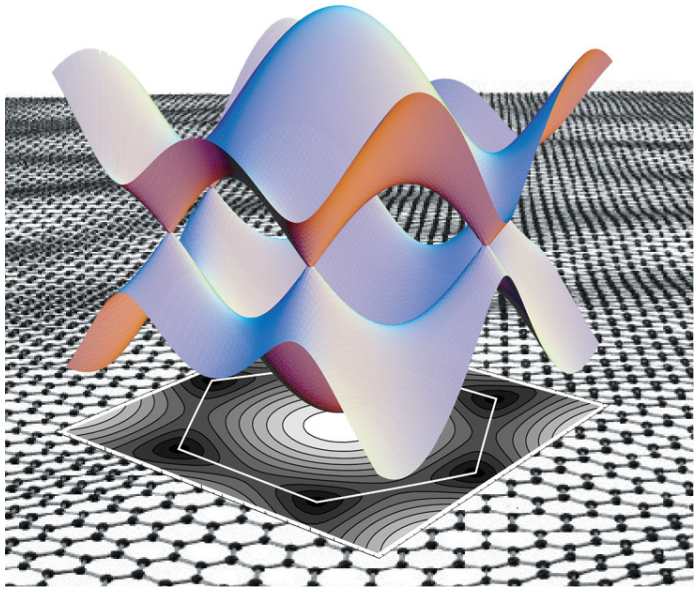
Report on Workshop

Computational Physics and Chemistry of Graphene



CECAM/Psi-k workshop, Lausanne, Switzerland
October 14-16, 2009

Organizers:

Oleg YAZYEV (University of California at Berkeley, USA)
Mikhail KATSNELSON (Radboud University Nijmegen, NL)
Annalisa FASOLINO (Radboud University Nijmegen, NL)

Supported by:

http://www.cecam.org/workshop-302.html
http://civet.berkeley.edu/~yazyev/Graphene2009

WORKSHOP SUMMARY

Graphene is a two-dimensional hexagonal allotrope of carbon. Since its isolation in 2004, this seemingly simple material has revealed a number of intriguing physical properties. Immediately, this series of discoveries ignited an ever-growing interest among researchers coming from various disciplines of basic and applied science.

This workshop was the first attempt to bring together computational scientists working on various aspects of graphene physics and chemistry under the roof of CECAM. The workshop aimed at a broad coverage of computational methods applied to study graphene and of its properties under investigation. In particular, the following topics have been addressed:

- Electronic structure and transport properties of graphene
- Magnetism, spintronics and quantum computing
- Optical properties of graphene
- Structure, defects and edges
- Interaction with substrates and adsorbates
- Chemical functionalization and reactivity

The workshop took place at the new location of CECAM headquarters in Lausanne, Switzerland. The program consisted of three full days of intensive talks and a poster session. The total number of registered participants was 45, including 3 organizers, 20 invited speakers and 1 representative of a sponsoring organization (QuantumWise A/S, Denmark). In fact, the number of applications for participating the workshop was significantly larger than the established limit of 50 participants. This illustrates very well the growing interest to graphene in the community of computational researchers. Geography of the workshop participants covers most of the countries in western and central Europe, USA, Singapore and South Korea.

The oral presentations were given by invited speakers. However, during a dedicated session all contributing participants were invited to give short talks summarizing their poster presentations. Many contributing participants used this opportunity to expose their research.

In addition to the researchers working in various fields of computational science, three talks were given by the leading experimentalists. In particular, Irina Grigorieva (University of Manchester, UK) spoke on the recent studies of the magnetic properties of graphene performed in the group of Andre Geim, where graphene has been isolated for the first time. Andrea Ferrari (University of Cambridge, UK) gave a talk on the optical properties of graphene with a particular emphasis on the applications of this material in optoelectronics. An

extensive overview of epitaxial graphene grown on a variety of metal surfaces was presented by Thomas Greber (University of Zurich, Switzerland).

Anders Blom (QuantumWise A/S, Denmark) offered a tutorial talk on the methodological aspects of Atomistix ToolKit, a software package for modeling electronic transport in nanostructures developed by QuantumWise A/S. Specific examples of the applications to graphene nanostructures have been shown.

Other invited speakers reported their latest progress in studying graphene *in silico*. The organizers didn't constrain the speakers in choosing the subjects of their talks. However, all major trends in the current computational research of graphene have been covered in the final program. Electronic transport of graphene still receives particular attention. This reflects the fact the current interest in graphene is clustered around its possible applications in the field of electronics. Several speakers have also covered a related field of spintronics and magnetic properties of graphene nanostructures. Another emerging topic covered by many participants is related to the chemical properties of this nanomaterial. Various aspects of graphene chemistry have been covered, in particular, graphene/substrate interactions, tuning the properties of graphene by adsorbates, impurities and chemical functionalization, chemical approaches to graphene production. Modeling defects in graphene and related carbon nanostructures was another major focus of computational research covered at the workshop. Topological defects such as grain boundaries and dislocations are now gaining increasing attention. Another emerging direction of computational research is related to tuning the properties of graphene by means of strain.

The workshop was sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the Psi-k Network, and QuantumWise A/S. The organizers and participants of the workshop thank these organizations for their generous support for the workshop.

We are pleased to conclude that the workshop was highly successful. The feedback from the workshop participants was very positive.

More information can be found at:

http://www.cecam.org/workshop-302.html
http://civet.berkeley.edu/~yazyev/Graphene2009

WORKSHOP PROGRAM

Day 1 - October, 14th 2009

08:30 to 09:00 – Welcome

09:00 to 09:40 – **Michele Lazzeri**
Transport properties of graphene in the high-current limit

09:40 to 10:20 – **Elisa Molinari**
Illuminating graphene nanostructures: nanoribbons and dots vs. nanotubes

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – **Alexander Lichtenstein**
Impurity states and electron scattering in graphene

11:30 to 12:10 – **Irina Grigorieva**
Magnetism in graphene-based systems: experiment

12:10 to 14:00 – Lunch Break

14:00 to 14:40 – **Oleg Yazyev**
Imperfect graphene: point defects, edges, dislocations and grain boundaries

14:40 to 15:20 – **Joaquin Fernandez-Rossier**
Spintronics and magnetism in graphene nanostructures

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – **Efthimios Kaxiras**
Graphene nano-flakes with large spin as structural elements for all-carbon spintronics devices

16:30 to 18:00 – Poster highlights

18:00 to 19:30 – Poster Session

Day 2 - October, 15th 2009

09:00 to 09:40 – **Tim Oliver Wehling**
Adsorbates and inhomogeneities on graphene: first principles studies

09:40 to 10:20 – **Biplab Sanyal**
Chemical functionalisation of graphene, experiment and theory

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – **Pablo Ordejon**
Transport properties of Carbon Nanotube links connecting Graphene layers

11:30 to 12:10 – **Anders Blom**
Modeling of graphene nanotransistors

12:10 to 14:00 – Lunch Break

14:00 to 14:40 – **Francisco Guinea**
Strains and electronic transport in graphene

14:40 to 15:20 – **Jean-Christophe Charlier**
Electronic Quantum Transport in Graphene Nanoribbons

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – **Thomas Greber**
Corrugated and Chiral Graphene and Boron Nitride single layers on transition metals

16:30 to 17:10 – **Andrea C. Ferrari**
Strain and Photoluminescence in Graphene

17:10 to 17:50 – **David Tomanek**
Probing and changing graphene with electric current and light

20:00 to 23:00 - Dinner

Day 3 - October, 16th 2009

09:00 to 09:40 - **Laurence Magaud**
Atomic and electronic structure of graphene on SiC

09:40 to 10:20 - **Young-Woo Son**
Electronic properties of graphene under external perturbations

10:20 to 10:50 - Coffee Break

10:50 to 11:30 - **Paul Kelly**
The ultimate HYPE: materials for HighlY Planar Electronics

11:30 to 12:10 - **Johan Carlsson**
Structural and Electronic Properties of Grain Boundaries in Graphene

12:10 to 14:00 - Lunch Break

14:00 to 14:40 - **Arkady Krasheninnikov**
Ion and electron irradiation of graphene

14:40 to 15:20 - **Daniel Gunlycke**
The effects of edges on the electronic and transport properties of graphene nanoribbons

15:20 to 16:20 - Closing word

LIST OF PARTICIPANTS

Organizers

Annalisa FASOLINO (Radboud University Nijmegen, NL)

Mikhail KATSNELSON (Radboud University Nijmegen, NL)

Oleg YAZYEV (University of California at Berkeley, USA)

Invited speakers

Anders BLOM (QuantumWise A/S, DK)

Johan CARLSSON (Fritz-Haber-Institut and Accelys GmbH, DE)

Jean-Christophe CHARLIER (University of Louvain, BE)

Joaquin FERNANDEZ-ROSSIER (University of Alicante, ES)

Andrea FERRARI (University of Cambridge, UK)

Thomas GREBER (University of Zurich, CH)

Irina GRIGORIEVA (University of Manchester, UK)

Francisco GUINEA (Instituto de Ciencia de Materiales de Madrid, ES)

Daniel GUNLYCKE (Naval Research Laboratory, USA)

Efthimios KAXIRAS (Ecole Polytechnique Fédérale de Lausanne, CH)

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Alexander LICHTENSTEIN (University of Hamburg, DE)

Laurence MAGAUD (Institut Néel, FR)

Elisa MOLINARI (Università di Modena, IT)

Pablo ORDEJON (CIN2 (CSIC-ICN), ES)

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Young-Woo SON (Korea Institute for Advanced Study, KR)

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Michiel VAN SETTEN (FZ Karlsruhe, DE)

Marco VANIN (Technical University of Denmark, DK)

Wei WANG (Harvard University, USA)

ABSTRACTS

Invited oral presentations

October 14, 09:00 to 09:40

Transport properties of graphene in the high-current limit

Michele Lazzeri
IMPMC, UMR CNRS, Universites Paris 6 et 7, IPGP

I will present a detailed study of the high-current transport properties of graphene devices patterned in a four-point configuration [1]. Measurements are compared to a transport model based on the Boltzmann equation, which includes electron-scattering processes due to charged and neutral impurities, and electron-scattering with graphene optical phonons. The current tends to saturate as the voltage across graphene is increased but never reaches the complete saturation as already observed in metallic carbon nanotubes, where high-bias electronic transport is associated with "hot phonon" generation [2]. Contrary to the case of metallic nanotubes, in graphene the saturation is incomplete because of the competition between disorder and optical-phonon scattering.
The actual value of the electron-phonon scattering coefficients plays a crucial role in this context and is computed from first-principles with DFT and GW which provide precise values in agreement with a large set of experimental data ranging from phonon dispersion from x-ray scattering on graphite and Raman spectroscopy data on graphene and nanotubes [3].

[1] A. Barreiro *et al.* PRL **103**, 076601 (2009);
[2] N. Vandecasteele *et al.* PRL **102**, 196801 (2009);
[3] A. Gruneis *et al.* PRB **80**, 085423 (2009); M. Lazzeri *et al.* PRB **78**, 081406 (2008)

October 14, 09:40 to 10:20

Illuminating graphene nanostructures: nanoribbons and dots vs. nanotubes

Elisa Molinari
Università di Modena

October 14, 10:50 to 11:30

Impurity states and electron scattering in graphene

Alexander Lichtenstein
University of Hamburg

Graphene has been attracting an increasing interest due to its remarkable physical properties ranging from the Dirac electron spectrum to ballistic transport under ambient conditions. The latter makes graphene a promising material for future electronics and the recently demonstrated possibility of chemical doping without significant change in mobility has improved graphene's prospects further. We address the question of impurity formation in graphene. Results of tight-binding calculations as well as DFT studies will be presented to explain the peculiar nature of impurity states in this material, the consequences for STM experiments as well as the possibility of strong exchange interactions between magnetic impurities. For the realistic case of Co on graphene, we discuss magnetic moment formation and chemical binding within GGA+U as function of the on-site Coulomb interaction. Depending on the adsorption site and interaction strength, we find Co in a spin 1/2 or spin 1 state.

October 14, 11:30 to 12:10

Magnetism in graphene-based systems: experiment

Irina Grigorieva
University of Manchester

There have been many reports predicting magnetic behaviour in graphene and graphene-based systems but very few experimental studies. We have succeeded in producing macroscopic graphene samples by ultrasonic exfoliation of graphite and subsequent deposition of graphene flakes to form the so-called graphene paper. Its magnetic properties have been studied using SQUID magnetometry and the results will be reviewed in this talk.

October 14, 14:00 to 14:40

Imperfect graphene: point defects, edges, dislocations and grain boundaries

Oleg Yazyev
University of California at Berkeley

In two dimensions, properties of materials can be heavily affected by structural irregularities. In this talk, I will review our recent efforts directed towards understanding various types of defects in graphene.

Firstly, I will present the results of first-principles studies of the magnetism induced by point defects and edges in graphene and graphite. We show that in graphene the single-atom defects (e.g. vacancies and hydrogen chemisorption) induce the spin-polarized defect states [1,2]. The coupling between the magnetic moments is either ferromagnetic or antiferromagnetic, depending on whether the defects correspond to the same or to different sublattices of the graphene lattice, respectively. These results are able to clarify the recent experimental observations of high-temperature ferromagnetism in proton-irradiated graphite. Similarly, the zigzag edges of graphene are predicted to induce localized magnetic moments which can serve as a basis for novel spintronic devices. We address the question of the spin correlation length at finite temperatures in this one-dimensional magnetic system and establish the limitations of the proposed spintronic devices [3].

Then, I will present our latest research on dislocations and grain boundaries in graphene [4], extended defects which are still poorly understood despites the growing number of experimental observations. I will introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors as well as grain boundaries, covering the whole range of possible misorientation angles. By using ab initio calculations we characterize thermodynamic and electronic properties of the proposed structures, finding energetically favorable large-angle grain boundaries, strong tendency towards out-of-plane deformation in the small-angle regimes, and pronounced effects on the electronic structure. Our results highlight an important role of dislocations and grain boundaries in practical graphene samples.

[1] O. V. Yazyev and L. Helm, Phys. Rev. B 75, 125408 (2007).
[2] O. V. Yazyev, Phys. Rev. Lett. 101, 037203 (2008).
[3] O. V. Yazyev and M. I. Katsnelson, Phys. Rev. Lett. 100, 047209 (2008).
[4] O. V. Yazyev and S. G. Louie, submitted.

October 14, 14:40 to 15:20

Spintronics and magnetism in graphene nanostructures

Joaquin Fernandez-Rossier
University of Alicante

A variety of graphene nanostructures, like ribbons and islands, present very peculiar spin properties, like magnetic order and spin Hall effect, according to both DFT calculations and model Hamiltonians. In this talk I will discuss three issues: 1) whether or not the graphene nanostructures with peculiar order are chemically stable 2) the competition (or cooperation) between spin orbit and interaction 3) the effect of curvature of the sample on its magnetic properties.

October 14, 15:50 to 16:30

Graphene nano-flakes with large spin as structural elements for all-carbon spintronics devices

Efthimios Kaxiras
Harvard University

π-electrons are responsible for many interesting electronic and magnetic properties of graphene. In the bulk, these electrons tend to pair with each other to stabilize the system and suppress the net magnetic moment. In the presence of edges, as in a finite graphene flake, a perfect pairing scheme may not be possible depending on the geometry. As a result, topological frustration could occur a net spin arises. In this talk, we combine graph theory and the Lieb theorem to classify arbitrary graphene nanoflakes depending on whether the frustration is on a single or both sublattices of the graphene lattice, which respectively give rise to a large net spin or to two groups of spins coupled antiferromagnetically. We carry out first-principles calculations to confirm these properties and illustrate how the general principle of topological frustration can be used to design all-carbon logic gates as the elementary components of spintronic devices. Finally, we review some current experimental progress and challenges in fabricating these nanometer scaled devices with focused electron beams.

October 15, 09:00 to 09:40

Adsorbates and inhomogeneities on graphene: first principles studies

Tim Oliver Wehling
1st Institute for Theoretical Physics, Hamburg University

We address adsorbate effects on the electronic properties of graphene. Based on density functional theory calculations, different interaction mechanisms of open- and closed-shell impurities with graphene are introduced.

The former impurities strongly interact with graphene and may from covalent or ionic to bonds. Within the class of monovalent impurities a relation between chemical bonding, the local electronic structure and migration barriers for the impurities is illustrated. Inert impurities like H_2O usually only physisorb on graphene and do not cause direct doping. They can, however, contribute local dipole moments and cause electrostatically mediated doping.

Finally, magnetic impurities on graphene and the particular importance of orbital symmetries are addressed. The implications for the Kondo screening of the impurity spin are discussed.

October 15, 09:40 to 10:20

Chemical functionalisation of graphene, experiment and theory

Biplab Sanyal
Dept. of Physics, Uppsala University

Graphene is a two dimensional carbon network with highly interesting properties. It has been shown that the electronic properties of graphene can be tuned by external agents. Here, we will present the electronic properties of chemically functionalized graphene studied by experiments and ab-initio density functional theory. Spectroscopic data will be analyzed by theoretical modeling of vacancy defects formed due to functionalization. Transport measurements and theoretical calculations show an increase in conductivity due to defect formation. Moreover, we will show the change in properties due to molecular adsorption in a defected graphene sheet. Finally, the magnetic properties of graphene nanoribbons in presence of transition metal adatoms will be presented.

October 15, 10:50 to 11:30

Transport properties of Carbon Nanotube links connecting Graphene layers

Pablo Ordejon
CIN2 (CSIC-ICN)

The study of electronic transport both in graphene and in carbon nanotubes has attracted a great deal of work, due to the interesting fundamental phenomena that these materials display and to the promise of outstanding applications in nanoelectronics. The two- and one-dimensional character of the two materials, respectively, confer them with sharply different electronic transport properties, and therefore different potential applications are envisioned.

In this work, we have considered the possibility of future devices that may use combinations of graphene layers and carbon nanotubes for electronic applications. For instance, nanotubes might be used to transmit electronic signals between two graphene-based devices, in the same way as copper wires do between traditional silicon-based transistors.

We present first-principles studies of the transport properties of a system consisting on two graphene sheets connected by a carbon nanotube. We consider different nanotubes with different chiralities and lengths, and also different types of connections between the tube and the sheet. We compute the ballistic transport between the two sheets through the nanotube, and show that the behavior of the conductance is qualitatively different for metallic and semiconducting nanotubes. We also show how the conductance depends on the link between the nanotube and the graphene sheet.

October 15, 11:30 to 12:10

Modeling of graphene nanotransistors

Anders Blom
QuantumWise A/S

This talk will discuss the latest developments in atomic-scale modeling of electron transport in nanoscale devices, with a focus on applications in graphene. Among other systems, we will present results of simulations of graphene nanoscale transistor structures, including the influence of an electrostatic gate and the (electron) temperature.

Over the last decade, a combination of DFT and NEGF methods has become a relatively established approach to describe the non-equilibrium transport properties of e.g. nanotubes, graphene, and molecular electronics structures. The majority of such studies involve system geometries with two leads, or electrodes, and the ballistic tunneling current at a finite bias applied between these electrodes, through the scattering or contact region, is computed. In order to simulate more realistic transistor-like device structures, it is however also necessary to consider the influence of various types of electrostatic gates and dielectric screening regions.

We will present an approach for handling such structures, as implemented in the latest version of our software package Atomistix ToolKit (ATK). It is based on a semi-empirical method (extended Hückel) to describe the electronic structure, combined with NEGF and scattering states methods for handling the non-equilibrium electron distribution. An arbitrary configuration of metallic and dielectric gates can be included in the system, and these are described fully self-consistently electrostatically, thus allowing for a realistic simulation of transistor characteristics of nanoscale device structures.

October 15, 14:00 to 14:40

Strains and electronic transport in graphene

Francisco Guinea
Instituto de Ciencia de Materiales de Madrid

One of the unique features of graphene is the fact that lattice strains induce effective gauge fields on the electronic carriers. We review different types of strains in mesoscopic graphene samples, and their effect on the electronic transport properties.

October 15, 14:40 to 15:20

Electronic Quantum Transport in Graphene Nanoribbons

Jean-Christophe Charlier
Université catholique de Louvain, Unité de Physico-Chime et de Physique des Matériaux (PCPM), European Theoretical Spectroscopy Facility (ETSF), 1348 Louvain-La-Neuve, Belgium.

Remarkable transport properties related to the very high electron/hole mobilities have been reported in graphene monolayers, suggesting their potential use in future nanoelectronic. However, since truly two-dimensional graphene is a zero gap semiconductor, its direct integration in active electronic devices such as field effect transistor seems prevented. The lithographic patterning of graphene into nanographites provides an easy way to overcome this drawback. Among the patterned nanographites, graphene nanoribbons (GNRs) have attracted considerable attention due to the strong relation between their electronic structure and their topology (more specifically the nature of their edges). Hydrogenated GNRs with armchair edges exhibit a band gap which arises from both quantum confinement and termination effects. In GNRs with zigzag shaped edges, an energy gap due to edge magnetization is found to depend on the hydrogen coverage of the terminations. Regarding their synthesis, bottomup fabrication techniques are very promising for the achievement of accurately defined ribbons geometries. However, GNRs produced are unlikely to be pristine graphene fragment with perfect atomic edges, but rather contains both topological and edges defects, playing the role of scattering centers. In the present work, the spin-polarized density functional theory is used to investigate the electronic and transport properties of GNRs with various edges geometries in the presence of topological and edge defects [1]. The nature and the position of the defect is found to play a key role in the band gap engineering of these graphene ribbons. In addition, pentagon and heptagon defect geometries are suggested to induce a strong electron-hole transport asymmetry owing to an effective chemical donor and acceptor character respectively. Single- or double-hydrogenation of single defects also affects the resulting conductance patterns dramatically. Consequently, large fluctuations of the conduction gap are induced by the disordered edge profile, as predicted by mesoscopic transport calculations based on accurately parameterized tight-binding models [2].

[1] Spin-Transport in Defective Graphene Nanoribbons, S.M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier, submitted for publication (2009).
[2] Electron-Hole Transport Asymmetry and Conduction Gaps in edge-defected Graphene NanoRibbons, S.M.-M. Dubois, A. Lopez-Bezanilla, A. Cresti, F. Triozon, J.-C. Charlier, and S. Roche, submitted for publication (2009).

October 15, 15:50 to 16:30

Corrugated and Chiral Graphene and Boron Nitride single layers on transition metals

Thomas Greber
University of Zurich

sp^2 hybridized single layers of hexagonal boron nitride and graphene on Rh(111) and Ru(0001) form corrugated superstructures with about 3nm lattice constant. [1] These structures are stable in air and may be used as templates for supramolecular architectures [2]. The peculiar trapping mechanism for single molecules with a diameter of 1 to 2 nm is traced back to strong lateral electric fields within the nanostructure that can be measured with photoemission from adsorbed xenon [3]. The adsorption of water in this nanostucture leads to the formation of bilayer ice clusters [4]. Graphene on Ru(0001) lowers the strain energy in breaking the mirror symmetry as it is inferred from surface X-ray diffraction and an analysis of the resulting elastic energies of chiral and achiral structural models [5].

[1] Brugger et al. Phys. Rev. B 79 (2009) 045407
[2] Berner et al. Angewandte Int. Ed. 46 (2007) 5115
[3] Dil et al. Science 319 (2008) 1826
[4] Ma et al. ArXiv:0908.0875
[5] Martoccia et al. ArXiv:0908.4517

October 15, 16:30 to 17:10

Strain and Photoluminescence in Graphene

Andrea C. Ferrari
University of Cambridge

Raman spectroscopy is one of the most powerful tools for graphene characterisation [1] I will first focus on the effects of uniaxial strain on its Raman spectrum [2]. The doubly degenerate E2g optical mode splits in two components, one polarized along the strain and the other perpendicular to it. This leads to the splitting of the G peak into two bands, which we call G+ and G-, by analogy with the effect of curvature on the nanotube G peak. Their variation with strain allows a direct measurement of the Gruneisen parameters [2]. Their relative intensities depend on light polarization determines the crystallographic orientation with respect to the applied strain [2]. I will then discuss the dependence of the 2D peak intensity on doping [4-6] and show that this is determined by a combination of electron-phonon and electron-electron scattering [6]. Under full resonance, the generated electron-hole pairs can scatter not just with phonons, but also with electrons and holes, and this affects the 2D peak intensity [7]. This explains quantitatively the experimental doping dependence of the 2D peak and can be used to determine its Electron Phonon Coupling, which is higher than previously predicted by density-functional theory, as a consequence of the renormalization by Coulomb interactions [7]. Finally I will discuss how to induce significant photoluminescence in graphene [8], and

how to exploit Pauli blocking to realise an ultrafast laser based on graphene as saturable absorber [9]. The latter examples show the viability of graphene for optoelectronics.

1. A. C. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006)
2. T. M. G. Mohiuddin et al. Phys Rev. B 79, 205433 (2008)
4. S. Pisana et al. Nature Mater. 6, 198 (2007)
5. A. Das et al, Nature Nano 3, 210 (2008).
6. C. Casiraghi et al. Appl. Phys Lett. 91, 233108 (2007)
7. D. M. Basko, S. Piscanec, A. C. Ferrari, arXiv:0906.0975 (2009)
8. T. Gokus, R. R. Nair, A. Bonetti, M. Bohmler, A. Lombardo, K. S. Novoselov, A. K. Geim, A. C. Ferrari, and A. Hartschuh; Arxiv 0909.3641v1(2009)
9. Z. Sun, T. Hasan, F. Torrisi, D. Popa, F. Bonaccorso, A. C. Ferrari, submitted (2009)

October 15, 17:10 to 17:50

Probing and changing graphene with electric current and light

David Tomanek
Michigan State University

Exposure to light is known to initiate desirable chemical reactions in nanostructures, such as photosynthesis, and cause permanent structural changes. Temporal reduction of the interlayer spacing in graphite irradiate by a femtosecond laser has been observed and interpreted by changes in the force field and suggested as a way to convert graphite to diamond. I will report results of time-dependent density functional calculations, coupled to molecular dynamics simulations [2] of a graphene slab exposed to laser irradiation. Our results indicate that by carefully tuning the laser fluence and pulse width, it should be possible to photo-exfoliate the topmost graphene layer from graphite [3], thus avoiding the shortcomings of mechanical and chemical exfoliation.

To harness the unique electronic properties of graphene such as high carrier mobility, it is sufficient to rotate the topmost layer without the necessity to physically separate it from the graphite substrate [4]. Also, spin injection does not necessitate the presence of ferromagnetic contacts or external fields, but may be achieved in graphene strips with asymmetrically rough edges [5] that may change due to Joule heating.

[1] Ramani K. Raman, Yoshie Murooka, Chong-Yu Ruan, Teng Yang, Savas Berber, and David Tománek, Direct Observation of Optically Induced Transient Structures in Graphite Using Ultrafast Electron Crystallography, Phys. Rev. Lett. 101, 077401 (2008).
[2] O. Sugino and Y. Miyamoto, Density-functional approach to electron dynamics: Stable simulation under a self-consistent field, Phys. Rev. B 59, 2579 (1999); 66, 089901(E) (2002).
[3] Youshiyuki Miyamoto, Hong Zhang, and David Tománek, Photo-exfoliation of graphite to graphene: An ab initio study (in preparation).
[4] K. S. Nagapriya, Savas Berber, Tzahi Cohen-Karni, Lior Segev, Onit Srur-Lavi, David Tománek and Ernesto Joselevich, Diameter-dependent conductance oscillations in carbon nanotubes upon torsion, Phys. Rev. B 78, 165417 (2008).

[5] Michael Wimmer, Inanc Adagideli, Savas Berber, David Tománek, and Klaus Richter, Spin transport in rough graphene nanoribbons, Phys. Rev. Lett. 100, 177207 (2008).

October 16, 09:00 to 09:40

Atomic and electronic structure of graphene on SiC

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Graphene is a topical material in condensed matter physics that offers outstanding electronic properties and a high potential for applications. We focus here on the graphene-on-SiC system where the annealing of a SiC surface leads to the formation of few graphitic layers. Though this system consists in several C layers on top of a SiC substrate, transport measurements, Raman and Landau Levels spectroscopies evidence properties expected for an isolated graphene sheet [1-3]. The question then is how the conducting graphene layer can be decoupled from its neighbourhood (substrate and other C layers). We have investigated the morphology and the electronic structure of the graphene-SiC interface on the basis of extensive ab initio calculations (VASP). In agreement with experiments, they are utterly different for the two polar faces of SiC -Si (0001) and C(000-1)-.
On the Si face, there is a strong interaction between the substrate and the first carbon layer [2]. This prevents any graphitic electronic properties for this layer. The graphitic nature of the film is recovered by the second and the third absorbed layers. They are dopped by a charge transfer from the substrate in agreement with ARPES experiments [3]. Interaction with the substrate is modelled in a very large supercell -more than 1200 atoms- that describes the actual experimental interface structure [4,5]. The effect of the complex first carbon layer geometry on the on top graphene like layer will also be discussed to show how it generates soft ripples in the honeycomb lattice.

On the C face, we propose a model for the interface, based on the SiC 2x2 native reconstruction that explains how the SiC surface is passivated by Si adatoms. Interaction between graphene and SiC is then much lower than on the Si face. Total energy calculations explain the rotational disorder of the graphene layers observed experimentally. Moreover, we will discuss the effect of a rotation between two graphene sheets to show how it leads to an effective decoupling of these layers and a linear free graphene like dispersion [6]. The renormalisation of the Fermi velocity for very small rotation angles will also be discussed [7].

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[2] F.Varchon, R.Feng, J.Hass, X.Li, B.Ngoc Nguyen, C.Naud, P.Mallet, J.-Y.Veuillen, C.Berger, E.H.Conrad, L.Magaud Phys. Rev. Lett. 99, 126805 (2007)
[3] T.Ohta et al, Science 313, 951 (2006)
[4] F.Varchon, P.Mallet, J.-Y.Veuillen, L.Magaud, Phys. Rev. B77, 235412 (2008)
[5] P.Mallet, F.Varchon, C.Naud, L.Magaud, C.Berger, J.-Y.Veuillen, Phys. Rev.B76, 041403 (2007)

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October 16, 09:40 to 10:20

Electronic properties of graphene under external perturbations

Young-Woo Son
Korea Institute for Advanced Study

In this talk, I will discuss my recent first-principles calculations on variations of electronic structures of graphene under uniform planar tensions [1] and on top of the SiC(0001) surface [2]. Both cases are shown to be deviated from an ideal description of the electronic structures of graphene and to exhibit many interesting electronic and electromechanical properties.

[1] S.-M. Choi, S. Jhi and Y.-W. Son, arXiv.org:0908.0977.
[2] S. Kim, J. Ihm, H. J. Choi and Y.-W. Son, submitted.

October 16, 10:50 to 11:30

The ultimate HYPE: materials for HighlY Planar Electronics*

Paul Kelly
Computational Materials Science, Faculty of Science and Technology, University of Twente

Measuring the transport of electrons through a graphene sheet necessarily involves contacting it with metal electrodes. We study the adsorption of graphene on metal substrates using first-principles calculations at the level of density-functional theory. The bonding of graphene to Al, Ag, Cu, Au, and Pt (111) surfaces is so weak that its unique “ultrarelativistic” electronic structure is preserved. The interaction does, however, lead to a charge transfer that shifts the Fermi level by up to 0.5 eV with respect to the conical points. The crossover from p-type to n-type doping occurs for a metal with a work function ~5.4 eV, a value much larger than the work function of free-standing graphene, 4.5 eV. We develop a simple analytical model that describes the Fermi level shift in graphene in terms of the metal substrate work function. Graphene interacts with and binds more strongly to Co, Ni, Pd, and Ti. This chemisorption involves hybridization between graphene pz states and metal d states that opens a band gap in graphene and reduces its work function considerably. The supported graphene is effectively n-type doped because in a current-in-plane device geometry the work-function lowering will lead to electrons being transferred to the unsupported part of the graphene sheet [1,3,5]. Cu has no states at the K-point for either spin while Co and Ni have the interesting property that they have only minority spin states at the K-point of reciprocal space making perfect spin filtering and injection possible [2,4]. Combination with the insulator h-BN [1] make it

possible to gate devices. A number of devices are discussed which have been studied with density functional based methods to predict their structural and electrical transport properties from first principles.

* Work carried out in collaboration with P. A. Khomyakov, G. Giovannetti, V.M. Karpan, P. C. Rusu, M. Bokdam, G. Brocks, M. Talanana, M. Zwierzycki, and J. van den Brink

October 16, 11:30 to 12:10

Structural and Electronic Properties of Grain Boundaries in Graphene

Johan M. Carlsson
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, and Accelrys Ltd, Cambridge Science Park 334, Cambridge CB4 OWN, United Kingdom

Graphene has been suggested as the ultimate material for nanoelectronics, but the extraordinary performance may be hampered by extended defects, such as grain boundaries(GB). GBs occur naturally in as-grown graphene, but relatively little is known about how the GBs affect graphene. Experimental results for small and large misorientation angles give a contradictory picture of the grain boundary structure as small GBs lead to buckling while large angle GBs are flat. We have developed a theory for the geometrical and electronic structure of GBs that is able resolve the experimental ambiguities. The theory is based on a combination of atomistic force field calculations and density functional calculations. These multiscale calculations show that the structure of low energy [0001] tilt boundaries in graphene can be identified as an periodic array of dislocation cores. The grain boundaries lead to an structural anisotropy that also impose an electronic anisotropy. The GBs open up band gaps for electrons travelling perpendicular to the grain boundary, but GB states occur parallel to boundary line. This indicates that GBs might have a strong influence on the electron transport in graphene.

October 16, 14:00 to 14:40

Ion and electron irradiation of graphene

Arkady Krasheninnikov
University of Helsinki

The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments [1] on the bombardment of carbon nanostructures with energetic particles demonstrate that irradiation can have beneficial effects and that electron or ion beams may serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of nanostructured carbon systems. Irradiation also gives rise to many interesting phenomena such as irradiation-

induced pressure build-up inside carbon nanotubes [2] and onions [3] encapsulated with metals.

We systematically study irradiation effects in graphene [4] and other forms of nano-structured carbon. By employing various atomistic models ranging from empirical potentials to time-dependent density functional theory we simulate collisions of energetic particles with carbon nanostructures, and calculate the properties of the irradiated systems. In this presentation, our latest theoretical (and first experimental) results on the response of graphene to electron and ion irradiation will be presented. I will also address the interaction of transition metal atoms with pristine and defected graphene sheets [5]. I will discuss the electronic structure of defected graphene sheets with adsorbed transition metal atoms and identify possible avenues for tailoring the electronic and magnetic structure of graphene by irradiation-induced defects and metal atoms.

1. For an overview, see A.V Krasheninnikov, F. Banhart, Nature Materials, 6 723-733 (2007).
2. L. Sun, F. Banhart, A.V Krasheninnikov, J.A. Rodriguez-Manzo, M. Terrones, and P.M. Ajayan, Science 312, 1199-1202 (2006).
[3] L. Sun, A.V. Krasheninnikov, T. Ahlgren, K. Nordlund, and F. Banhart, Phys. Rev. Lett., 101, 156101 (2008).
4. A.V. Krasheninnikov, Y. Miyamoto, and D. Tomanek, Phys. Rev. Lett. 99 (2007) 016104.
5. A.V. Krasheninnikov, P.O. Lehtinen, A.S. Foster, P. Pyykko, and R. M. Nieminen, Phys. Rev. Lett. 102, 126807(2009).

October 16, 14:40 to 15:20

The effects of edges on the electronic and transport properties of graphene nanoribbons

Daniel Gunlycke
Naval Research Laboratory

The presence of edges in graphene ribbons provide degrees of freedom that, when uncontrolled, can inhibit ballistic conduction, and when controlled, could provide great flexibility in tuning the electronic properties of the materials. In this talk, both armchair- and zigzag-edge nanoribbons terminated with different chemical species are covered. The effects of unevenness along the edges will also be considered. Presented calculations have been performed both/either at the local-density functional level and/or at the tight-binding level.

(*)This work has been funded by the Office of Naval Research, directly and through the Naval Research Laboratory.

Contributed presentations

P1

Coronene XPS spectrum: electron dynamics simulations

Angela Acocella
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Coauthor(s) : Francesco Zerbetto

Over the last twenty years, the potential for applications of carbon-based materials has constantly grown, both for systems such as fullerenes, nanotubes, and graphene, produced by a variety of physical means, and for molecules with carbon frameworks that are synthesized chemically. Coronene is a baby-graphene sheet at the cross road of the two types of systems, as it displays an abundance of high quality experimental and theoretical data, typical of molecules, as well as a wide variety of behaviours, typical of complex systems.

Several properties exploitable for practical applications of carbon-based materials depend on charge transport that takes a surprising turn in graphene with the relativistic velocity of its carriers, which is 1/300 of that of light.1 Spectroscopy monitors the motions of molecules, atoms and electrons, as a function of the energy of photons. In particular, X-ray photoelectron spectroscopy, XPS, is a quantitative spectroscopic technique that is often used for measuring the elemental composition, empirical formula, chemical and electronic states of the elements present in a material. Since the physics under XPS is extremely rich, the simulation of an XPS spectrum requires sophisticated quantum chemical models with a strong quantum mechanical basis2-4. The final ionized state is non-stationary. In practice, the high energy of the photon triggers a complicated re-organization of the wavefunction where the usually dominant one-photon contribution is combined with all the possible many-photon contributions of the same energy together with the continuum states of the ionized electron. Here we investigate the onset of the ionization dynamics with a quantum-mechanical time-dependent propagator used to evolve the electronic wavefunction5-7 and we also attempt to correlate it to the spectral analysis of XPS spectra.

(1) Geim, A. K.; Novoselov, K. S. Nat Mater 2007, 6, 183-191.
(2) Deleuze, M. S. The Journal of Physical Chemistry A 2004, 108, 9244-9259.
(3) Michael, D.; Markus, K. S.; Lorenz, S. C. The Journal of Chemical Physics 1995, 103, 3578-3588.
(4) Golod, A.; Deleuze, M. S.; Cederbaum, L. S. The Journal of Chemical Physics 1999, 110, 6014-6024.
(5) Acocella, A.; Jones, G. A.; Zerbetto, F. Journal of Physical Chemistry A 2006, 110, 5164-5172.
(6) Jones, G.; Acocella, A.; Zerbetto, F. Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) 2007, 118, 99-106.
(7) Jones, G. A.; Acocella, A.; Zerbetto, F. Journal of Physical Chemistry A 2008, 112, 9650-9656.

P2

Control of magnetization direction in molecules formed by π-ligands and 4f-metals

Nicolae Atodiresei
Research Centre Juelich, Institute of Solid State Research (IFF) and Institute for Advanced Simulation (IAS)

By means of ab initio calculations we predict that it is possible to manipulate the magnetization direction in organic magnetic molecules by changing their oxidation state. We demonstrate this novel effect on the Eu2(C8H8)3 molecule, in which the hybridization of the outer π -ring states with the Eu 4f-states causes a redistribution of the orbitals around the Fermi level leading to a strong ferromagnetism due to a hole-mediated exchange mechanism. As a key result, we predict an oscillatory behavior of the easy axis of the magnetization as a function of the oxidation state of the molecule [1] —a new effect, which could lead to new technological application.

[1] N. Atodiresei et al., "Controlling the Magnetization Direction in Molecules via Their Oxidation State", Phys. Rev. Lett. 100, 117207 (2008).

P3

Structural properties and elasticity of graphene flakes: density functional study

Soumya Bera
Institute for Nanotechnology, FZK

Under generic experimental conditions graphene sheets exhibit a surface corrugation ("ripples"), which are believed to leave a pronounced signature in the electronic structure. To better understand the origin of ripples, elastic properties of graphene membranes and flakes should be investigated.

We present a detailed study of thermodynamic properties of edge hydrogenated graphene flakes in the presence of surface ripples, which is based on the density functional theory. In particular, we calculate the flake's free energy and disentangle the surface and bulk contributions. We discover, that the surface contribution exerts a pressure which substantially diminishes the carbon-carbon distance even in the flake's interior. Furthermore, we also compute all elastic constants ("Lame'e parameters") and determine the quantum corrections by including the contribution of phonons to the free energy. Our analysis of the long range phonon modes reveals the characteristic flexural dispersion.

P4

Electron transport simulations through organic adlayers on metal surfaces

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ICMAB
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Molecular entities at the interface with an inorganic surface are the basis for new hybrid functional materials for microelectronics. In most cases, strong bonding of molecules to metal surfaces perturbs the discrete molecular energy levels leading to a broadening of the molecular density of states. Deposition of C60 on a Au(111) surface previosly exposed to tetraphenyl adamantane give rises to a nanostructured organic layer where the electronic coupling between the C60 and the Au(111) surface is significantly reduced compared to C60 on a clean Au(111) surface (1). In this case molecular states of C60 remain more localized and less broadened, thus giving rise to strong non-linearities in the electron transport through the organic-inorganic interface. Calculations based on Density Functional Theory reveal that intermolecular interactions lock C60 into a particular orientation. Scanning tunneling spectroscopy experiments on such system exhibit the presence of negative differential resistance that motivated the simulation of the transport properties at ab-initio level using TRANSIESTA.

KJ. Franke, G. Schulze, N. Henningsen, I. Fernandez-Torrente, JI. Pascual, S. Zrwell, K. Ruck-Braun, M. Cobian, N. Lorente Physical Review Letters 2008, 100, 036807

P5

Spin relaxation time in graphene induced by impurities

Martin Gradhand
Max Planck Institute of Microstructure Physics
Coauthor(s) : Dmitry Fedorov, Peter Zahn, Michael Czerner, Ingrid Mertig

Recent experiments [1,2] have shown that spins in graphene relax faster than it was expected taking into account the low atomic number of carbon atom. A possible explanation was that the Elliot-Yafet spin relaxation mechanism is dominating. In addition, an anisotropy of the spin relaxation time was found to be about 20%. We present an ab initio treatment of the Elliott-Yafet mechanism with spin scattering induced by impurities. The electronic structure of graphene with point defects is calculated in the framework of density-functional theory using a multiple scattering Green's function Korringa-Kohn-Rostoker scheme. The spin-life time is obtained by applying Fermi's golden rule. The anisotropy of the spin relaxation time is evaluated, also.

[1] N. Tombros et al., Nature 448, 571 (2007)
[2] N. Tombros et al., Phys. Rev. Lett. 101, 046601 (2008)

P6

Nonlinear screening of charges induced by metal contacts in graphene

Petr Khomyakov
IBM Research Division - Zurich Research Laboratory
Coauthor(s) : A. A. Starikov, G. Brocks, P. J. Kelly

To understand the band bending caused by metal contacts, we study the potential and charge density induced in graphene in response to contact with a metal strip [1, 2]. We find that the screening is weak by comparison with a normal metal as a consequence of the ultra-relativistic nature of the electron spectrum near the Fermi energy. The induced potential decays with the distance from the metal contact as x^(-1/2) and x^(-1) respectively, for undoped and doped graphene, breaking its spatial homogeneity. In the contact region the metal contact can give rise to the formation of a p-p, n-n, p-n junction (or with additional gating, even a p-n-p junction) that contributes to the overall resistance of the graphene sample, destroying its electron-hole symmetry.

[1] G. Giovannetti, P. A. Khomyakov, G. Brocks, V. M. Karpan, J. van den Brink, and P. J. Kelly , Phys. Rev. Lett. 101, 026803 (2008).
[2] P. Khomyakov, G. Giovannetti, P. C. Rusu, G. Brocks, J. van den Brink, and P. J. Kelly, Phys. Rev. B 79, 195425 (2009).

P7

Simulations of electron beam damage on graphene

Jani Kotakoski
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Coauthor(s) : Arkady Krasheninnikov

Recent advances in high resolution transmission electron microscopy (HRTEM) have revealed a welth of interesting atomic scale processes occurring under the electron beam, hitherto only accessible by atomistic simulations. While the computational power has also increased in the meanwhile, we can now join the ab initio calculations and HRTEM experiments in order to fully understand how light atoms, such as carbon in graphene, behave in these conditions. Furthermore, by carefully designing the experimental conditions and electron currents, aided by computational methods, it is possible to directly modify the atomic structure of graphene - or carbon nanotubes - by using the electron beam. This can for instance allow creating novel nanoscaled materials for future electronics.

Although some of the produced defects and their properties have been known for some time, e.g. Stone-Wales defects, several possible vacancy configurations (mono- and divacancy, 555-777) and carbon adatoms, several questions are still unanswered. By combining density functional theory (DFT) and DFT-based tight binding (DFTB), we have described experimentally seen complex radiation damage patterns on graphene, and explained how they

may have been formed during the exposure of graphene to the electron beam. Furthermore, we have studied recombination of Frenkel pairs (adatom-vacancy pair) on graphene by DFT, and described the most likely trajectories of the point defects close to each other. We also use DFT calculations in order to explain the surprisingly high concentration of Stone-Wales defects seen in the experiments, despite their high formation energy.

P8

Infrared observation of the bandgap and phonon anomalies in gated bilayer graphene

Alexey Kuzmenko
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Coauthor(s) : I. Crassee, E. van Heumen, D. van der Marel, P. Lerch, L. Benfatto, E. Cappelluti, P. Blake, K.S. Novoselov, A.K. Geim

Bilayer graphene is the simplest system where the electronic coupling between stacked graphene layers can be studied and exploited. Although this coupling is much weaker than the in-plane chemical bonding, it gives rise to several new spectacular phenomena, resulting from extra electronic and lattice degrees of freedom. Some of these effects, such as the opening of a bandgap in a perpendicular electric field [1], make bilayer graphene promising for applications. Infrared spectroscopy, which is a powerful technique to study electronic and lattice dynamics in solids, additionally benefits in graphene from a possibility to combine it with electrostatic gating. We have measured infrared reflectivity spectra of bottom-gated exfoliated bilayer graphene in the range of photon energies between 0.08 and 1 eV and carrier concentrations up to 1013 cm-2 [2,3]. By a simultaneous fitting of the whole 3D set of spectra with the tight-binding Slonzewski-Weiss-McClure (SWMcC) model, we extracted the bandgap as a function of the gate voltage and determined the SWMcC parameters $\gamma 0$, $\gamma 1$, $\gamma 3$, $\gamma 4$ and Δ. Our study demonstrates an important influence of electrostatic self-screening on the value of the bandgap.

This study reveals also several anomalies of the infrared peak corresponding to the anti-symmetric Eu in-plane mode (~ 0.2 eV). We observe an unexpected giant increase of the peak intensity and its softening as a function of the gate voltage. Interestingly, the phonon peak has a pronounced Fano-like asymmetry. We suggest that the intensity growth and the softening originate from the coupling of the phonon mode to the narrow electronic transition between parallel bands of the same character ($\gamma 1$ - transition), while the asymmetry is due to the interaction with the continuum of transitions between the lowest hole and electron bands. The amplification of the peak can be interpreted as a "charged-phonon" effect [5] observed previously in organic chain conductors and doped fullerenes.

[1] E. McCann and V.I. Fal'ko, Phys. Rev. Lett. 96, 086805 (2006).
[2] A B. Kuzmenko et al., Phys. Rev. B 79, 115411 (2009).
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[4] A B. Kuzmenko et al., Phys. Rev. Lett. 103, 116804 (2009).
[5] M. J. Rice, N.O. Lipari and S. Strassler, Phys. Rev. Lett. 39, 1359 (1977).

P9

Graphene on Ir(111) surface: From van der Waals to strong chemical bonding

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Even though the bonding in graphene sheet is very strong and of chemical character, when graphene is adsorbed on different surfaces a variety of phenomena may arise with respect to the bonding mechanism. On some surfaces it gets chemisorbed, but on others (e.g. when it bonds to other graphene sheets into graphite) it is physisorbed, similarly as on Ir(111). Putting additional metal atoms on top of graphene/Ir(111) results in locally chemical bonds due to the change from sp2 to sp3 hybridization in carbon atoms. Current DFT implementations, due to semi-locality of the functionals used, do not describe properly long range correlation effects which are crucial for van der Waals forces (physisorption). However, some five years ago a new truly nonlocal ab initio functional was proposed, named vdW-DF. We applied this functional in order to study different regimes of graphene adsorption on metal surfaces.

P10

Hydrogenation of bilayer graphene

Ortwin Leenaerts
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Coauthor(s) : B. Partoens, F. M. Peeters

We studied the process of hydrogenation of a bernal stacked (AB) bilayer of graphene using density functional theory. As for single layer graphene, hydrogenation of a bilayer causes the opening of a band gap in the electronic structure at the K point [1] which might be important for possible applications in electronics. In our work we focussed on the formation of chemical bonds between the two graphene layers as a consequence of hydrogen adsorption at higher concentrations.
The most stable position of a hydrogen atom adsorbed on a single graphene layer is on top of a single carbon atom of the graphene sheet inducing the formation of a chemical bond between the carbon and hydrogen atom. The hybridisation of this carbon atom changes from sp2 to sp3 in forming this bond and also the neighbouring carbon atoms will slightly change their hybridisation. In case of a bilayer of graphene with hydrogenation taking place at both sides, the changed hybridisation of the neighbouring carbon atoms can induce chemical bonds between the two layers. Whether this will happen or not depends strongly on the concentration of the adsorbed hydrogen atoms. In an AB stacked graphene bilayer the interlayer chemical bonds are formed between the carbon atoms located on top of each other and having at least two hydrogenated neighbours. At high hydrogen concentrations one hydrogenated neighbour may also suffice.

[1] D. W. Boukhvalov, and M. I. Katsnelson, Phys. Rev. B 78, 085413 (2008).

P11

Ballistic-Ohmic quantum Hall plateau transition in graphene pn junction

Tony Low
Purdue University

Recent quantum Hall experiments conducted on graphene pn junction provide evidence that the junction resistance could be described by a simple Ohmic sum of the individual resistances of the n and p medium. On the other hand, theory predicts the existence of different quantum Hall plateaus in a ballistic pn junction. Although it is highly suggestive that disorders are responsible for the Ohmic behavior observed in experiments, the underlying mechanism responsible for the ballistic-Ohmic plateau transition is not well understood. In this work, we performed a series of magneto-transport calculations on a 0.1um-wide disordered graphene pn junction within the tight-binding model. Two types of disorders, namely pn interface and edge roughness, are considered in this work. The former plays the role of equilibrating the Landau modes along the pn interface. We found that pn interface disorder with a root-mean-square roughness of only 10nm is sufficient to completely equilibrate the Landau modes propagating along the pn junction under typical experimental conditions. On the other hand, edge disorder plays the role of diluting the valley iso-spin information of the lowest Landau level. We show that these two mechanisms are sufficient in recovering the simple ohmic sum rule observed in experiments, in both armchair and zigzag ribbons for all Landau level filling factor combinations. Lastly, we benchmark our numerical results against recent experimental data.

P12

Disorder-induced pseudodiffusive transport in graphene nanoribbons

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We study the transition from ballistic to diffusive and localized transport in graphene nanoribbons in the presence of binary disorder, which can be generated by chemical adsorbates or substitutional doping. The interplay between the induced average doping and the impurity scattering modifies the traditional picture of phase-coherent transport. Close to the Dirac point, intrinsic evanescent modes produced by the impurities dominate transport at short lengths giving rise to a regime analogous to pseudodiffusive transport in clean graphene. This intrinsic pseudodiffusive regime precedes the traditional ballistic, diffusive, and localized regimes. The latter regimes exhibit an anomalously large mean free path close to the Dirac point.

P13

Exploring the two-dimensional Brillouin zone of the electronic and the vibrational band structure of uniaxially strained graphene

Marcel Mohr
Technical University Berlin
Coauthor(s) : Papagelis, Janina Maultzsch, Christian Thomsen

We report ab initio calculations of uniaxially strained graphene. Strain is applied in arbitrary directions and the effect on the electronic and vibrational spectrum is analyzed. Under small strains graphene remains semimetallic. The Fermi surface points move away from the K-points, thus favoring electronic transport in specific directions. The Raman-active E2g and 2D-mode are red-shifted. The shift rates are independent on the strain direction. Due to the loss of the three-fold symmetry of the Dirac-cones, the 2D-mode becomes broadened by 10 cm^(-1) per 1% strain.

P14

Nonequilibrium phase transitions and shot noise as all-electrical probes of magnetism in zigzag graphene nanoribbons

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Recent chemical derivation [X. Li *et al.*, Science **319**, 1229 (2008)] of sub-10-nm wide semiconducting graphene nanoribbons with ultrasmooth edges has opened new avenues to explore magnetic ordering along zigzag edges and potential applications in carbonbased nanoelectronics and nanospintronics. While numerous density functional theory calculations predict magnetism in zigzag graphene nanoribbons (ZGNR), this has remained an elusive phenomenon for direct experimental observations. Here I overview our recent proposal to use *all-electrical* transport measurements to detect this low-dimensional *s-p* magnetism: (i) if the length of the sub-10-nm wide GNRs in decreased from 100 nm [as in recent experiments on GNRFETs, Wang *et al.*, Phys. Rev. Lett. **100**, 206803 (2008)] to 10 nm, one should observe a nonequilibrium phase transition between magnetic insulator at low bias voltage and nonmagnetic metal at bias voltage around 1 V whose principal signature is a jump in the corresponding I-V characteristics and possibly a hysteresis due to nonequilibrium-driven collapse of magnetic ordering induced band gap [1]; (ii) when wide and short GNRs are attached to metallic electrodes they become doped by injected evanescent wave functions which leads to "pseudodiffusive" transport with Ohmic-like conductance and the Fano factor (noise-to-current ratio) of the shot noise being the same as in the diffusive metallic wires, as observed in recent experiments [R. Danneau *et al.*, Phys. Rev. Lett. **100**, 196802 (2008)]—however, zigzag edges and localized magnetic ordering around them could enhance

this Fano factor so that shot noise acts as edge sensitive all-electrical probe of magnetic degree of freedom [2]. I also discuss possible applications of GNRs in spintronics [3].

[1] D. A. Areshkin and B. K. Nikolić, Phys. Rev. B **79**, 205430 (2009).
[2] R. L. Dragomirova, D. A. Areshkin, and B. K. Nikolić, Phys. Rev. B **79**, 241401(R) (2009).
[3] S.-H. Chen, B. K. Nikolić, and C.-R. Chang, arXiv:0904.2192 (2009).

P15

Computational Nanomechanics of Graphene

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Coauthor(s) : Romain Perriot

The unique properties of graphene are the subject of intense theoretical and experimental investigations. In recent nanoindentation experiments, graphene was found to be the strongest material ever investigated. In this presentation, we discuss the results of atomistic modeling of mechanical properties of graphene. The computational nanoindentation experiments were focused on studies of the elastic properties, as well as the dynamics of the plastic deformations and defect formations that result in membrane breaking. The onset of defect appearance allowed us to determine the true elastic limit of graphene and the corresponding yield strength which was not accessible experimentally. The defects consist of vacancies and Stone-Wales type defects. Long stable linear chains of bonded carbon atoms (carbynes) were observed under the indenter at the advanced stages of indentation. The dynamics of fracture propagation is governed by the shear stresses developed in the sample. Comparison with experiment will also be discussed.

P16

Ab-Initio Study of the Graphene/SiC Interface

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Coauthor(s) : Oleg Yazyev, Alfredo Pasquarello

Epitaxial graphene grown on silicon carbide (SiC) surfaces is one of the promising approaches towards realizing graphene-based electronic at industrial scales [1]. Interactions with the SiC substrate play crucial role in the transport properties of electronic devices based on epitaxial graphene [2]. In our work, we investigate the local interface structures by using first-principles approach. In particular, our structural models involve both unreconstructed C- and Si-terminated surfaces of SiC as well as adatoms and ad-tetramers at the interface [3,4].

Variations of the stoichiometry have been addressed by systematically changing the nature of the atoms at the interface. The relative stabilities of different models are analyzed in terms of the grand canonical potential [5]. We found that silicon atoms compose the most stable ad-structures over a wide range of chemical potential. While silicon adatoms seems to be preferred in SiC environment, more silicon-rich condition seems to favor silicon tetramer. Only Carbon-rich environment allowed carbon ad-structure to exist. The electronic band structures and work functions of stable structures are further considered in details. The results of our work allow understanding the basic atomic and electronic structure features of realistic graphene/SiC interfaces.

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P17

Linearly doped graphene by charge transfer complex

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Based on density functional theory (DFT), the doping behaviors of graphene by molecular adsorption have been investigated extensively through detailed analysis of interfacial electronic structures. Strong donor (acceptor) molecules give (attract) electron to make n(p)-doped graphene due to the mismatch between the ionization potential of single molecule and the work function of graphene. It is also found that acceptor molecules change the electronic structure of inert graphene significantly, while donor molecule doesn't alter that much. The doping behavior of graphene can be controlled by tuning the ratio of donor and acceptor molecules. This provides a noncovalent and nondestructive method for functionalizing graphene, which is very easy for experimental realization.

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Co dimers on graphene proposed as magnetic storage bits

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It is shown by density functional calculations that transition metal - carbon systems may exhibit a huge magnetocrystalline anisotropy, and thus have the potential to enhance the present area density of magnetic recording by three orders of magnitude. As a model system, Co2-benzene is investigated and a magnetic anisotropy energy between 50 meV (lower estimate by GGA) and 330 meV (upper estimate by GGA with orbital polarization corrections) is found, large enough to store permanently one bit of information at temperatures accessible to industrial technology. The origin of such a huge anisotropy is explained and it is demonstrated that it can be achieved without heavy metal substrates. Thus, deposition of cobalt dimers on graphene or on graphite (0001) is predicted to result in a similarly large anisotropy. Finally, it is proposed that such subnanometer bits can be written by a combination of moderate magnetic and strong electric fields.

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Band structure engineering in graphene Ribbons by edge chemistry

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Edge termination is an important topic for graphene ribbons. This aspect has been appreciated by many authors in the context of edge localized transport modes, edge magnetization etc.. What has not been studied systematically is the effect of edge chemistry on the interior modes of the ribbon. One of the reasons why these bulk modes are especially interesting is, that it is them who are most susceptible to chemical functionalization and therefore most promising for chemical sensing applications. In addition, these modes are also carrying the main current for wider ribbons and therefore dominate the low temperature transport properties.
In our contribution we present studies where we have looked at various experimentally motivated possibilities for edge terminations. We investigate their effect on the atomic structure of the ribbon and how these geometrical changes effect the electronic structure. To get an improved quantitative estimate for the emergent band gaps we apply the GW methodology.

Graphene on metals

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The discovery in 2004 [1] of a method to prepare free-standing graphene, a monoatomic layer of graphite, has stimulated enormous scientific and technological interests. Due to its exotic electronic properties, graphene is currently been considered as a promising candidate in the field of molecular, carbon based, electronics. Understanding the interaction of graphene with metal surfaces is important since graphene growth on transition metal catalysts is one of the major method for graphene preparation [2,3,4]. Moreover, transport measurements and actual devices necessarily involves making contacts with metals.

The main theoretical challenge in modelling the graphene-substrate interface is that methods based on the density functional theory with common local and semi-local approximations for the exchange and correlation effects are not able to reproduce the long range dispersive interaction, i.e. van der Waals. The most common approach is then to use the simple local density approximation (LDA) which at least provide some binding, contrary to most gradient corrected functionals (GGAs) [5].

In this work we apply the recently developed VDW-DF [6] which includes non-local contributions in order to account for the long ranged van der Waals forces. Within this approximation, we find that all the investigated metals interact weakly with the metal surfaces. This is in contrast with what is predicted by the LDA approximation, which is most often employed with these systems.

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Graphene nanostructures and their fabrication

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Finite graphene such as graphene nanoribbon and graphene nanoflakes are attractive nanostructures for electronics and spintronics applications. Realization of these applications however put server challenge on device fabrication and complicated by issues such as structural instability and functionalization of unexpected species. In this talk, we discuss the electronic and magnetic properties of various graphene nanoflakes structures and the theoretical modeling of producing these structures with controlled electron beam in vacuum.