TT 83: Graphene: Adsorption, Intercalation and Doping (organized by O)

Time: Wednesday 18:15–21:00 Location: Poster A

TT 83.1 Wed 18:15 Poster A

Defects and oxygen adatoms on graphene — •Jan Gesenhues and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, 48149 Münster, Germany

Oxygen adatoms on graphene are one of the ingredients of graphene oxide and are being discussed as building blocks to open a band gap in the Dirac cone of graphene. In our work we study graphene and oxygen adatoms within the theoretical framework of Tight-Binding and Density Functional Theory (DFT). The SIESTA program was used to carry out the DFT calculations.

In order to study defects in the graphene-layer a supercell approach is used. We take a closer look at the 5-7 defect and its effect on the electronic structure, in particular on the local density of states near the Fermi level. Furthermore we investigate the absorbtion of a single oxygen atom on the graphene-layer. Structure optimisations for various unit-cell sizes show that the oxygen atom equilibrium position is approximatly 2 Å above the layer, also resulting in a perpendicular displacement of the surrounding carbon atoms of a few 0.1 Å. The effetcs on the electronic structure are studied in comparison with the undisturbed system via the (local) density of states.

TT 83.2 Wed 18:15 Poster A

High Energy Ion Irradiation of Graphene — Philipp Ernst[1], •Tobias Foller[1], Oliver Ochedowski[1], Roland Kozubek[1], Johannes Hopster[1], Jan Weber[2], Thorsten Balgar[2], and Marika Schleberger[1] — [1]Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Fakultät für Chemie and CeNIDE, Universität Duisburg-Essen, 45117 Duisburg, Germany

In this presentation we show that single high energetic ions can be used as a tool to locally modify the properties of graphene. For this graphene samples are irradiated with swift heavy ions (typical kinetic energies in the rage of 100 MeV) and slow highly charged ions (potential energies up to 45 keV). By combining various analytical techniques like AFM, TEM, and Raman spectroscopy it is shown that depending on the irradiation parameters (ion energy, angle of incidence, choice of substrate for graphene) various modifications like local defective areas, pores in form of origami-like foldings and even doping can be introduced into the graphene sheet. Remarkably graphene field-effect measurements revealed that irradiation with swift heavy ions under perpendicular incidence with small fluences doubles the mobility of holes compared to the unirradiated sample. In contrast to this, irradiation with highly charged ions decrease the mobility. In this case defects are created which are subsequently hydrogenated as strongly suggested by sum frequency generation spectroscopy.

TT 83.3 Wed 18:15 Poster A

Initial stages of hydrogen intercalation of epitaxial graphene studied by XPS and LEEM — •Julia Krone, Florian Speck, Felix Fromm, Martina Wanke, and Thomas Seyller — TU Chemnitz, Institut für Physik, Reichenhainer Straße 70, 09126 Chemnitz, Germany

During graphitization of SiC(0001) surfaces, a buffer layer (BL) is formed at the interface between graphene and the substrate. The BL is a graphene-like layer covalently bound to the SiC [1]. Hydrogen intercalation underneath the BL has been shown to decouple it from the substrate, thus converting it into quasi-freestanding monolayer graphene (QFMLG) [2]. This modification of the interface results in improved charge carrier mobility as compared to regular epitaxial graphene on SiC [3], making it an interesting material for electronic applications. Investigation of short-time annealing of the BL in molecular hydrogen could help to elucidate the initial stages of hydrogen intercalation and BL decoupling. In this work, we employ a combination of X-ray photoelectron spectroscopy, low-energy electron microscopy and low-energy electron diffraction to study the onset of QFMLG formation.

[1] K. V. Emtsev *et al.*, Phys. Rev. B **77**, 155303 (2008).
[2] C. Riedl *et al.*, Phys. Rev. Lett. **103**, 246804 (2009).
[3] F. Speck *et al.*, Appl. Phys. Lett. **99**, 122106 (2011).

TT 83.4 Wed 18:15 Poster A

XPS-investigation of the interaction of Lanthanides with epitaxial graphene — •Sarah Roscher, Martina Wanke, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz, Germany

Large-scale epitaxial graphene on silicon carbide is promising for electronic applications. Recently, interface engineering by intercalation of various elements underneath the buffer layer has been studied by several groups and it was demonstrated that elements of the Lanthanides are able to intercalate through epitaxial graphene [1-3]. In this study, erbium was deposited onto different graphene layers epitaxially grown on SiC(0001) and subsequently annealed in a temperature range of 300-950°C. X-ray photoelectron spectroscopy (XPS) was employed to determine the chemical composition of the sample, the intercalation, and the amount of doping. The XPS data indicate that subsequent heating to 850°C results in partial intercalation of the buffer layer. Because of erbium's high reactivity the influence of oxygen on the sample preparation demanded particular attention.

[1] S. Schumacher et al., Nano Lett. 13 (2013) 5013.
[2] S. Watcharinyanon et al., Graphene 2 (2013) 66.
[3] L. Huang et al., Appl. Phys. Lett. 99 (2011) 163107.

TT 83.5 Wed 18:15 Poster A

Structure and thermodynamic stability of graphene oxide — •Sebastian Gsänger and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

A large set of possible atomic configurations of graphene oxide with different composition and coverage were investigated by density functional theory. The adsorption of hydroxyl groups and the formation of epoxides and endoperoxides was systematically evaluated. In a first series of calculations the mutual interaction and the preferred relative position of pairs of adsorbates was determined. Based on these results, promising low-energy adsorption pattern at high coverage were derived and their thermodynamic stability was analyzed in terms of a surface phase diagram. Finally, the possibility for formation of 1,4-endoperoxides on graphene oxide was investigated in detail.

TT 83.6 Wed 18:15 Poster A

Investigation of the molecular doping of graphene on 6H-SiC(0001) — •Christian Raidel[1], Christian Heidrich[1], Julia Krone[1], Florian Speck[1], Peter Wehrfritz[1], Felix Fromm[1], Roland J. Koch[1], Peter Robaschik[2], Francisc Haidu[2], Ovidiu Gordan[2], Zoran Mazej[3], Dietrich R. T. Zahn[2], Thomas Seyller[1], and Martina Wanke[1] — [1]Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Halbleiterphysik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [3]Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Graphene is characterized by two linear bands crossing each other at the K-point of the hexagonal Brillouin zone. In neutral graphene, the Fermi level lies exactly at the crossing point where the density of states is zero. For certain applications, it is desirable to choose both charge carrier type and density which can be accomplished by electrostatic gating or doping. While substitutional doping alters the graphene lattice, charge transfer doping using adsorbates keeps the lattice intact.

In this work, we investigate charge transfer doping of graphene on 6H-SiC(0001) by organic molecules. Angle-resolved photoelectron spectroscopy (ARPES) was used to determine the position of the Dirac point and thus charge carrier type and density. It was observed that fluorinated fullerenes, mainly C60F48 can effectively induce p-type doping [1]. Thereby, the charge transfer is influenced by electron affinity of the adsorbed molecule and by the work function of the graphene, which was investigated in these studies. A model for the doping efficiency [1] of the various adsorbates was tested.

[1] Tadich, et al., APL 102, 241601 (2013)

TT 83.7 Wed 18:15 Poster A

Theoretical NMR signatures of water and ice on graphene — •Achraf Jaadouni, Eva Rauls, Wolf Gero Schmidt, and Uwe Gerstmann — University of Paderborn, Paderborn Germany

Since the discovery of graphene the adsorption of water has been discussed as a possibility for doping [1], while changing the electron mobility surprisingly little. Theoretical studies have shown that the electronic properties of the resulting system strongly depends on the microscopic details of the substrate [2].

In this theoretical work we investigate the influence of thin layers of ice using density functional theory (DFT) whereby van-der-Waals interaction has been taken into account. We demonstrate that an adsorption of at least two layers of ice on free standing graphene results in a charge transfer between the ice and graphene layers and, thus, can lead to a doping of graphene. The sign of the charge transfer and by this the type of doping, however, depends on the orientation of the water molecules. As a consequence, a mixture of two phases can result in a cancellation of the doping effect. Whereas the two configuration differ only slightly in total energies, the NMR chemical shifts calculated for both types of nuclei, O as well as H, are significantly different. Hence, a control of the orientation of the ice layers should be experimentally possible via nuclear magnetic resonance (NMR).

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science 306, 666 (2004).

[2] T.O. Wehling, A.I. Lichtenstein, and M.I. Katsnelson, Appl. Phys. Lett. 93, 202110 (2008).