweitzer — Physikalisch-Technische Bundesanstalt (PTB), Bundesalee 100, 38116 Braunschweig, Germany

We study theoretically the confinement of electrons in a graphene quantum dot created by an electrostatic gate potential applied to single-layer graphene. In the low-energy limit, the electronic properties of graphene are given by a two-dimensional Dirac-like equation for massless chiral electrons. The graphene quantum dot is described by a radially symmetric confining potential with a sharp boundary and that makes the problem analytically integrable. Also, couplings between the graphene layer and the substrate and atomic scale defects and impurities are taken into account by adding a sub-lattice anisotropy and an inter-valley scattering to the Hamiltonian. These terms open a gap in the energy spectrum and allow for the existence of true bound states, forbidden otherwise due to the Klein tunneling phenomenon in an ideal, clean graphene. Considering a wave function with four components (two valleys times two sub-lattice indices), we discuss the conditions for the existence of bound and scattering states for different regimes of the confinement potential. Furthermore, we calculate the energies of the bound states and the scattering matrix. The influence of disorder in the graphene sheet and in the quantum dot is also discussed.

O 43.5 Wed 11:30 H31

Ab-initio determination of the electronic and optical properties of functionalized group IV monolayers for optoelectronic and photovoltaic devices. — •Margherita Marsili — ETSF, Dipartimento di Fisica Università di Roma 'Tor Vergata' (Italy)

Graphene, one of the most intensively material studied recently, is well known as being metallic. The absence of an electronic gap limits its possible use in electronic and optoelectronic devices. A route to the opening of a gap is the functionalization of graphene through the absorption of molecules. In particular a reversible metal-insulator transition of graphene upon hydrogenization has been experimentally achieved, after it was theoretically predicted. Graphane, the fully hydrogenated graphene, has indeed a wide gap of almost 6 eV. The extent of the electronic gap of graphane limits its use in photovoltaic devices, one of the key technologies for the attainment of green energy. Possible solutions are either to functionalize graphene with other molecules, or to change the backbone material looking at the other group IV elements such as Si and Ge. Here we present results exploring both paths: the optical properties of different molecules on graphane and on polysilane and polygermyne (Si and Ge counterparts of graphane) monolayers are investigated also including many-body effects beyond density functional theory. Many-body effects are also crucial in the quantitative description of a material's electron affinity. Hydrogenated diamond surfaces are known to have negative electron affinity, therefore the effect of hydrogen on graphene's electron affinity is also determined taking into account self-energy effects.

O 43.6 Wed 11:45 H31

Adsorption of water on graphene from first principles — •Elena Voloshina[1], Krzysztof Rosciszewski[2,3], and Beate Paulus[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [3]Institute of Physics, Jagiellonian University, 30059 Krakow, Poland

Although current density functionals are able to describe quantitatively different systems at much lower computational cost than other first principles methods, they fail to do so for the consideration of van der Waals (vdW) interactions. The problem of restoring the vdW interactions in DFT methods has been addressed by a number of authors. However, all these works are based on approximations leaving the main lack of systematic improvability within the DFT framework.

Furthermore, even in the case of investigation of similar systems under similar conditions DFT can predict quite different results, e.g., as in the case of adsorption of H_2O on graphene [1]. Therefore ab initio wavefunction-based correlation methods are desirable. A possibility to apply them to extended systems is to use the so-called local correlation methods, e.g. method of increments [2]. Recently this method has been extended to the description of interaction between molecules and surface (see e.g. [3]). Here we present the results for the adsorption of H_2O on a graphene layer using a CCSD(T) correlation treatment.

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O 43.7 Wed 12:00 H31

Optical detection of single graphenes on mica with a contrast as high as 14% — •Martin Dorn, Phillipp Lange, Alexei Chekushin, Nicolai Severin, and Jürgen Rabe — Humboldt-Universität zu Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany

Graphene is a one atom thick material with unique properties arising from its two dimensional crystal lattice. Most of graphene devices are fabricated on silicon wafers covered with a SiO2 layer necessary for optical detection of single graphenes. Graphene adhering to a SiO2 layer follows the intrinsic roughness of the latter and therefore cannot be considered strictly two dimensional. Mica is a natural crystal with perfect atomically flat cleavage planes. We demonstrate here a simple optical microscopy method for the detection of graphenes on mica with up to 14% of single graphene optical contrast. The experimental results are rationalized with a Fresnel-law based model. The contrast is only weakly wavelength dependent, i.e. white light contrast of single graphenes is sufficiently high for easy detection. The theory predicts also a high contrast for single graphenes on different transparent substrates with refractive indices close to that of mica, e.g. lime glass and ITO.

O 43.8 Wed 12:15 H31

Local work function of defective graphene probed by Kelvin Probe Force Microscopy — •Liang Yan[1], Sasa Vinaji[1], Christian Punckt[2], Ilhan Aksay[2], Hanna Bukowska[3], Marika Schleberger[3], Gerd Bacher[1], and Wolfgang Mertin[1] — [1]Werkstoffe der Elektrotechnik & CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany — [2]Department of Chemical Engineering, Princeton University, Princeton, New Jersey, USA — [3]Fakultät für Physik & CeNIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

Graphene is currently one of the hottest topics in research due to its unique properties. In particular for electronic applications, the influence of defects on its electronic properties such as work function is of great interest since it might be possible to taylor these properties by changing the type and density of defects. In this work we demonstrate local work function measurements on thermally exfoliated graphene on HOPG and on mechanically exfoliated graphene on SrTiO3 and SiO2 using Kelvin Probe Force Microscopy, which allows us to correlate the electronic properties with the topography of the defective areas. We find that in case of thermally exfoliated graphene, where the presence of defects and functional groups leads to wrinkling of the sheets, the work function at defective areas is increased compared to non-defective regions. In mechanically exfoliated graphene, a partial overflipping of the graphene layer is achieved by swift heavy ion bombardment, which results in a pronounced change of the local work function and thus in the electrical properties as compared to the non defective areas.

O 43.9 Wed 12:30 H31

Electrical transport measurements in graphene and graphenoids from pyrolized self-assembled monolayers — •Andrey Turchanin[1], Dirk Weber[2], Matthias Büenfeld[1], Joachim Mayer[3], Christian Kisielowski[4], Thomas Weimann[3], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig — [3]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen — [4]National Center for Electron Microscopy, Berkeley

We investigate the transition of insulating ultrathin (~1 nm) carbon nanosheets (graphenoid sheets) to conducting graphene. Self-assembled monolayers (SAM) of aromatic biphenyl molecules are cross-linked by electrons. The cross-linking results in mechanically stable graphenoid sheets with the thickness of a single molecule and arbitrary sizes. The nanosheets can then be lifted from their surface and transferred to another solid substrate or holey structure, where the nanosheets become suspended free-standing nanomebranes [1]. Upon annealing (pyrolysis) at higher temperatures (up to ~1300K) the nanosheets transform into a graphitic phase that consists of nanosize graphene patches. This transformation is accompanied by a drop of the sheet resistivity from $\sim 10^8$ to 10 kΩ/sq [2]. We characterize the insulator to conductor transition by complementary spectroscopic and microscopic techniques and electrical transport measurements.

[1] C. T. Nottbohm et al, Ultramicroscopy 108, 88 (2008)

[2] A. Turchanin et al, Adv. Mater. 21, 1233 (2009)