Towards Reality in Nanoscale Materials VI

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Organizers

Prof. Adam Foster
Department of Applied Physics, Aalto University

Dr. Teemu Hynninen
Department of Applied Physics, Aalto University

Dr. Arkady Krasheninnikov
Department of Applied Physics, Aalto University
Department of Physics, University of Helsinki

Prof. Risto Nieminen
Department of Applied Physics, Aalto University

Prof. Kai Nordlund
Department of Physics, University of Helsinki

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Programme

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	chair: Schwarz	9:00	**Grigorieva**	9:00	**Caro**
9:00	**Repp**	9:40	**Yazyev**	9:40	Djurabekova
9:40	**Berndt**	10:20	Casartelli	10:00	Philipp
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	chair: Repp	11:20	**Kis**		*chair: Seifert*
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17:00	Björkman			16:40	Landers
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9:40	-	10:20	**Berndt** Plasmons, forces and currents in atomic and molecular contacts
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11:20	-	12:00	**Schwarz** Magnetic Exchange Force Microscopy and Spectroscopy - A Novel Technique to Study Magnetism with Atomic Resolution
12:00	-	12:20	Eder Poking from both sides - Reshaping Graphene Landscape Via Face-To-Face Dual Probe Microscopy
12:20	-	12:40	Weymouth The Phantom force
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16:40	-	17:00	Mittendorfer Growth and magnetic properties of lowdimensional oxide films on a support: CoO/Ir(100)
17:00	-	17:20	Björkman Adsorption and defects of 2-dimensional silica
17:20	-	18:00	*Coffee*
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18:00	-	18:40	**Gale** Extending the scope of force field methods: reactivity and multiple scales
18:40	-	19:00	Jonsson Calculations of electronic defects and excitons in oxides

Scanning Probe Spectroscopy of Individual Molecules on Thin Insulating Films

J. Repp[1]

[1] Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Ultrathin insulating films on metal substrates facilitate the use of the scanning tunneling microscope (STM) to study the electronic properties of single atoms and molecules, which are electronically decoupled from the metallic substrate. This setup enables to perform spatially resolved vibronic spectroscopy in a double barrier tunnelling junction geometry. We show that the spatial position of the electron injection as well as the local wave function symmetry dramatically affect the electron-vibron coupling. We observe that the energy dissipation associated with the electron attachment, the so-called reorganization energy, spatially varies by more than a factor of two. We investigated $C_{20}S_2H_{12}$ molecules adsorbed on ultrathin layers of NaCl by means of atomic force-microscopy (AFM) in a combined STM/AFM based on the qPlus-sensor. These non-planar molecules exist in two stable conformations. By means of excitations from inelastic tunneling electrons we can switch between both conformations. We present atomic force microscopy (AFM) measurements with submolecular resolution directly revealing the conformational changes. From AFM data and taking the chirality of the molecules into account, we could unambiguously determine the pathway of the conformational change. Hence, the AFM channel reveals additional information that is truly complementary to the STM data set. Finally, we formed artificial metal-organic complexes on the same substrate by means of inelastic excitations. The electronic decoupling of the ultrathin NaCl films enabled the study of the molecular electronic structure of the constituents and the complex by means of scanning tunnelling spectroscopy. The actual bonding geometry was determined from AFM images with submolecular resolution. Exploiting the symmetry of the complex its electronic structure can be rationalized from considering the linear combinations of the constituents' orbitals.

Plasmons, forces and currents in atomic and molecular contacts

R. Berndt[1]

[1] Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The electron transport through single atoms, molecules and molecule-molecule contacts is investigated with low-temperature scanning probe microscopy. In the experiments, which aim at maximizing the control over the junction properties, the conductance, the acting force and the emission of photons are probed. The talk will address the role of molecular structure and bonding as well as localized plasmons and quantum noise properties.

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy

J. van der Lit[1] M. P. Boneschanscher[1] M. Ijäs[2] A. Harju[2] P. Liljeroth[2]
D. Vanmaekelbergh[1] I. Swart[1]

[1]Debye Institute for Nanomaterials Science, Utrecht University, 3508 TA Utrecht, the Netherlands
[2]Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland

Many applications have been envisioned for graphene, a monolayer of carbon atoms packed in a hexagonal lattice [1,2]. However, the fact that graphene remains metallic even at the neutrality point is a major problem for applications in (opto-)electronic devices. One possible way to introduce a bandgap in graphene is by fabricating narrow gaphene ribbons. The electronic and magnetic properties of such nanostructures sensitively depend on the atomic structure of the edges. Recent advances in the on-surface synthesis of graphene nanoribbons (GNRs) have made it possible to manufacture atomically well-defined, narrow, GNRs with arm-chair edges and a band-gap in excess of 2 eV [3-5].

By combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with reactive and non-reactive tips, we can relate the electronic properties of the GNRs with their atomic structure. Furthermore, we can use the STM tip to (i) deliberately create well-defined atomic scale defects and (ii) control the interaction with the substrate. Hence, we are able to directly study the robustness of the properties of the graphene nanostructures.

[1] A. K. Geim, *Science* **324**, 1530 (2009).
[2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Re. Mod. Phys.* **81**, 109 (2009).
[3] J. Cai, et al. , *Nature* **466**, 470 (2010).
[4] P. Ruffieux, et al. , *ACS Nano* **6**, 6930 (2012).
[5] M. Koch, F. Ample, C. Joachim, L. Grill, *Nat. Nanotechnol.* **7**, 713 (2012).

Magnetic Exchange Force Microscopy and Spectroscopy - A Novel Technique to Study Magnetism with Atomic Resolution

A. Schwarz[1]

[1]Institute of Applied Physics, University of Hamburg, 20355 Hamburg, Germany

Magnetism on the nanoscale exhibits new phenomena due to the reduced dimensionality and the presence of surfaces as well as interfaces. For example, single atoms often exhibit a very strong anisotropy energy, e.g., Co adatoms on Pt(111), which can exceed bulk values by orders of magnitude. At interfaces spin-orbit coupling between a non-magnetic substrate and a magnetic overlayer can induce a new magnetic order, e.g., Fe, the prototypical bulk ferromagnet, orders antiferromagnetically if deposited as a monolayer on W(001). Some non-magnetic surfaces show a rather exotic magnetic behavior on its own, e.g., the pseudospin in graphene and the spin-orbit coupling in the surface state of topological insulators.

In this presentation magnetic exchange force microscopy (MExFM), which is a rather new technique that can be used to study magnetism with atomic resolution, will be introduced [1,2]. Unlike spin-polarized scanning tunneling microscopy (SP-STM) this technique is not restricted to conductive samples, but can be applied on insulating surfaces, e.g., oxides, as well [1]. Moreover, with its spectroscopic mode (MExFS) it is possible to directly measure the distance dependence of the magnetic exchange interaction [3]. This knowledge can then be utilized to manipulate the magnetic state by adjusting the strength via the distance dependence [4]. Recent results on NiO(001) and Fe/W(001) will be reported.

[1] U. Kaiser, A. Schwarz, and R. Wiesendanger, *Nature* **446**, 522 (2007).
[2] R. Schmidt et al., *Nano Letters* **9**, 200 (2009).
[3] R. Schmidt et al., *Phys. Rev. Lett.* **106**, 257202 (2011).
[4] R. Schmidt, A. Schwarz, and R. Wiesendanger, *Phys. Rev. B* **86**, 174402 (2012).

Poking from both sides - Reshaping Graphene Landscape Via Face-To-Face Dual Probe Microscopy

F. R. Eder[1] J. Kotakoski[1] K. Holzweber[1] C. Mangler[1] V. Skakalova[1]
J. C. Meyer[1]
[1]University of Vienna - Faculty of Physics

Probing and manipulating single atoms or chemical bonds requires a technique where atomic-scale probes are positioned and controlled with sub-nanometer accuracy. Here, we describe how this can be achieved by using a sample—in our case few-layer graphene—which can be simultaneously accessed from opposing sides. We use a specifically designed dual-probe scanning tunneling microscopy (STM) setup, in which the two probes are at the closest point separated only by the thickness of graphene. This allows us for the first time to directly measure the deformations induced by the STM probe on a free-standing membrane. We reveal different regimes of stability of few-layer graphene, and show how the STM probes can be used as tools to shape the membrane in a controlled manner. Our work also opens new avenues to study mechanical and electronic properties of two-dimensional materials.

The Phantom force

A. J. Weymouth[1] F. J. Giessibl[1]

[1]University of Regensburg

The Phantom force is a phenomenon that we took note of when performing simultaneous current and force microscopy (STM and AFM) on a system with limited conductance. Our first observations were on the Si(111)-7x7 surface. While unsaturated Si atoms should appear attractive, when we applied a bias, and thus also a tunnelling current, the adatoms appeared relatively repulsive [1]. We were able to explain our observations with a model incorporating an ohmic voltage drop near the tip-sample junction [1, 2]. This model described the effect of the current on the electrostatic attractive force between tip and sample: With higher current, more of the applied bias dropped outside the tip-sample junction, decreasing the attractive electrostatic force. It has proven to be quite robust at explaining our observations, even explaining inversion of parabolae when performing Kelvin Probe Microscopy [3]. Ohm's law can explain the high resistance required for this effect, howeve r it is unintuitive that this model should be successful when describing transport on the atomic scale. It does seem likely, however, that this Phantom force can be used to measure conductance on the atomic scale.

[1] A. J. Weymouth, T. Wutscher, J. Welker, T. Hofmann and F. J. Giessibl, *Phys. Rev. Lett.* **106**, 226801 (2011).
[2] T. Wutscher, A. J. Weymouth and F. J. Giessibl, *Phys. Rev. B* **85**, 195426 (2012).
[3] A. J. Weymouth and F. J. Giessibl, *Appl. Phys. Lett.* **101**, 213105 (2012).

Crystal phase QWs design in pure and doped ZnO nanostructures

V. Khranovskyy[1] L. Hultman[1] B. Monemar[1] R. Yakimova[1]

[1] Linköping University, Department of Physics, Chemistry, and Biology (IFM), 583 81 Linköping, Sweden

Semiconductor nanowires (NWs) are considered an important technology for future advanced devices. Carrier confinement in semiconductor nanostructures, namely, quantum wells (QWs) or quantum dots (QDs) has the well-known advantage of increasing radiative recombination efficiency, making them of particular interest for optoelectronic applications. Crystal phase engineering is an alternative approach, which practically enables engineering of the electronic structure of a single material [1]. Due to the existing band offsets at wurtzite (WZ) / zinc blende (ZB) materials interface, the hetero-interface WZ/ZB/WZ can define a QW in a single material. While growing of such a structure in a NW allows confinement of charges in two other dimensions, forming a crystal phase QD. ZnO is a wide direct band gap semiconductor (Eg = 3.36 eV), with large exciton binding energy (60 meV), which makes it potential material for design of high-efficiency optoelectronic and photonic devic es [2]. Both bulk material and NWs of ZnO exhibit single phase WZ crystal structure at normal conditions. However, at certain conditions the stacking faults (SF) as a specific structural defect are observed in ZnO. Particularly, basal plane stacking faults (BSF) are the most common type of SFs (90%). Imperative is that BSFs in wurtzite-structure (WZ) ZnO, can be considered as a sheet of zinc blende structure (ZB) embedded in the parent crystal. Due to the smaller bandgap of the ZB modification, these BSFs form perfect ZB/like quantum wells in a WZ matrix [3]. Thus, once the formation of SF can be engineered, it could transform a challenging defect-related problem into a groundbreaking advantage for crystal phase band gap engineering [4, 5]. We have studied the formation of SFs in pure and Ag doped ZnO NWs and investigated their photoluminescence (PL) properties in comparison high quality ZnO NWs of pure wurtzite structure. The light emission peculiarities of pure ZnO NWs have been studied by temperature-dependent micro-PL in the temperature range of 4 – 300 K. It is revealed that via growth at high supersaturation, the BSFs form the quantum wells in WZ ZnO nanowires, providing additional characteristic peak of excitonic luminescence at 3.329 eV in the LT PL spectrum. The observed peak is explained as indirect exciton transition due to the recombination of electrons in the QW conduction band to holes localized near BSF. The binding energy of electrons is estimated to be around 100 meV, while the excitons are found to be localised with binding energy of holes 5 meV, which is due to the coupling of BSFs, which form QW-like structures. It is revealed, that acceptor doping of ZnO by Ag promotes formation of the BSFs. Furthermore, BSFs concentration was found to be proportional to the dopant concentration, which is explained as due to accumulation of the local strain caused by Ag substitution of Zn in the host crystal lattice. The presence of SFs affect the luminescence properties of Ag:ZnO by creating additional peak at 3.321 eV (at 4 K). This peak co-exists with the common donor bound excitonic (D0X) and free excitonic recombination's peaks as well as their respective phonon replicas. Furthermore, the SFs related peak is stable at least up to 350 K, providing splitting of the near band edge emission of ZnO into two peaks: FX emission appears at 375 nm and this of SFs at 386 nm. We demonstrate the simultaneously existence of both emission lines from different regions of NWs by CL mapping: the two types of emission are spatially resolved. These radiative recombination processes are has different kinetics, as it is revealed by time-resolved PL. The nature of the PL of Ag:ZnO is explained as indirect exciton transition from the electrons, localized in the QW in conduction band of zinc blende ZnO with hole, localized near the acceptors in the proximity of SF. The data obtained are compared to similar phenomena that have recently been reported in GaN, InGan, AlGaN as well as single and multiply quantum wells structures. The results obtained demonstrate the original approach to tailor the electronic structure of semiconductor materials via control of their polytypism and defect engineering on the nanoscale interface.

[1] N. Akopian, G. Patriarche, L. Liu, J.-C. Harmand and V. Zwiller, *Nano Letters* **10**, 1198 (2010).
[2] A. Djurisic, A. M. C. Ng, X. Y. Chen , *Progr. Quant. Electr.* **34**, 191 (2010).
[3] Lähnemann, O. Brandt, U. Jahn, C. Pfuller, C. Roder, P. Dogan, F. Grosse, A. Belabbes, F. Bechstedt, A. Trampert, and L. Geelhaar, *Phys. Rev. B* **86**, 081302 (2012).
[4] P. Caroff, J. Bolinsson and J. Johansson, *IEEE Journal of Selected Topics in Quantum Electronics* **17**, 829 (2010).
[5] Perfectly imperfect , *Nature Nanotechnology* **5**, 311 (2010).

Two-dimensional charge trapping in metal-oxide materials

K. P. McKenna[1] A. L. Shluger[2] M. J. Wolf[2]

[1]Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom
[2]Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, United Kingdom

The trapping of electrons and holes in oxides is a fundamental effect critical to the performance of materials in microelectronics, energy generation, and photocatalysis. In highly polarisable oxides, electrons and holes can self-trap in the perfect lattice (i.e. polaron formation), but can also be trapped by pre-existing defects, such as impurities, surfaces and interfaces [1]. Since separating these effects in order to characterise charge trapping in real materials experimentally remains extremely challenging, theoretical models can be invaluable.

In this talk, I will give an overview of the main theoretical challenges to accurate prediction of charge trapping in oxides before presenting several examples of systems where the nature of electron and hole trapping is predicted to be two-dimensional. These will include the polaronic trapping of holes in bulk HfO_2 [2], hole trapping at the surface of ZrO_2 nanocrystals [3], and electron and hole trapping by grain boundaries in MgO and HfO_2 [4-6]. In many ways the two-dimensional properties of these systems are similar to those pronounced in numerous layered oxides as well as in 2D electron gases that can be formed at oxide heterointerfaces and in the high-Tc superconducting cuprates.

[1] K. P. McKenna *et al*, *Model. Simul. Mater. Sci. Eng.* **17**, 084004 (2009).
[2] K. P. McKenna *et al*, *Phys. Rev. Lett.* **108**, 116404 (2012).
[3] M. J. Wolf, K. P. McKenna and A. L. Shluger, *J. Phys. Chem. C* doi:10.1021/jp309525g (2012).
[4] K. P. McKenna and A. L. Shluger, *Nat. Mater.* **7**, 859 (2008).
[5] K. P McKenna and A. L. Shluger, *Proc. Roy. Soc. A* **467**, 2043 (2011).
[6] Z. Wang, M. Saito, K. P. McKenna *et al*, *Nature* **479**, 380 (2011).

Growth and magnetic properties of lowdimensional oxide films on a support: CoO/Ir(100)

F. Mittendorfer[1]
[1]TU Vienna

The support of epitaxial films frequently determines their crystallographic orientation, which is of crucial importance for their electronic and magnetic properties. Although the surface stress in the oxide layer is usually seen as the main driving force for its orientation, we could recently show in a combined theoretical and experimental study that the interface chemistry can play a crucial role [1]. This allows for a novel way to alter the film orientation without changing the substrate. I will present our results for the growth of CoO on the Ir(100) surface, obtained on the basis of DFT calculations with the Vienna Ab-initio Simulations Package (VASP). While the oxide grows in (111) orientation on the bare substrate, the orientation switches to (100) by introducing a single (or a few) monolayer(s) of Co between the oxide and substrate due to the enhances interaction at the interface.

In addition, I will report on the the magnetic ordering in the ultrathin hexagonal c($10\bar{1}2$) CoO(111) film supported on Ir(100) [2]. In that case, we find a close relationship between the local structural properties of the oxide film and the induced magnetic order, leading to alternating ferromagnetically and antiferromagnetically ordered segments. While the local magnetic order is directly related to the geometric position of the Co atoms, the mismatch between the CoO film and the Ir substrate leads to a complex long-range order of the oxide.

[1] M. Gubo et al., *Phys. Rev. Lett.* **108**, 066101 (2012).
[2] F. Mittendorfer, at el., *Phys. Rev. Lett.* **109**, 015501 (2012).

Adsorption and defects of 2-dimensional silica

T. Björkman[1] A. V. Krasheninnikov[1]

[1]Aalto University School of Science

The recent finding of a 2-dimensional (2D) SiO_2 bilayer structure has recently attracted attention, both for being a stable 2D compound and for its existing in amorphous forms as a 2D glass[1,2]. In the present study, we investigate the binding to different metal surfaces by non-local correlation functionals, a sophisticated density functional theoretical method that properly accounts for van der Waals interactions[3]. Furthermore, we study the formation energy of defects similar to those that appear in graphene, another honeycomb lattice, and which have also been found experimentally in pristine 2D SiO_2. The results show large qualitative similarities with the defect structures in graphene, but also quantitative differences that arise from the differences in the binding structure compared with graphene. The strain fields around the defects are studied and found to be exceptionally long ranged, a serious practical problem which is overcome by a careful compari son of results obtained with classical potentials with first-principles data. We also study so-called Haeckelite structures, hypothetical structures obtained by periodically reproducing the defect throughout the lattice. When allowing for full relaxation of the structure, the total energies of the Haeckelite structures exceed those of the ideal honeycomb lattice by surprisingly small amount, showing that formation of amorphous structures should indeed be expected.

[1] P. Y. Huang et al., *Nano Letters* **12**, 1081 (2012).
[2] L. Lichtenstein et al., *Angewandte Chemie International Edition* **51**, 404 (2012).
[3] T. Björkman, *Physical Review B* **86**, 165109 (2012).

Extending the scope of force field methods: reactivity and multiple scales

P. Raiteri[1] S. Piana[1] J. D. Gale[1] A. G. Stack[2]

[1]Nanochemistry Research Institute/Department of Chemistry, Curtin University, PO Box U1987, Perth, WA 6845, Australia

[2]Chemical Sciences Division, Oak Ridge National Laboratory, PO Box 2008, MS-6110, Oak Ridge, Tennessee 37831, United States

For complex dynamical systems, such as interfaces and surfaces in contact with solution, force field methods are often the only computationally feasible technique. However, even these methods face limitations for many important problems of interest relating to the description of the energy surface or the length- and time-scales involved. This talk will give examples of work within our group to address both of these challenges:

1) Reactivity: Here the proton conductivity of Y-doped $BaZrO_3$ will be examined. A comparison of two reactive force field approaches to describe proton diffusion will be made based on ReaxFF [1] and Empirical Valence Bond (EVB) theory [2] parameterised from first principles. This allows proton trapping by point defects and grain boundaries to be addressed, while connecting to experimental diffusion rates. Comments regarding some of the issues facing reactive force fields for interfacial systems involving water will be made.

2) Multiscale: The use of kinetic Monte Carlo methods makes it possible to overcome some of the problems associated with length- and time-scale associated with force fields. It has been shown that the crystallisation and evolution of particles in solvents can be simulated in this manner leading to agreement with direct experimental comparisons at the micron-scale [3]. However, the challenge of determining the rate constants remains a problem for many cases. Here the combined use of multiple rare-event theories to determine accurate rate constants for multistep pathways will be presented [4].

[1] A.C.T. van Duin, B.V. Merinov, S.S. Han, C.O. Dorso and W.A. Goddard III, *J. Phys. Chem. A* **112**, 11414 (2008).
[2] P. Raiteri, J.D. Gale and G. Bussi, *J. Phys. Cond. Matter* **23**, 334213 (2011).
[3] S. Piana, M. Reyhani and J.D. Gale, *Nature* **438**, 70 (2005).
[4] A.G. Stack, P. Raiteri and J.D. Gale, *J. Am. Chem. Soc.* **134**, 11 (2012).

Calculations of electronic defects and excitons in oxides

H. Jonsson[1,2]
[1]Dept. of Applied Physics, Aalto University
[2]Faculty of Physical Sciences, Univ. of Iceland

An overview will be given of calculations of self-trapped holes and excitons in amorphous and crystalline silica using the DFT/PBE approximation [1-3]. Processes leading to network degredation and the formation of oxygen interstitials as well as surface desorption have been identified. But, it is clear that this level of approximation is too crude in particularly for quartz where delocalized electronic states are lower in energy than localized ones. The reason is the spurious self-interaction in the DFT/GGA approximations to the energy functional. An implementation of Perdew-Zunger self-interaction correction [4] will be described and recent results on test systems (molecules) [5] as well as vacancy on a TiO2 surface discussed [6]. This correction makes the functional orbital density dependent (ODD) and unitary invariance of the orbitals no longer applies, giving rise to some additional challenges in the implementation. While significant, qualitative as well as qu antitative improvements in the calculated results are found, problems remain and more work is needed to make optimal use of the functional form where orbital density dependence is included.

[1] R. Van Ginhoven, H. Jonsson and L. R. Corrales, *J. Non-Cryst. Solids* **352**, 2589 (2006).
[2] R. M. Van Ginhoven, L. R. Corrales and H. Jonsson, *Phys. Rev. B* **71**, 024208 (2005).
[3] R. M. Van Ginhoven, H. Jonsson, K. A. Peterson, M. Dupuis, and L. R. Corrales, *J. Chem. Phys.* **118**, 6582 (2003).
[4] P. J. Klupfel, S. Klupfel, K. Tsemekhman and H. Jonsson, *Lecture Notes in Computer Science* **7134**, 23 (2012).
[5] S. Klupfel, P. Klupfel and H. Jonsson, *J. Chem. Phys.* **137**, 124102 (2012).
[6] A. Valdes, et al., *Phys. Chem. Chem. Phys.* **14**, 49 (2012).

Tuesday 12.02.2013

			chair: Falko
9:00	-	9:40	**Grigorieva**
			Defect-induced magnetism in graphene
9:40	-	10:20	**Yazyev**
			Polycrystalline graphene: atomic structure and electronic transport properties
10:20	-	10:40	Casartelli
			Spin-coupling around a carbon vacancy in graphene
10:40	-	11:20	*Coffee*
			chair: Yazyev
11:20	-	12:00	**Kis**
			Single-layer MoS2 electrical transport and devices
12:00	-	12:40	**Seifert**
			Defects and edges in metal chalcogenide layers
12:40	-	13:00	Komsa
			Defects in two-dimensional transition metal dichalcogenides: From vacancies to substitutional random alloys
13:00	-	16:00	*Lunch*
16:00	-	18:00	*Posters*
18:00	-	20:00	*Dinner*

Defect-induced magnetism in graphene

I. V. Grigorieva[1]

[1]School of Physics and Astronomy, University of Manchester, UK

I will review our recent experiments on inducing and controlling magnetic response of graphene via introduction of point defects such as vacancies and adatoms. Graphene is hailed as potentially an ideal material for spintronics due to its weak spin-orbit interaction and the ability to control its electronic properties by the electric field effect. We have demonstrated that point defects in graphene - both vacancies and adatoms carry magnetic moments, leading to pronounced paramagnetic behaviour that dominates graphene's low-temperature magnetic properties. Even better, we show that the defect magnetism is itinerant (i.e. due to localisation of conduction electrons) and can be controlled by doping, so that the induced magnetic moments can be switched on and off. This not only adds important functionality to potential graphene devices but also has profound implications for spin transport.

Polycrystalline graphene: atomic structure and electronic transport properties

O. V. Yazyev[1]

[1]Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

There is growing evidence of the polycrystalline nature of graphene samples at micrometer length scales. Grain boundaries and dislocations, intrinsic topological defects of polycrystalline materials, inevitably affect all kinds of physical properties of graphene. This talk reviews our theoretical efforts directed towards understanding atomic structure and electronic transport properties of polycrystalline graphene. Recent experimental works on this subject are also covered in my lecture.

We introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors and grain boundaries covering the whole range of possible misorientation angles [1]. By using ab initio calculations we investigate thermodynamic properties of grain boundaries finding energetically favorable large-angle symmetric configurations as well as dramatic stabilization of small-angle configurations via the out-of-plane deformation, a remarkable feature of graphene as a truly two-dimensional material. Charge-carrier transport across periodic grain boundaries in graphene is shown to be governed primarily by a simple momentum conservation law [2]. Two distinct transport behaviors are predicted - either perfect reflection or high transparency for low-energy charge carriers depending on the grain boundary structure. Beyond the momentum conservation picture we find that the transmission of low-energy charge carriers can be dramatically suppressed in the sma ll-angle limit [3]. This counter-intuitive behavior is explained from the standpoint of resonant backscattering involving electronic states localized at the dislocations. Finally, my talk will cover advances of a joint experiment-theory project on controlled engineering of a degenerate grain boundary defect exhibiting valley-filtering properties [4].

These results demonstrate that dislocations and grain boundaries are important intrinsic defects in graphene which can be used for engineering novel functional devices.

[1] O. V. Yazyev and S. G. Louie, *Phys. Rev. B* **81**, 195420 (2010).
[2] O. V. Yazyev and S. G. Louie, *Nature Mater.* **9**, 806 (2010).
[3] F. Gargiulo and O. V. Yazyev, *in preparation* (2012).
[4] J.-H. Chen, G. Autes, N. Alem, F. Gargiulo, A. Gautam, M. Linck, C. Kisielowski, O. V. Yazyev, S. G. Louie, and A. Zettl, *submitted* (2012).

Spin-coupling around a carbon vacancy in graphene

M. Casartelli[1] S. Casolo[1] S. Pellegrini[1] G. F. Tantardini[1,2] R. Martinazzo[1,2]
[1]Dept. of Chemistry, Universita degli Studi di Milano, via Golgi 19, 20133 Milan, Italy
[2]Istituto di Scienze e Tecnologie Molecolari, CNR, via Golgi 19, 20133 Milan, Italy

Recent magnetization measurements of C atom vacancies in graphene have provided conflicting results, with both spin$-1/2$ and spin-1 paramagnetic responses observed[1,2]. Spin-half paramagnetism is consistent with C vacancies behaving like simple p_z-defects[3] but it is at odds with chemical intuition which suggests that (at least) one unpaired σ electron has to be left upon vacancy formation, in addition to the π electron common to any p_z-defect. Here, in order to shed light on this issue, we investigate in detail the electronic structure of a bare C-vacancy in graphene, and its interaction with possible simple contaminants typically present in the environment. We employed magnetization-constrained density-functional-theory on periodic models and spin-exact, multireference, second-order perturbation theory on large clusters, and explored the energy landscape of the two low-lying spin states around their equilibrium configurations. In accordance with expectations, we find that the ground state is a triplet with a planar equilibrium geometry, and the excited state is an open-shell singlet with a non-planar structure. The singlet lies $\sim 0.2\,eV$ above the ground-state, $i.e.$ at an energy which is yet too high for the two electrons to decouple into independent spin$-1/2$ paramagnetic species at ordinary temperatures. Thus our results show that a $bare$ C-vacancy behaves as a $spin-one$ species. Next, we investigated the role that simple adsorbed species such as H adatoms may play in modifying the paramagnetic response of the defective graphene substrate, by following ($ab\ initio$) the sticking dynamics of H atoms in the neighbourhoods of a C-vacancy. Results show that the sticking cross-section is large ($\sim 19\,\mathring{A}^2$, $i.e.$ comparable to the geometric cross-sectional area of the defect), and essentially independent of the collision energy. The resulting hydrogenated vacancy has one electron left and behaves as a spin$-1/2$ defect. Overall, our results suggest that foreign species may play an important role in determining the observed magnetic properties of defective carbon compounds, even when magnetic species have been ruled out by a careful sample preparation.

[1] Nair R. R. et al., *Nat. Phys.* **8**, 199-202 (2012).
[2] Ney A. et al., *Appl. Phys. Lett.* **99/102505**, 1-3 (2011).
[3] Yazyev O. V., *Rep. Prog. Phys.* **73/056501**, 1-16 (2010).

Single-layer MoS2 electrical transport and devices

A. Kis[1]
[1]EPFL

After quantum dots, nanotubes and nanowires, two-dimensional materials in the shape of sheets with atomic-scale thickness represent the newest addition to the diverse family of nanoscale materials. Single-layer molybdenum disulphide (MoS_2), a direct-gap semiconductor is a typical example of these new graphene-like materials that can be produced using the adhesive-tape based cleavage technique originally developed for graphene. The presence of a band gap in MoS_2 allowed us to fabricate transistors that can be turned off and operate with negligible leakage currents. Furthermore, our transistors can be used to build simple integrated circuits capable of performing logic operations and amplifying small signals.

I will report here on our latest 2D MoS_2 transistors with improved performance due to enhanced electrostatic control, showing improved currents and transconductance as well as current saturation. We also record electrical breakdown of our devices and find that MoS_2 can support very high current densities, exceeding the current carrying capacity of copper by a factor of fifty. Furthermore, I will show optoelectronic devices incorporating MoS_2 with sensitivity that surpasses similar graphene devices by several orders of magnitude. Finally, I will present temperature-dependent electrical transport and mobility measurements that show clear mobility enhancement due to the suppression of the influence of charge impurities with the deposition of an HfO_2 capping layer.

Defects and edges in metal chalcogenide layers

G. Seifert[1] A. Enyashin[1] E. Erdogan[1]
[1] Physikalische Chemie, TU Dresden

In addition to Graphene 2D transition metal chalcogenide, as for example MoS2 and WS2, nanostructures are promising materials for applications in electronics and mechanical engineering. Though the structure of these materials results in a highly inert surface with a low defect concentration, defects and edge effects can strongly influence the properties of these nanostructures. Therefore, a basic understanding of the interplay between electronic and mechanical properties and the influence of defects and edge states is needed. We demonstrate on the basis of atomistic quantum mechanical simulations of several types of MoS2 nanostructures how the edge structure and defects influence the mechanical behavior, the electronic properties of such systems.

Defects in two-dimensional transition metal dichalcogenides: From vacancies to substitutional random alloys

H-P. Komsa[1] J. Kotakoski[2] S. Kurasch[3] O. Lehtinen[1,3] U. Kaiser[3]
A. V. Krasheninnikov[1,4]

[1]Department of Physics, University of Helsinki, Finland
[2]Department of Physics, University of Vienna, Austria
[3]Central Facility for Electron Microscopy, University of Ulm, Germany
[4]Department of Applied Physics, Aalto University, Finland

Transition metal dichalcogenides (TMDs) are a class of layered materials, similar to graphite and BN, with promising future in nanoelectronic and photonic applications. Due to recent advances in succesful production of two-dimensional monolayers they have started to attract considerable attention. In order to take full advantage of the promise of these materials, a good control over the defect production is required. In particular, defects could be produced intentionally during chemical vapor deposition growth or by ion irradiation, whereas unintentional production may be expected during transmission electron microscope (TEM) imaging.

In this work, we first investigate vacancy formation under electron irradiation in TMD materials. Displacement thresholds are evaluated from molecular dynamics calculations and compared to the experiments in the case of S vacancy formation in MoS_2 [1]. Isolated vacancies are stable, but with increasing exposure and vacancy concentration, they are found to agglomerate to form lines. With the help of first-principles calculations, we determine their atomic structure and also discuss possible formation mechanisms.

Filling of the vacancies is observed in TEM images. Thus, we examine chalcogenide substitution processes within these materials. Substitution by other atomic species is found to be energetically favorable, thereby suggesting a way for doping of these materials [1]. Finally, as extended substitution by isoelectronic ions leads to alloying, we study the stability and electronic structure of alloys consisting of MoS_2, $MoSe_2$, and $MoTe_2$ [2].

[1] H.-P. Komsa et al., *Phys. Rev. Lett.* **109**, 035503 (2012).
[2] H.-P. Komsa and A. V. Krasheninnikov, *J. Phys. Chem. Lett.* **3**, 3652 (2012).

Wednesday 13.02.2013

			chair: Gale
9:00	–	9:40	**Caro** What do electrons do when ions collide?
9:40	–	10:00	Djurabekova Flow of Molten Material and Recrystallization Explains the Swift Heavy Ion Shape Transformation of Au Nanoclusters
10:00	–	10:20	Philipp MD simulation study of nanolayer formation by continuous carbon deposition on a silicon (100) surface
10:20	–	10:40	Langer Giant non-contact friction observed on $NbSe_2$ measured with pendulum AFM
10:40	–	11:20	*Coffee*
			chair: Seifert
11:20	–	12:00	**Harju** Recent results on electronic properties of graphene
12:00	–	12:20	Kotakoski Realistic atomic-scale model for polycrystalline graphene and the related mechanical and electronic properties
12:20	–	12:40	Standop Ion Impacts on Graphene/Ir(111): From Vacancy Funnels to a Nanomesh
12:40	–	13:00	Drost Hetero-epitaxial monolayers of graphene and hexagonal boron nitride on Ir(111)
13:00	–	16:00	*Lunch*
			chair: Grigorieva
16:00	–	16:20	Sachs First-Principles Simulations of Graphene Hybrid Structures
16:20	–	16:40	Gomes da Rocha Graphene-based nanosensors for perceiving molecular systems
16:40	–	17:00	Landers Tandem influence of two classes of defects on graphene: An experimental and theoretical perspective
17:00	–	17:20	Pereira Thermal transport in strained, isotopically engineered and functionalized graphene
17:20	–	18:00	*Coffee*
			chair: Harju
18:00	–	18:40	**Falko** Moiré minibands in graphene heterojunctions with hexagonal 2D crystals.
18:40	–	19:00	*Closing*

What do electrons do when ions collide?

A. Caro[1]
[1] Los Alamos National Laboratory

The keystone to molecular dynamics simulations of radiation damage is the Born-Oppenheimer or adiabatic approximation. In this talk I will discuss recent progress on going beyond this approximation and the new phenomena that could be possible to describe when electrons and ions are treated simultaneously as out of equilibrium.

Flow of Molten Material and Recrystallization Explains the Swift Heavy Ion Shape Transformation of Au Nanoclusters

A. A. Leino[1] O. H. Pakarinen[1] F. Djurabekova[1] K. Nordlund[1] P. Kluth[2]
M. C. Ridgway[2]

[1]Helsinki Institute of Physics and Department of Physics, University of Helsinki
[2]Research School of Physics and Engineering, Australian National University

Heavy ions accelerated to very high kinetic energies Ekin > MeV / amu can be used to transform the shape of metal nanoclusters with diameters 5-30 nm into elongated ones not easily achievable by other means. This effect is analogous to the well established possibility to use multiwall carbon nanotubes inside an electron microscope as pressure vessels to modify and study the properties of metal nanoclusters. The swift ion processing has, however, the major advantage that the end result is stable over macroscopic timescales when taken out of the experimental processing chamber. Using atom-level multiscale modelling and experiments, we show here that the elongation is caused by melting and subsequent flow of initially crystalline metal into an underdense ion track core. The minor axis of the elongated particle is shown to saturate at a width comparable to the width of the ion track, in good agreement with the experiments.

MD simulation study of nanolayer formation by continuous carbon deposition on a silicon (100) surface

A. Jana[1,2] L. Briquet[1] P. Philipp[1] T. o. m. Wirtz[1] G. Henrion[2]

[1]Department Science and Analysis of Materials (SAM), Centre de Recherche Public Gabriel Lippmann, 41 rue du Brill, L-4422 Belvaux, Luxembourg
[2]Institut Jean Lamour, UMR CNRS Université de Lorraine, Department Chemistry and Physics of Solids and Surfaces, Parc de Saurupt, CS 50840, F-54011 Nancy, France

One of the most important aspects in case of particle surface interaction is to observe surface deformation, defects along with reorganization and distribution of matter at the surface in the sub-monolayer range. By using molecular dynamics (MD) simulations and DFT calculations, a better understanding of distribution of atoms on the surface, surface deformation and defects information can be achieved. Level-three force fields capable of simulating the breaking and formation of chemical bonds have recently been conceived for a more realistic simulation of systems involving reactive species. In this presentation, we will use MD simulations coupled to the reactive force field developed by J. Kieffer's group [1-3] to investigate how carbon atoms deposit onto the Si(100) surface and a SiC thin film forms [4]. A (100) silicon surface having size of a 4nm x 4nm was created and continuous carbon deposition at 300K was modeled to study the formation of thin SiC films. 100 carbons were sent to the surface in a continuous manner and in such a way to have a fluence similar to experimental conditions for carbon deposition. Deposition energies ranging from 1 to 30eV were simulated with several incidence angles. The evolution of the sticking coefficient with the progressive coverage of the surface is monitored. It varies in between 0.86 to 0.99 for the variation of the fluence from 1.0×10^{14} to 5.0×10^{14} $atoms/cm^2$. The variation of the sticking coefficient with increasing fluence is not uniform. Implantation of C and distribution of C atoms in the sample as well as the amount of defects caused by the carbon implantation are monitored, showing an amorphization of the top monolayers of the sample. The damaged depth increases to 3 monolayers at 5eV and 4 monolayers at 10eV, compared to 1 monolayer at 1eV. The different properties are compared for the different angles and energies.

[1] L. P. Huang and J. Kieffer, *J. Chem. Phys.* **118**, 1487 (2003).
[2] L. P. Huang and J. Kieffer, *Phys. Rev. B* **74**, 224107 (2006).
[3] J. H. Zhou and J. Kieffer, *J. Phys. Chem. C* **112**, 3473 (2008).
[4] L. G. V. Briquet, A. Jana, L. Mether, K. Nordlund, G. Henrion, P. Philipp, and T. Wirtz, *Journal of Physics: Condensed Matter* **24**, 395004 (2012).

Giant non-contact friction observed on $NbSe_2$ measured with pendulum AFM

M. Langer[1] M. Kisiel[1] R. Pawlak[1] R. Buzio[2] E. Meyer[1]

[1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056, Switzerland
[2]INFM-Dipartimento di Fisica, Universita di Genova, Via Dodecaneso 33, 16146 Genova, Italy

The mechanism of friction and accompanied energy dissipation is a widely studied field. Sophisticated techniques, like atomic force microscopy (AFM), made it possible to get insight into the energy dissipation mechanism on the atomic scale. In addition, we got also the insight into the dissipation mechanism in the non contact regime [1]. Here, we present an example of giant non-contact friction measured below the charge density wave (CDW) phase transition of $NbSe_2$. Measurements were mainly carried out by means of an Atomic Force Microscope (AFM) in pendulum geometry. In this cantilever alignment one has extremely good force sensitivity of $10\text{aN}/\sqrt{\text{Hz}}$ and very high dissipation resolution of $1.7 \cdot 10^{-12}\text{Kg/s}$. Giant non-contact friction maxima was also confirmed with a tuning fork AFM. All shown measurements were carried out in Ultra-High Vacuum and low temperatures of 6K.

[1] M. Kisiel, E. Gnecco, U. Gysin, L.Marot, E. Meyer, *Nature Materials* **10**, 199 (2011).

Recent results on electronic properties of graphene

A. Harju[1]

[1]Aalto University, Helsinki, Finland

This talks present some new results on interesting electronic properties of graphene. In the first direction, the collective electronic states are shown to exhibit interesting many-particle interference of the Fabry-Perot type [1] that differ from the more traditional single-particle Fabry-Perot experiments. The measurements are done on suspended graphene samples and the reflection is caused by the connections to leads. Theoretical modeling for these can be done on the tight-binding level that reliably models the collective states in graphene structures [2] and electronic transport properties [3,4]. The second direction deals with well-defined graphene nanostructures on gold substrate, where finite ribbons interact more weakly than, e.g., on iridium [2]. The STM/STS experiments are used to probe the electronic structures both with metallic and CO tip, and theoretical work is based on tight-binding, density functional theory, and exact diagonalizations using a new re alistic model for long-range interacting graphene. We show some evidence for magnetic zigzag edge state and study the effects of structural defects on electronic and magnetic properties.

[1] P. Hakonen et al., (collaboration).
[2] S. Hämäläinen et al., *Phys. Rev. Lett.* **107**, 236803 (2011).
[3] A. Uppstu et al., *Phys. Rev. B* **85**, 041401(R) (2012).
[4] A. Uppstu and A. Harju, *Phys. Rev. B* (accepted).
[5] P. Liljeroth, D. Vanmaekelbergh et al., (collaboration).
[6] N. B. Kopnin et al., (http://arxiv.org/abs/1210.7595).

Realistic atomic-scale model for polycrystalline graphene and the related mechanical and electronic properties

J. Kotakoski[1] J. C. Meyer[1] D. van Tuan[2] T. Louvet[2] F. Ortman[2] S. Roche[2,3]
[1]University of Vienna, Austria
[2]CIN2 (ICN-CSIC) and Universitat Autonoma de Barcelona, Spain
[3]ICREA, Barcelona, Spain

Large-scale production of graphene relies on chemical vapor deposition (CVD), which unfortunately leads to samples which have properties that are markedly different from those of mechanically exfoliated mono-layers. One reason for this is that CVD-growth initiates spontaneously on several different locations and often with random lattice orientations. When the separately grown grains meet, the structure gets patched with grain boundaries (GB) which consist of non-hexagonal carbon rings to make up for the mismatch in lattice orientations.

Although experimental studies have recently brought light onto the atomic structure of grain boundaries as well as their effect on the magnitude of changes in properties due to their influence, detailed atomic-scale understanding of the origin of the different properties has remained unknown. For this reason, we have established a method to create realistic atomistic models of polycrystalline graphene structures which have random misorientation angles between the different grains and exhibit serpent-like meandering GB structures similar to the experimental images. Using this model, we have shown that—unlike has often been expected—mechanical failure upon stretching a graphene sheet does not start from within individual GBs but rather at points where several GBs meet. From there, the cracks them propagate through the grains (not along the GBs), again similar to recent experimental findings. Our atomistic models have further allowed us to study the charge transport characte ristics in realistic polycrystalline graphene samples. Our calculations revealed a remarkably simple scaling law which relates several of the transport properties to the average grain sizes in the sample, establishing quantitative foundations for estimating transport features in polycrystalline graphene.

Ion Impacts on Graphene/Ir(111): From Vacancy Funnels to a Nanomesh

S. Standop[1] O. Lehtinen[2] C. Herbig[1] J. Kotakoski[2] T. Michely[1]
A. V. Krasheninnikov[2] C. Busse[1]
[1]University of Cologne
[2]University of Helsinki

Ion bombardment is a powerful tool to create nanostructured surfaces [1]. Often even regular patterns appear spontaneously due to a complex interplay of creation and thermally activated diffusion or annihilation of defects, thereby constituting an example of self-organization [2]. In case of graphene a periodic arrangement of vacancies, i.e. a nanomesh [3], may cause a bandgap opening making it suitable for a wide range of applications.

By combining ion beam experiments and atomistic simulations we study the production of a nanomesh in graphene on Ir(111) by low energy Xe ion bombardment. Based on our findings on single ion impacts causing arrays of defects under grazing incidence we explore the possibilities of tuning the defect pattern via thermal treatment.

While the graphene vacancies obtained by interface channeling persist up to 900K we find their edges bent down to the substrate, giving rise to a funnel-like shape. This shape is due to the formation of C-Ir-bonds saturating the dangling bonds of the vacancies. We further demonstrate that with the onset of vacancy cluster mobility around 800K, vacancies tend to move in certain areas within the moiré supercell formed by the graphene layer with the incommensurate Ir metal substrate. This observation corroborates our simulation findings of a strongly varying vacancy formation energy landscape, depending on the exact position of the defect with regard to underlying metal atoms. These tools at hand we are able to create a graphene nanomesh adopting the periodicity of the moiré pattern.

[1] W. L. Chan, E. J. Chason, *J. Appl. Phys.* **101**, 121301 (2007).
[2] S. Facsko, T. Dekorsy, C. Koerdt, C. Trappe, H. Kurz, A. Vogt, H. Hartnagel, *Science* **285**, 1551 (1999).
[3] J. Bai, X. Zhong, S. Jiang, Y. Huang, X. Duan, *Nat. Nanotechnology* **5**, 190 (2010).

Hetero-epitaxial monolayers of graphene and hexagonal boron nitride on Ir(111)

R. Drost[1] S. K. Hämäläinen[1] F. Schulz[1] P. Liljeroth[1]
[1]Department of Applied Physics, Aalto University School of Science, Espoo, Finland

After almost a decade of intensive research, the interest in graphene is unabated. The material's many exceptional properties make it very attractive as a candidate for industrial and technological applications, while fundamental researchers are especially fascinated by the rich electronic structure of graphene[1]. Hexagonal boron nitride (h-BN), a large bandgap insulator structurally similar to graphite, has emerged as a promising support material for graphene, with with electron mobilities of graphene samples on h-BN approaching those measured in suspended graphene[2]. Furthermore, the combination of h-BN and graphene within a single layer, both in the form of domain structures as well as the use of B and N as dopants, offer routes to engineer the graphene band structure[3][4][5]. It is clear that the interface of graphene with h-BN in a hetero-epitaxial monolayer will play an important role in it's electronic properties. In order to fully understand the possibili ties offered by mixing the two materials, a detailed study of the interface region is necessary.

Both graphene and h-BN samples of high qulity can be readily grown by chemical vapour deposition (CVD) on transition metal surfaces under UHV conditions. The growth of graphene has been studied in depth especially on the Ir(111) surface, making it a good testing ground for hetero-epitaxial layers of graphene and h-BN[6][7]. We grow a single layer of hybridised graphene and h-BN domains on the Ir(111) surface in a two-step process. In a first step, small islands of graphene are formed from an ethylene precursor by temperature controlled growth. Following the deposistion of graphene, the remainder of the surface is covered in h-BN through thermal cracking of borazine ($B_3N_3H_6$) on Ir(111). Both processes are self-limiting, so that monolayer coverage is ensured. The resulting films are characterised by standard surface science techniques such as AES and LEED, followed by thorough study with a low-temperature STM with a focus on the geometric and electronic structure of th e graphene/h-BN interface.

[1] K. S. Novoselov et al., *Science* **306**, 666 (2004).
[2] C. R. Dean et al., *Nature Nanotechnology* **5**, 722 (2010).
[3] L. Ci et al., *Nature Mat.* **9**, 2010 (430).
[4] M. P. Leven et al., *Nature* **488**, 627 (2012).
[5] W. H. Brito et al., *Physical Review B* **85**, 035404 (2012).
[6] J. Coraux et al., *New Journal of Physics* **11**, 023006 (2009).
[7] S.K. Hämäläinen et al., *Physical Review Letters* **107**, 2011 (236803).

First-Principles Simulations of Graphene Hybrid Structures

B. Sachs[1] T. O. Wehling[2] M. I. Katsnelson[3] A. I. Lichtenstein[1]

[1] I. Institut fuer Theoretische Physik, Universitaet Hamburg, Jungiusstrasse 9, D-20355 Hamburg, Germany
[2] Institut fuer Theoretische Physik, Universitaet Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany
[3] Radboud University of Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

The design of graphene heterostructures is a research field of rising importance. It is nowadays possible to combine graphene with other layered 2D materials which offers promising possibilities for novel nanodevices[1]. Here, we present first-principles simulations of interfaces between graphene and other layered 2D materials, such as boron nitride[2] or the transition metal dichalcogenide MoS2. We discuss electronic and structural properties of the hybrids and compare the results to experiments.

[1] K. S. Novoselov, V. I. Fal'ko, L. Colombo, P. R. Gellert, M. G. Schwab & K. Kim, *Nature* **490**, 192 (2012).
[2] B. Sachs, T. O. Wehling, M. I. Katsnelson & A. I. Lichtenstein, *Phys. Rev. B* **84**, 195414 (2011).

Graphene-based nanosensors for perceiving molecular systems

S. M. Avdoshenko[1] C. G. Rocha[2] G. Cuniberti[3]

[1]Purdue University, School of Materials Engineering, West Lafayette, IN 47907-2045, USA
[2]University of Jyväskylä, NanoScience Center, Jyväskylä, FI 40014, Finland
[3]Dresden University of Technology, Institute for Materials Science, Dresden, 01062, Germany

Although most of the buzz created after graphene discovery points mainly to the idea that a promising substitute for silicon perhaps has emerged, still we are far away from fabricating graphene transistors at commercial level. Nonetheless graphene can act in many other application fields and some of them are about to reach commercial-scale production. For instance, sensor industry has been looking at graphene with great interest. Previous works have reported that graphene is an excellent host material for sensing numerous chemicals and gaseous molecules [1,2]. Moreover, the sensing abilities of graphene can also benefit other important scientific fields such as medicine and biology since graphene can also successfully perceive the presence of biomolecules, e.g. DNA strands [3]. In this research front we use robust numerical methods to model graphene reaction while stimulated by foreign objects. A host graphene sheet is exposed to different types and amounts of impur ities such as organic- and bio- molecules. The adsorption processes are treated dynamically or statically from where prominent information about the graphene/molecule interaction is inferred. In particular, we illustrate in detail how graphene membranes can effectively work as nanoelectromechanical mass-sensor devices [4]. Our results confirm the potential use of graphene as promising mass/chemical sensors operating with molecular precision and selectiveness.

[1] F. Schedin, A.K. Geim, S.V. Morozov, E.W. Hill, P. Blake, M.I. Katsnelson, and K.S. Novoselov, *Nature Materials* **6**, 652 (2007).
[2] C. Chen, S. Rosenblatt, K.I. Bolotin, W. Kalb, P. Kim, I. Kymissis, H.L. Stormer, T.F. Heinz, and J. Hone, *Nature Nanotechnology* **4**, 861 (2009).
[3] Y. Dan, Y. Lu, N.J. Kybert, Z. Luo, and A.T. Charlie Johnson, *Nano Letters* **9**, 1472 (2009).
[4] S.M. Avdoshenko, C.G. Rocha, and G. Cuniberti, *Nanoscale* **4**, 3168 (2012).

Tandem influence of two classes of defects on graphene: An experimental and theoretical perspective

J. Landers[1] J. Coraux[2] L. Magaud[2]
[1]Institut NEEL, CNRS, BP166, F-38042 Grenoble Cedex 9, France
[2]Institut NEEL, CNRS & Universite Joseph Fourier, BP166, F-38042 Grenoble Cedex 9, France

The exceptional transport properties of a 2-dimensional sheet of graphene has endeared it to great promise for an array of prospective applications ranging from ultra-high frequency transistors, gas sensors and transparent flexible electrode materials. However graphene's use in these applications has been limited due to either the presence of intrinsic defects, such as vacancies and Stone-Wales configurations; or due to extrinsic defects such as adsorbed species. Both of which can introduce a bandgap and alter the transport properties[1]. Some have already taken advantage of this fact by investigating either one or the other[2,3]. However, to date there is a dearth of literature that investigates the coupling of both classes of defects and its effects on the transport properties of graphene. In this work we examine the tandem influence of first creating intrinsic defects in graphene grown on Ir(111) followed by functionalizing these defects with adsorbed species. In trinsic defects are introduced into the system by irradiation and precisely controlled by irradiation time, voltage and ion concentration. Extrinsic defects are further added by pumping in an adsorbate at low concentrations. The defective system is then characterized by scanning tunneling microscopy (STM) in order to identify any modification of the Moire patterns. We combine these experimental studies with DFT and MD calculations in order to unveil a better understanding of the mechanism of the adsorbed species onto defective sites and its resultant effect on the density of states and transport properties.

[1] F. Banhart, J. Kotakoski, A.V. Krasheninnikov, *ACS Nano* **5**, 26 (2011).
[2] T.O. Wehling, M.I. Katsnelson, A.I. Lichtenstein, *Chemical Physics Letters* **476**, 125 (2009).
[3] M.M. Ugeda, I. Brihuega, F. Hiebel, P. Mallet, J.Y. Veuillen, J.M. Gomez-Rodriguez, F. Yndurain, *Physical Review B* **85**, 121402 (2012).

Thermal transport in strained, isotopically engineered and functionalized graphene

L. F. C. Pereira[1] D. Donadio[1]

[1]Max Planck Institute for Polymer Research

Unique heat transport properties make graphene a strong candidate to applications in future thermal management devices. At room temperature its thermal conductivity is dominated by phonons and values as large as 5000 W/m-K have been measured for suspended graphene at $\approx$ 300 K. In order to build functional devices it is necessary to be able to manipulate and tailor these properties, which requires a deep understanding of the behavior of phonons in graphene. We perform extensive equilibrium molecular dynamics simulations to understand the mechanism of heat transport in suspended graphene in various conditions. Studying size convergence we demonstrate that low-frequency out-of-plane vibrational modes act as scatterers and limit the thermal conductivity to a large but finite value. We then show that the thermal conductivity of an extended periodic graphene model under uniaxial tensile strain diverges. This behavior stems from strain-induced changes in the dispe rsion relations and population of low-frequency phonon modes. Divergence would lead to a strong size dependence of experimental measurements of thermal conductivity. Finally, in view of the recent fabrication of graphene with predefined concentrations of carbon isotopes and of functionalized graphene, we investigate the effect of isotopic mass disorder and functionalization on the thermal conductivity of unstrained and strained graphene.

Moiré minibands in graphene heterojunctions with hexagonal 2D crystals.

V. Falko[1] J. Wallbank[1] A. Patel[1] M. Mucha-Kruczynski[1] A. Geim[2]
[1]Physics Department, Lancaster University, Lancaster, LA1 4YB, UK
[2]School of Physics and Astronomy, Manchester University, Oxford Road, Manchester, UK

The transformation of the linear Dirac spectrum of electrons in monolayer graphene and parabolic spectrum in bilayer graphene due to the influence of a tightly bound insulating or semiconducting layer is studied. We present a symmetry-based classification and quantitative analysis of generic miniband structures for electrons in graphene heterojunction with a 2D crystal with the hexagonal Bravais symmetry, such as boron nitride. In particular, we identify conditions at which the first moire miniband is separated from the rest of the spectrum by either one or a group of three isolated mini Dirac points and is not obscured by dispersion surfaces coming from other minibands. In such cases the Hall coefficient exhibits two distinct alternations of its sign as a function of charge carrier density. Then, we study the Hofstadter spectrum of electrons in a magnetic field.

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Engineering Quantum Spin Hall Effect in Graphene Nanoribbons via Edge Functionalization

G. Autes[1] O. V. Yazyev[1]

[1] Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Kane and Mele predicted that in presence of spin-orbit interaction graphene realizes the quantum spin Hall (QSH) state [1]. However, exceptionally weak intrinsic spin-orbit splitting in graphene ($\approx 10^{-5}$eV) inhibits experimental observation of this topological insulating phase. To circumvent this problem, we propose an approach towards controlling spin-orbit interactions in graphene by means of covalent functionalization of graphene edges with functional groups containing heavy elements.

By using a modification of the Kane-Mele model we show that by introducing spin-orbit interactions only at the edges it is possible to realize the QSH state in narrow graphene nanoribbons. To prove the experimental relevance of this idea, we perform first principle calculations of tellurium (Te) terminated graphene nanoribbons which can be produced using current methods of synthetic organic chemistry. Our calculations show that these configurations exhibit the presence of a parabolic band with strong Rashba splitting and the robust QSH state, respectively. These results provide guiding principles towards engineering topological electronic phases in graphene nanostructures by means of bottom-up chemical techniques.

[1] C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 226801 (2005).

Molecular dynamics simulations of phase transformation in Al-Ru nanolayers

K. A. Avchaciov[1] F. Djurabekova[1] K. Nordlund[1]
[1]University of Helsinki

Thin films, formed as multilayers of pure polycrystalline metals, can show spontaneous intermixing with formation of metallic glasses or binary alloys phases. Recently discovered compound of Al-Ru with enormous high positive enthalpy of mixing reveals self-propagating reactions at the high heating rates. We report on MD simulation of phase transformation in crystalline Al-Ru nanolayers. Obtained characteristic values of self-propagating reaction such as the reaction velocity and maximum temperature are in good agreement with experiments.

Bond directionality in boron nitride nanotubes probed by STXM-NEXAFS

C. Bittencourt[1] C. Karunakaran[2] J. Wang[2] Y. Lu[2] A. Hitchcock[3]

[1]ChIPS, University of Mons, Mons, Belgium
[2]Canadian Light Source Inc., University of Saskatchewan, Saskatchewan, Canada
[3]B.I.M.R, McMaster University, Ontario, Canada

Boron Nitride nanotubes (BNNTs) represent an important new wide band gap nanomaterial, primarily due to their homogeneous electronic behavior: tubes of different chiralities are all semiconductors with almost the same optical band gap experimentally determined at 5.8 eV and they all show chemical and thermal stabilities. Existing literatures on BNNTs based on conventional bulk spectroscopy where the π-type partial density of empty states are probed by Near-Edge X-ray Absorption Fine Structure spectroscopy (NEXAFS) is almost completely insensitive to the orientation of the hexagonal layers, namely whether they are flat or rolled up into nanotubes. The similarity reported between BNNTs and hexagonal BN (h-BN) as probed by both NEXAFS and electron energy loss spectroscopy (EELS) is somewhat surprising considering the drastic changes of the band structure and dimensionality of the two allotropes.

Here we used NEXAFS spectroscopy combined with Scanning Transmission X-ray Microscopy (NEXAFS-STXM) to study the effect of the dimensionality in the electronic states of BN nanostructures. The spatial resolution of the NEXAFS-STXM allows studying isolated nanostructures without the interference of impurities, while the linear polarized X-rays can be used as a searching tool to probe the bonding directionality. We observed a strong dichroism at the B 1s edge. Results will also be discussed taking into account the presence of carbon at the nanostructure surface.

The influence of bulk or interface disorder on the magnetic anistropy energy

K. Carva[1] I. Turek[1]

[1]Department of Condensed Matter Physics, Charles University in Prague, Czech Republic

We employ fully relativistic first-principles theory of metallic ferromagnetic systems to calculate magnetic anisotropy energy (MAE) of chemically disordered systems. The theory is based on the all- electron tight-binding linear muffin-tin orbital (LMTO) method and the coherent potential approximation (CPA). Particular attention is devoted here to the spin and orbital magnetic moments, total energies, and transport properties.

The properties of random Fe-Co alloys in tetragonal structures will be presented. These alloys were predicted to exhibit a giant uniaxial MAE which would make them a promising material for magnetic recording. It will be shown that a correct treatment of the chemical randomness present in real samples reduces dramatically the MAE; the effect of a perfect and partial atomic long-range order on the MAE will be shown as well [1].

Another interesting example represents thin Fe layers on top of GaAs surface. A surprisingly high value of in-plane MAE has been predicted in this system, while the experimental value vary by more than an order of magnitude [2]. We examine the influence of intermixing between Fe and GaAs at the interface on the MAE.

[1] I. Turek, J. Kudrnovsky, K. Carva, *Phys. Rev. B* **86**, 174430 (2012).
[2] M. Kosuth, V. Popescu, H. Ebert, G. Bayreuther, *EPL (Europhysics Letters)* **72**, 816 (2005).

NaCl dissolution from first principles

J. Chen[1,2] A. Foster[1] K. Laasonen[2]
[1]Department of Applied Physics, Aalto University
[2]Department of Physical Chemistry, Aalto University

By employing ab initio molecular dynamics (AIMD), we have simulated the liquid water-solid surface interaction of 256 water water on a (4x4) NaCl(100) unitcell. In this system, our AIMD results show that the liquid water density distribution has a maximum peak of 1.40 g/cm^3 at 2.8 Å above the NaCl surface, these 256 water molecules occupy approximately in four layers. To understand the dissolving process of NaCl into water, we have calculated the dissolve barrier of Cl- and Na+ ions from flat, vancancies,stepped and the corner of the island on the NaCl(100) surfaces using constraint method. The barriers for producing Cl- or Na+ ions on flat NaCl(100) surface are 0.78 eV and 0.75 eV, respectively. The dissolve barriers for Cl- and Na+ ions on stepped surface are 0.19 eV and 0.13 eV respectively. The barriers for producing Cl- or Na+ ions from the corners of island on NaCl(100) surface are 0.17 eV and 0.05 eV, respectively.

Manipulating the Electronic Structure and Magnetic Properties of Graphene by Adsorbing Atomic Clusters

P. A. Clayborne[1] C. G. Rocha[2] H. Hakkinen[1,2]

[1]Department of Chemistry, NSC University of Jyvaskyla
[2]Department of Physics, NSC University of Jyvaskyla

Graphene collects a multitude of striking properties that make it a suitable material for various technological applications. When integrated in electronic devices, for instance, graphene samples are incorporated in complex circuit architectures in which they must endure numerous environmental conditions and interact with distinct materials. From single atom adsorption to bulky substrates, graphene susceptibility to external agents, given its one-atom-thick dimensions, is simply remarkable. An almost unexplored and promising scientific arena opens up when graphene is probed to interact with a special class of materials, atomic (ligand functionalized) clusters, which are aggregates of several atoms (or molecules) that possess interposed properties between their respective monomer and solid-state forms. In this work, we perform a systematic theoretical investigation about how the electronic and magnetic features of graphene structures are affected by the presence of atomic clusters. Ligand-stabilized aluminum clusters $[Al_4Cp_4]$ and BTA copper complexes $[Cu_6(BTA)_4]$ are adsorbed on two- and one-dimensional graphene hosts and their electronic structure is treated within density functional theory. Our results point out that the clusters affect weakly the properties of two-dimensional graphene. This scenario is significantly altered when graphene nanoribbons are used as platforms for the clusters. The former has one of its dimensions comparable with the cluster size. In this sense, nanoribbons turn to be more sensitive to the cluster presence than their two-dimensional counterpart. In addition, we demonstrate that atomic clusters can act as a prominent tool to manipulate spin-polarized states in graphene ribbons from which novel spin-filter devices could be designed.

Control of the exchange coupling in granular CoPt/Co recording media

W. J. Fan[1] R. F. L. Evans[1] R. W. Chantrell[1]

[1]Department of Physics, University of York, Heslington, York, YO10 5DD, United Kingdom

In order to control the exchange coupling between the grains in a perpendicular recording media, a simple method is to totally decouple the grains using a thick oxide and apply a continuous magnetic capping layer to improve the uniformity of the coupling. An atomistic spin model is used to calculate a system of CoPt grains coupled with a Co layer. We show that the exchange coupling between the CoPt grains and the Co layer has an impact on the reversal process of the grains, as well as causing a reduction in the coercivity of the whole system. Further, we have studied the coercivity of the whole system as a function of the exchange coupling parameter between the grains and the exchange layer, and have found a sharp decrease in the coercivity. The coercivity as a function of the exchange layer thickness is also studied for different exchange coupling parameters.

Friction Anisotropy Investigations: Development of a New UHV-SPM and First Measurements

G. Fessler[1] S. Messmer[1] Y. Pellemont[1] T. Glatzel[1] E. Meyer[1]

[1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

We developed a new Scanning Probe Microscope (SPM) which operates in Ultra-High Vacuum (UHV) and in room temperature. The design is based on the microscope developped by L. Howald[1] ten years ago. Various changes for further improvements were done at the optical sensing part, the platform of the microscope, the electrical connections and the electronics were implemented. Some additional connections to the sample are also new providing additional functionality. This enables us to rotate the sample in situ. In this way it is possible to do friction measurements along different directions. Anisotropic effects of friction on the nanoscale can therefore be investigated in UHV environment. The first measurements on NaCl and BNL[2] are presented.

[1] L. Howald, *Appl. Phys. Lett.* **63**, 117 (1993).
[2] G. Fessler, *Appl. Phys. Lett.* **98**, 083119 (2011).

Spectral and Transport Parameters of Electron-Transporting Material Bis(10-hydroxybenzo[h]qinolinato)beryllium (Bebq2) Calculated by Ab Initio Methods

A. Y. Freidzon[1] A. A. Safonov[1] A. A. Bagaturyants[1]

[1]Photochemistry Center, Russian Academy of Sciences

Bis(10-hydroxybenzo[h]qinolinato)beryllium (Bebq2) is an electron-transporting and fluorescent material used in organic light-emitting diodes. The structures of its monomer and several dimers are considered in order to study its spectral (absorption and emission) and transport parameters, such as reorganization energy and hopping integral, as well as its electron affinity and ionization potential. Transport parameters and spectra are calculated by high-level ab initio method CASSCF/XMCQDPT both for holes and for electrons, because holes should also be present in the material to ensure light emission. The calculated spectra agree well with the experiment. We have shown that the lowest excited states, electrons, and holes are localized on individual ligands of the complex. Carrier transfer consists of two steps, intramolecular and intermolecular hopping. For holes, there is a substantial difference between intra- and intermolecular hopping barriers. Intramolecular hole hopping proceeds easier than intermolecular. For electrons, the difference between intra- and intermolecular hopping barriers is small. As a whole, electron hopping proceeds easier than hole hopping.

[1] A.A. Granovsky, *J. Chem. Phys.* **134**, 214113 (2011).

Investigation of the thermal stability of Cu nanowires using atomistic simulations

F. Granberg[1,2] S. Parviainen[1,2] F. Djurabekova[1,2] K. Nordlund[1,2]

[1]Department of Physics, Helsinki University
[2]Helsinki Institute of Physics

We present a method for determining the melting point of copper nanowires based on classical molecular dynamics simulations and use it to investigate the dependence of the melting point on wire diameter. The melting point is determined as the temperature at which there is a significant change in the fraction of liquid atoms in the wire, according to atomic bond angle analysis. The results for the wires with diameters in the range 1.5 nm to 20 nm show that the melting point is inversely proportional to the diameter while the cross-sectional shape of the wire does not have a significant impact. Comparison of results obtained using different potentials show that while the absolute values of the melting points may differ substantially, the melting point depression is similar for all potentials. The obtained results are consistent with predictions based on the semi-empirical liquid drop model.[1] In the thinnest wires a spontaneous growth of a reconstruction was seen. This phenomenon is systematically examined with atomistic simulations. The spontaneous growth of reconstructions were found in all used potentials and for instance a 7.2 nm long and 1 nm thick wire had a 60 % probability to reconstruct in a wide temperature range.

[1] K. K. Nanda et al, *Phys.Rev.A* **66**, 013208 (2002).

Gold-embedded zigzag graphene nanoribbons as spin gapless semiconductors

X. Hu[1] W. Zhang[2] L. Sun[1] A. Krasheninnikov[3,4]

[1]SEU-FEI Nano-Pico Center, Key Lab of MEMS of Ministry of Education, Southeast University, 210096 Nanjing, China
[2]Shanghai Institute of Applied Physics, Chinese Academy of Sciences,201800 Shanghai, China
[3]Department of Physics, University of Helsinki, FI-00014 Helsinki, Finland
[4]Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland

Recently, the new concept of spin gapless semiconductor (SGS)[1] has been proposed by Xiaolin Wang, who analyzed the electronic properties of doped PbPdO2 systems using first-principles calculations. The SGS materials have unique band structures. The top of the valence band of one spin channel and the bottom of the conduction band of at least one spin channel touch at the Fermi level. The SGS materials have more interesting features than the conventional semiconductors[2, 3]. For example, no energy is required to excite electrons from the valence band to the conduction band, while the density of states at the Fermi level is zero, and both electrons and holes can be 100% spin polarized at the Fermi level, which is the most desirable property of semiconductors in spintronics. Using density-functional theory calculations, we studied the electronic and magnetic properties of zigzag graphene nanoribbons (ZGNRs) with gold (Au) atoms embedded into different sites of the ZGNRs[4]. Strong site dependence was found, and the system had the ferromagnetic or antiferromagnetic ground state depending on the Au atom position. Spin gapless semiconductor (SGS) behavior was observed when the Au atom was embedded into the center and edge sites of the ZGNRs. The simulations showed that the electronic structure of the ribbon strongly depends on ZGNR width, but the SGS behavior is always present when the Au atom is embedded into the center and edge sites. The SGS properties were also found to be dependent on impurity atom concentration, so that they can be tuned by either selecting the proper positions of Au atoms or changing their concentration. Our results suggest a flexible way of designing SGSs, which could be used in various spintronic, electronic, and optoelec tronic applications.

[1] X. L. Wang, *Phys. Rev. Lett.* **100**, 156404 (2008).
[2] X. L. Wang, G. Peleckis, C. Zhang, H. Kimura, and S. X. Dou, *Adv. Mater.* **21**, 2196 (2009).
[3] X. L. Wang, S. X. Dou, C. Zhang, *NPG Asia Mater.* **2**, 31 (2010).
[4] X. H. Hu, W. Zhang, L. T. Sun, and A. V. Krasheninnikov, *Phys. Rev. B.* **86**, 195418 (2012).

Synergy of Graphene and ZnO properties for optoelectronics

R. Yakimova[1] V. Khranovskyy[1]

[1]Linköping University, Department of Physics, Chemistry, and Biology (IFM), 583 81 Linköping, Swewden

Graphene (Gr) is widely reported due to its unique properties and possible respective applications. Furthermore, combination of Gr with other inorganic materials enables modification and improvement or enhancement of its key properties. Potentially, a novel type of hybrid structures may be created and a new beyond graphene area may appear. Zinc oxide is a wide band gap semiconductor material with a large potential for applications in optoelectronics for UV and blue light emitting devices. Intense light emission therefore is critical and may be facilitated by efficient light extraction from the material. Alternatively, the efficiency of light emission may be improved due to enhanced internal efficiency by intensification of the radiative recombination processes. Surface plasmons (SPs) have been earlier reported to enhance the luminescence efficiency of semiconductor materials and devices [1]. Traditionally, the plasmons related phenomena are studied on metals, as a source of abandoned charge carriers. However, Graphene, being a two-dimensional system, enables excitation of surface plasmons (SP) similar to the surface plasmons on metal/dielectric interfaces [2]. We have studied peculiarities of photoluminescence of the ZnO/Gr heterostructures in comparison to conventional ZnO samples by temperature and power dependent micro-photoluminescence (μ-PL). Monolayer (ML) graphene was prepared on SiC substrates by thermal decomposition at 2000°C in an argon atmosphere [3] and used as a substrate template for subsequent ZnO growth by MOCVD at 500 °C [4]. Growth of ZnO on Gr at common conditions results in a conventional thin polycrystalline ZnO film formation, while via respective growth regime modifications different morphologies nanorods (NRs) or nanowires (NWs) - can be obtained. We demonstrate, that: i) despite the significant in-plane lattice mismatch ($\delta\alpha$ ZnO/Gr $= +\ 32\%$) growth on Gr promotes high quality of the ZnO material in comparison to other substrates, e. g. such of less lattice mismatch, like SiC ($\delta\alpha$ ZnO/SiC $= +5\%$); ii) independently of the thickness of the ZnO films they reveal higher PL intensity in comparison to the similar films, grown on other substrates; iii) the light emission ability of ZnO depends non-linearly on the film thickness. Via HR TEM and XRD analysis we observed experimentally that Gr tends to decompose under longer deposition time of the ZnO. This, however, is assisted by relaxation of ZnO due to accommodation its crystal lattice with SiC substrate. The observed light emission enhancement phenomena can be explained as that the process of excitonic emission from ZnO is enhanced the by exciton-plasmon coupling. Responsible for the observed phenomena can be the surface plasmons, which appears on the interface ZnO/Gr. Finally, we demonstrate a particularly designed ZnO/Gr heterostructure, that reveals superior light emission properties. At room temperature the PL signal from ZnO/Gr was found to be 4 times larger in comparison to conventional ZnO samples. Furthermore, the PL enhancement was found to increase at low temperatures - up to 18 (at 4 K), which is due to increased density of states (DOS) at lower temperatures. The local enhancement of the electromagnetic field occurs due to the surface plasmons resonance on the ZnO/Gr interface. Thus, light emission enhancement occurs due to increased ratio of the radiative recombination processes. However, the issue of need of SPs media surface corrugation for efficient light extraction still has to be clarified for this system. For the optoelectronics such light emission enhancement is of vital importance. Thus, Gr is a proper template for growth of ZnO/Gr hybrid structures with tailored light emission properties and ZnO-Graphene system is prospective for investigation of SPs related phenomena since a substantial practical profit may be expected.

[1] Koichi Okamoto, Isamu Niki, Alexander Shvartser, Yukio Narukawa, Takashi Mukai & Axel Scherer, *Nature Materials* 3, 601 (2004).
[2] A. N. Grigorenko1, M. Polini and K. S. Novoselov, *Nature Photonics* **6**, 749 (2012).
[3] C. Virojanadara, M. Syväjarvi, R. Yakimova, and L. I. Johansson A. A. Zakharov and T. Balasubramanian, *Physical Review B* **78**, 245403 (2008).
[4] V. Khranovskyy and R. Yakimova, *Physica. B, Condensed matter* **407**, 1533 (2012).

Birth, motion, interaction, and annihilation of dislocations in graphene at the atomic scale

O. Lehtinen[1,2] S. Kurasch[1] A. V. Krasheninnikov[2,3] U. Kaiser[1]

[1]Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm
[2]Department of Physics, University of Helsinki, Finland
[3]Department of Applied Physics, Aalto University

The life cycle of dislocations, from creation to annihilation via motion and interaction is a concept of fundamental importance in materials science. Dislocations play a central role in determining a materials properties and influence the behavior of any material. Investigating the underlying mechanism of dislocation creation and annihilation in a 3D object, atom-by-atom, is well beyond the spatial and temporal resolution limits of current characterization techniques, and therefore has been reserved for computer simulations and analytical theory. Here, we overcome the conventional experimental limits by investigating a 2D material, graphene, in an aberration-corrected transmission electron microscope, exploiting the impinging energetic electrons both to image and stimulate atomic scale structural transformations. The resulting morphological changes are followed in situ, showing the full life cycle of a dislocation from birth to annihilation. The underlying mechanism of interaction is revealed by atomistic simulations. To our surprise we found that the interaction is driven by out-of-plane buckling, rather than previously assumed in-plane strain, which leads to markedly long range interactions of the point defects observed in our experiment.

Optical properties of a dye solar cell with high-absorption layers by using the transfer-matrix method

J. M. Luque-Raigon[1,2] J. Halme[1] H. Miguez[2]

[1]Department of Applied Physics, Aalto University, Finland
[2]Instituto de Ciencias de Materiales de Sevilla, CSIC, Spain

Abstract Dye-sensitized solar cells (DSSC) are electro-optic devices that convert the incident light radiation to current with an optical efficiency that depends on the light intensity distribution inside the device structure [1]. We intend to represent optic-energetic calculations through the transfer matrix method (TMM) to obtain the total reflectance, total transmittance and layer-by-layer absorptance of a DSSC when very high-absorption layers (metallic, polymers, carbon nanotubes) are included at the back electrode. These highly absorbing layers are characterized with a high imaginary part of the complex refractive index. However, at this condition TMM calculations show a numerical exponential instability (inaccuracy or singularity) [2]. We avoid the numerical instability by developing a new TMM solution, based on the symmetries of the TMM, which is specifically tailored for the numerical well-conditioning [3]. The represented calculations with this new solution work correctly in DSSC with metallic layers, when the standard TMM formulation fails. At the moment, we are investigating how to apply this TMM solution to the experimental and theoretical characterization of the optical properties of complex nanostructured materials like a DSSC composed of a layer of single-wall carbon nanotubes (SWNT) [4]. However, the SWNT layer shows collective electrons waves excited in its surface by the electromagnetic radiation, called surface plasmons, which enhances the SWNT absorption at some wavelengths [5]. In this meeting, we look forward to discuss our work on optical characterization and modeling of these nanomaterials and propose possible applications of this TMM solution to other related problems.

[1] S. Wenger, M. Schmid, G. Rothenberger, A. Gentsch, M. Grätzel and J. O. Schumacher, *J. Phys. Chem. C* **115**, 10218-10229 (2011).
[2] M. G. Moharam, D. A. Pommet, E. B. Grann and T. K. Gaylord, *J. Opt. Soc. Am. A* **12**, 1077-1086 (1995).
[3] J. M. Luque-Raigon, J. Halme, H. Miguez, *J. Opt. Soc. Am. B* submitted (2012).
[4] S. Iijima, *Physica B* **323**, 1-5 (2002).
[5] W. Que, *J. Phys.: Condens. Matter* **14**, 5239–5253 (2002).

Dynamic Charge Transfer Potential for Modeling Oxide Interfaces

T. Musso[1] T. Hynninen[1] A. S. Foster[1]
[1]Aalto University
[2]Tampere University of Technology

In this work the charge-optimized many-body potential (COMB) has been implemented using Pysic. Pysic is an ASE calculator in an object-based Python environment that allows the implementation of advanced variable charge potentials. The COMB potential is an empirical potential that allows atomic charges to vary, in response to changes in the atomic environment. It has been parameterized for Si, O and Hf. In this work the COMB potential has been implemented with Pysic (using COMB10 parameters [1]) and tested simulating Si3Oy (y = 1:6) clusters. Comparing the final bond lengths and charges with the ones obtained with ab-initio and DFT methods [2,3], with our implementation the final bond lengths appear to be too short. This can be due to some initial approximations used in the implementation of the potential and to probably bugs still present. Once these problems will be solved, the COMB potential will be implemented also for HfOn (n=2:6) clusters. The final objective is to simulate new kind of semiconductor/oxide interfaces, like Si/HfO2, that can be used to study new-generation CMOS devices.

[1] Shan, Devine et all, *PHYSICAL REVIEW B* **82**, 235302 (2010).
[2] Wang et al, *Phys. Rev. Lett.* **78**, 4450 (1997).
[3] MORDRED, *MORDRED Deliverable* **1.1.1**, 5 (2010).

Sensitivity of the amorphous silicon / crystalline silicon hetero-interface to electron and proton irradiation

H. C. Neitzert[1] M. Ferrara[2]

[1]Salerno University, Dept. of Industrial Engineering (DIIn), Via Ponte Don Melillo 1, 84084 Fisciano (SA) - Italy
[2]Centro Ricerche ENEA Portici, P.le Enrico Fermi - Localita Granatello, 80055 Portici (Na) - Italy

Silicon solar cells, based on the combination of a crystalline silicon base as absorption layer combined with a thin hydrogenated amorphous silicon emitter, are among the best performing solar cells for terrestrial applications. Space solar cells are, besides high efficiency GaAs and III-V multijunction solar cells, dominated by conventional homojuction crystalline silicon solar cells. The c-Si / a-Si heterostructure solar cell [1] is known to have a better performance at elevated temperatures and this makes them eventually also attractive for space applications, where, however, the radiation tolerance is an additional requirement. In the presented study the influence of electron and proton irradiation in the MeV energy range on the performance of this type of solar cells with special respect to the properties of the interface region has been investigated. While for large particles doses the decrease of the effective minority carrier lifetime in the c-Si base is st rongly decreasing the hetero-junction solar cell efficiency, for lower doses the hetero-interface near region modification is of major influence. In particular it has been observed that for small doses of electrons even a slight increase of the efficiency can occur, if the the hetero-interface contains an ultrathin intrinsic a-Si:H layer between the base and the doped a-Si:H hetero-emitter. This result can be explained by the better collection efficiency of the electrons due to defect assistant tunnelling through a spike in the conduction band. Particular information regarding the defect formation has been obtained by electroluminescence measurements on the degraded devices, a technique that has already been demonstrated to be very useful for the degradation monitoring of homojunction crystalline solar cells after proton-irradiation [2].

[1] M. Tanaka, M. Taguchi, T. Matsuyama, T. Sawada, S. Tsuda, S. Nakano, H. Hanafusa and Y. Kuwano, *Jpn. J. Appl. Phys.* **31**, 3518 (1992).
[2] H.C. Neitzert, M. Ferrara, M. Kunst, A. Denker, Z. Kertesz, B. Limata, L Gialanella and M. Romano, *Phys. Stat. Sol. (b)* **245**, 2877 (2008).

MD simulation of DLC-carbon nanotube hybrid materials

K. Nordlund[1] W. Ren[1]

[1]Department of Physics, University of Helsinki

Since both carbon nanotubes and diamond-like carbon (DLC) have excellent mechanical properties, and nanotubes also have very interesting electrical properties, forming composites between the two could provide for a very durable electrically active material. Since vacuum arc discharge deposition is a standard way to make DLC, DLC composites could be formed by doing vacuum arc deposition on carbon nanotubes. We will present results of molecular dynamics simulations of vacuum arc deposition on carbon nanotube bundles and in particular examine the sp3/sp2 ratio of the forming materials and the amount of damage in the nanotubes.

d^0 Ferromagnetic Interface Between Non-Magnetic Perovskites

R. Oja[1] R. M. Nieminen[1]

[1]COMP Centre of Excellence, Department of Applied Physics, Aalto University, P. O. Box 11100, 00076 Aalto, Finland

d^0 magnetism results from spin-polarized p orbitals, whereas conventional magnetic materials have partially filled d or f states. Magnetic effects in hole-doped oxides are a common experimental observation, and holes in oxygen p orbitals have been widely predicted to result in magnetic moments [1]. In perovskite oxides, oxygen p bands are narrow and have a high density of states just below the band gap. Also, oxygen p electrons have a strong exchange coupling. Hence, Stoner's criterion for itinerant ferromagnetism is fulfilled, if the hole density is high enough [2].

Obtaining such high hole densities, moving the Fermi level to the oxygen p band, is easily done by so-called intrinsic doping, by a charge-imbalanced interface between two d^0 perovskites. In our model $KTaO_3$/$SrTiO_3$ interface, SrO and TiO_2 layers are nominally neutral, but (KO)$^{\&}$8722; and (TaO2)$^+$ layers have preferred ionic charges. To retain charge neutrality and compensate for interface dipole, 0.5 holes per p type interface unit cell are localized in the interface oxygen p orbitals. The n type interface, on the other hand, introduces 0.5 electrons per unit cell above the band gap, on the Ti d orbitals. Usually, a 2D electron gas is formed at a charge-imbalanced perovskite interface [3].

We demonstrate GGA+U and hybrid functional results on magnetism in p and n type $KTaO_3$/$SrTiO_3$ interfaces [5]. The hole on oxygen $2p$ orbitals is partially magnetized even without on-site Coulomb interaction U. Nonlocal (hybrid) exchange or small local Coulomb repulsion U stabilize complete spin-polarization and half-metallic, ferromagnetic holes. For the n type interface, on the other hand, the electrons on Ti d orbitals do not magnetize completely, and doped electrons can have a variety of competing magnetic states [4]. The density of states at the top of the O p band is higher than at the bottom of the Ti d band, making p type interfaces between d^0 perovskites candidate materials for combining ferromagnetism and ferroelectricity. Experimental results indicate presence of room-T ferromagnetism in the system [5].

[1] O. Volnianska and P. Boguslawski, *J. Phys.: Condens. Matter* **22**, 073202 (201).
[2] H. Peng, H. J. Xiang, S.-H. Wei, S.-S. Li, J.-B. Xia and J. Li, *Phys. Rev. Lett.* **102**, 017201 (2009).
[3] A. Brinkman, M. Huijben, M. van Zalk, U. Zeitler, J. C. Maan, W. G. van der Wiel, G. Rijnders, D. H. A. Blank and H. Hilgenkamp, *Nature Materials* **6**, 493 (2007).
[4] S. Okamoto, A. Millis and N. Spaldin, *Phys. Rev. Lett.* **97**, 56802 (2006).
[5] R. Oja, M. Tyunina, L. Yao, T. Pinomaa, T. Kocourek, A. Dejneka, O. Stupakov, A. Jelinek, V. Trepakov, S. van Dijken and R. M. Nieminen, *Phys. Rev. Lett.* **109**, 127207 (2012).

Real-space Ehrenfest dynamics with projector augmented-waves: A powerful approach for modeling nonadiabatic phenomena

A. Ojanperä[1] A. V. Krasheninnikov[1,2] O. Lopez-Acevedo[1] M. Puska[1]

[1]Department of Applied Physics, Aalto University, P. O. Box 11000, FI-00076 AALTO, Finland
[2]Materials Physics Division, University of Helsinki, P. O. Box 43, FI-00014, Finland

Many processes in nature, such as ignition of chemical reactions and ion-atom collisions, are related to excited electronic states and their time development. Modeling such nonadiabatic processes in principle requires a full quantum-mechanical approach, which is feasible only for very small systems. Ehrenfest dynamics in the time-dependent density functional theory (TDDFT) framework offers a computationally affordable method for simulating nonadiabatic processes. We have implemented [1] Ehrenfest dynamics in the powerful and accurate real-space approach using projector augmented-waves in the electronic structure program GPAW [2].

In the present work, we have applied our method to two different types of problems: 1) electronic stopping in carbon and 2) photo-induced dynamics of a small gold cluster. In the first case, we demonstrated that Ehrenfest dynamics can be used as an ab initio tool for studying electronic stopping processes even when core electron excitations are important. In the second case, we discovered that the changes in the probability of emission are related to charge transfer processes between the metal core and the ligands. In conclusion, we demonstrated the applicability of our Ehrenfest dynamics method to simulating different types of nonadiabatic processes in nanostructures.

[1] A. Ojanperä, V. Havu, L. Lehtovaara, and M. Puska, *J. Chem. Phys.* **136**, 144103 (2012).
[2] J. Enkovaara et al., *J. Phys. Condens. Matter* **22**, 253202 (2010).

Understanding contrast in nc-AFM imaging of insulators in water

B. Reischl[1] F. Federici Canova[2] A. S. Foster[1] M. Watkins[3] N. Kobayashi[4] T. Fukuma[4]

[1]COMP Centre of Excellence, Dept. of Applied Physics, Aalto University, Finland
[2]WPI-AIMR, Tohoku University, Sendai, Japan
[3]London Centre for Nanotechnology and Dept. of Physics and Astronomy, University College London, United Kingdom
[4]Bio-AFM Frontier Research Center and Division of Electrical and Computer Engineering, Kanazawa University, Kanazawa, Japan

We study the AFM imaging mechanism of insulators in water, using the examples of the calcite $(10\bar{1}4)$ and calcium fluoride (111) surfaces. The system, consisting of several layers of surface material, water, and the tip apex represented by a nanocluster, is simulated at room temperature, using molecular dynamics simulations with empirical atomistic interaction potentials. We compute a continuous free energy profile of the system, as a function of the tip-surface separation, for different lateral tip positions. The derivative of this free energy with respect to the tip-surface distance is the best estimate for the force acting on the AFM tip, as the important entropic contributions from interactions with hydration layer water molecules are correctly taken into account in the free energy calculation [1]. We also compare different approaches to simulate the free energy for each system, and comment on the advantages and disadvantages for general simulations of AFM in liquids [2]. With the virtual AFM developed in our group, we use the calculated 3D force field to simulate the oscillation of a cantilever with the same resonance frequency, amplitude, force constant, and Q-factor as in the experiment. The frequency shift images and spectroscopy data obtained agree well with the experimental results. Analysis of the molecular dynamics trajectories gives insight into the atomistic details responsible for the contrast observed in the images, and establishes the relation between the real water-insulator interface and that seen by AFM [3, 4].

[1] M. Watkins and A. L. Shluger, *Phys. Rev. Lett.* **105**, 196101 (2011).
[2] B. Reischl, M. Watkins, and A. S. Foster, *J. Chem. Theory Comput.* accepted (2012).
[3] S. Rode, N. Oyabu, K. Kobayashi, H. Yamada, and A. Kuehnle, *Langmuir* **25**, 2850 (2009).
[4] B. Reischl, F. Federici Canova, A. S. Foster, N. Kobayashi, and T. Fukuma, in preparation (2012).

Plasmonic excitations in atomic nanostructures

T. Rossi[1] A. Sakko[1] R. M. Nieminen[1]
[1]COMP Centre of Excellence, Department of Applied Physics, Aalto University

The optical properties of metals are strongly affected by nearly-free valence electrons that interact with light collectively as plasma oscillations, i.e. plasmons. When confined into a nanoscale structure, the plasma interacts strongly with wavelengths much larger than the dimensions of the nanostructure, which enables focusing of light into subwavelength spatial area. The excitation frequencies of the confined plasma, and hence the optical response of the nanostructure, can be diversely tuned by the size, shape and composition of the nanostructure. These properties have shown their usefulness in multitude of applications in e.g. spectroscopy and biomedicine. Further developments necessitate deeper, quantum mechanical understanding of plasmonic excitations as the precision of nanofabrication techniques keep improving. [1]

In the present work, we study plasmonic excitations in atomically small structures with linear-response time-dependent density-functional theory. In addition to examining photoabsorption spectra, we also visualize the optical response in terms of electron density fluctuations that light induces in the system. Our results show that the induced densities give insight in the plasmonic nature of the excitations and help to understand both classical and quantum aspects of the phenomenon.

A metallic linear atom chain is used as a tractable model system for the study of plasmonics. [2] Longitudinal and transversal plasmonic excitations are observed in the system. The oscillator strengths, energies and induced densities of the excitations show systematic trends as a function of the chain length. Comparison of the results for sodium and silver chains demonstrates how the excitations emerge from the properties of the confined electron gas formed by the s-electrons of the metal atoms, and how the d-electrons of silver affect these excitations. Comparable excitations are expected to be present also in more complex nanostructures that exhibit similar characteristics in their electronic structure.

[1] N. J. Halas, S. Lal, W.-S. Chang, S. Link, and P. Nordlander, *Chemical Reviews* **111**, 3913 (2011).
[2] J. Yan, Z. Yuan, and S. Gao, *Physical Review Letters* **98**, 216602 (2007).

Tunable optical properties of graphene nanoflakes

A. Sakko[1] T. Rossi[1] R. M. Nieminen[1]
[1] COMP Centre of Excellence, Department of Applied Physics, Aalto University

Confining and controlling light in the nanoscale attracts significant interest in present day science and technology. Metallic nanoparticles, which are easy to synthesize and whose electronic and optical properties can be accurately tailored, have numerous applications in spectroscopy, sensing, and light harvesting.[1] Also graphene-based nanoscale materials, such as graphene nanoribbons and nanoflakes, have started to attract interest in nano-optics: they have favorable and tunable optical properties as well, and their fabrication techniques develop rapidly.[2]

In this work we study the optical properties of small graphene nanoflakes that contain 100–500 atoms. We present the photoabsorption spectrum of the graphene flakes as a function of their size. Systematic spectral changes are observed, demonstrating the desirable tunability of the material's optical properties. We analyze the changes in terms of their plasmonic properties, and discuss the implications of our results for the possible applications of nanoscale graphene.

[1] V. Giannini, A. I. Fernández-Domínguez, S. C. Heck, and S. A. Maier, *Chemical Reviews* **111**, 3888 (2011).
[2] C. Cocchi, D. Prezzi, A. Ruini, M. J. Caldas and E. Molinari, *The Journal of Physical Chemistry Letters* **2**, 1315 (2011).

Nanoscale Friction of Ice

N. Samadashvili[1] A. S. Foster[1] T. Hynninen[1,2]

[1]Department of Applied Physics, Aalto University School of Science and Technology, Espoo, Finland
[2]Department of Physice, Tampere University of Technology, Tampere, Finland

The freezing of water and melting of ice are among the most dramatic examples of phase transitions is nature. Everyday experience suggests why ice surface should be slippery: water spilled on a kitchen floor or rainwater on asphalt creates some kinds of hazards for walkers. Presumably, the liquid makes the surface slippery because liquids are mobile. Since the ice crystal structure demonstrates lower friction coefficient than other solids, asking why ice is slippery is thus roughly equivalent to asking how a liquid or liquid-like layer can appear on the ice surface. Significant efforts have been made to understand the properties of this liquid layer, particularly its thickness and atomic structure. However, very little work has been done to study the friction or slipperiness at the atomic scale. This contrasts strongly with the development of the field of atomic friction in general (AFM). The overall goal of this work is to use simulations to provide better understanding of the surface structure of ice and then look at the friction itself. In order to establish a good model for study, we have performed molecular dynamics simulations with Tip4p, Tip4p/2005 and Tip4p/Ice potentials. Our results for all three potentials, show a structural distortion of the lattice at the surface well below its melting temperature. Here we present temperature dependence of the disordered layer thickness and its role in the calculated friction along with other influencing parameters such as sliding velocity and applied load.

Formation of structures smaller than 100 nm by focused ion beam milling

A. Savenko[1,2] I. Yildiz[1] D. L. Lorenzen[2] Z. I. Balogh[2] P. Boggild[1]
[1]DTU Nanotech
[2]DTU Center for Electron Nanoscopy

Fabrication of small structures by FIB milling is limited by effects occurred in region of scattering of ions inside matter. For example 30 kV Ga ions produce defects in Si within 45 nm near the surface that includes implantation of ions, amorphisation and significant increase of temperature. These effects impose restrictions on minimal size of structures that can be produces. It also depends on the shape of structure (e.g. 1D or 2D, supported or not). When the size of the structure is comparable to ion penetration depth then the structure becomes unstable under ion beam irradiation and may shrink, be melted or bended. An example of description of small and thin structures behavior basing on simulations and experiments was given by Holmström [1]. FIB milling of sharp tips for AFM is one of the possible applications that is currently elaborated [2]. 200 nm thin suspended Si membranes are utilized for fabrication of AFM exchangeable tips by milling from the side. The smallest diameter of the tip that is currently obtained is 10 nm. Advanced strategy of FIB milling is used in order to eliminate influence of redeposition, drift of the beam and to preserve stability of structure. Further improvements are expected to be achieved by using additional methods (e.g. lower ion beam energies, wet etching). Study of these structures in TEM allows to understand better the changes in crystal structure and distinguish crystalline and amorphousized regions. It is known that thin membranes can be bended under ion beam irradiation [3]. Recently we have shown that 70 nm Si_xN_y membranes (strips) are bended upwards (towards the beam source) by FIB induced stress by 30 kV Ga ions [4]. Appropriate dose can result in controllable bending of the structures between 0 and 90 degrees. The basis of this effect is a joint influence of amorphisation and implantation in surface layer as well as transfer of atoms from top surface towards back surface. One of the targeted applications [2] is formation of the out-of-plane bended structures that are more easily accessible for manipulation and assembly. Additionally an experiment on fabrication of thin lamella films in single crystalline silicon by FIB for TEM study was done at different energies of Ga ions. It is shown that lower energies of ions can help to fabricate thinner lamellas with a thinner damaged layer on the surface.

[1] E. Holmström, *AIP Advances* **2, no. 1**, 012186, 1-13 (2012).
[2] "Nanobits", *EU FP7* **project**, www.nanobits-project.eu (2010-2013).
[3] Y.R. Kim, *J. Appl. Phys.* **110**, 104322, 1-9 (2006).
[4] A. Savenko, *Microelectronic Engineering* **-**, submitted (2013).

Computional insights on the FM-AFM experiments of the p-nitroaniline solid-liquid interface

P. Spijker[1] R. Nishioka[2] T. Hiasa[2] A. S. Foster[1]

[1]Surfaces and Interfaces at the Nanoscale, Department of Applied Physics, Aalto University, Helsinki, Finland
[2]Department of Chemistry, Kobe University, Kobe, Japan

Solid-liquid interfaces play a fundamental role in many biomolecular and electrochemical applications at the nanoscale. Although spectroscopy and diffraction techniques can provide very accurate information about such interfaces, atomic force microscopy (AFM) has the advantage of probing the investigated system locally, thus allowing a deeper understanding of interfaces. Latest developments in frequency modulated AFM (FM-AFM) have opened up a way to observe interfacial liquid structures as a function of the vertical and lateral coordinates [1]. Recently experiments on the p-nitroaniline (101) crystal surfaces in water have been performed in order to better understand the stability and the mechanisms of nucleation or dissolution at crystal surfaces. p-Nitroaniline is an organic compound containing polar NH_2 and NO_2 groups at opposite ends of a benzene ring. This crystal surface is quite simple but contains still more complex areas making it suitable as an experimental test case.

In the experiments clear structuring of the water at the interface is observed. In order to enhance the insight obtained through the FM-AFM experiments on these p-nitroaniline-water interfaces, we performed both DFT and large-scale molecular dynamics simulations of this system. In these simulations we observed that the (101) crystal surface differs considerably from the same surface based on existing crystallographic data [2,3], giving rise to a more elaborate description of the water interface structure observed in the experiments. As such the computer simulations proved to be useful for better understanding the AFM experiments.

[1] K. Kimura, S. Ido, N. Oyabu, K. Kobayashi, Y. Hirata, T. Imai, and H. Yamada, *J. Chem. Phys.* **132**, 194705 (2010).
[2] S.C. Abrahams and J. Monteath Robertson, *Acta Cryst.* **1**, 252 (1948).
[3] K.N. Trueblood, E. Goldish, and J. Donohue, *Acta Cryst.* **14**, 1009 (1961).

Nearly half-metallic ferromagnetism in CuCrTe2

D. Srivastava[1] G. Tewari[1] M. Karppinen[1]
[1]Department of Chemistry, Aalto University, FI-00076 Aalto, Finland

Spin-polarized density-functional theory within the generalized-gradient approximation (GGA) is employed on ferromagnetic state of $CuCrTe_2$. For the calculations we have adopted hexagonal rhombohedral crystal structure with space group R3m in which all the atoms occupy $00z$ positions with the rhombohedral lattice translations (2/3, 1/3, 1/3) and (1/3, 2/3, 2/3). We predict $CuCrTe_2$ is nearly half-metallic ferromagnet with polarization $3.6083\mu_B$ per formula unit. In a nearly half-metallic ferromagnet, majority spin subband is metallic, whereas in minority spin subband, very few states are available for the conduction near the Fermi edge. Hence, in electronic conduction majority spin bands dominate. These materials show colossal magnetoresistance behavior and are useful for spintronic applications.

Atomistic description of electron beam damage in nitrogen-doped graphene and carbon nanotubes

T. Susi[1] J. Kotakoski[2,3] R. Arenal[4,5,6] S. Kurasch[7] H. Jiang[1] V. Skakalova[2,8] O. Stephan[9] A. V. Krasheninnikov[1,3] U. Kaiser[7] E. I. Kauppinen[1]

[1] Department of Applied Physics, Aalto University, Espoo, Finland
[2] Department of Physics, University of Vienna, Austria
[3] Department of Physics, University of Helsinki, Finland
[4] LMA, Instituto de Nanocienciade Aragon, U.Zaragoza, Spain
[5] Fundacion ARAID, 50004 Zaragoza, Spain
[6] LEM, UMR 104 CNRS-ONERA, Chatillon, France
[7] Central Facility for Electron Microscopy, University of Ulm, Germany
[8] Max Planck Institute for Solid State Research, Stuttgart, Germany
[9] LPS, UMR 8502 CNRS, Université Paris Sud XI, Orsay, France

By combining ab initio simulations with state-of-the-art electron microscopy and electron energy loss spectroscopy (EELS) [1], we study the mechanism of electron beam damage in nitrogen-doped graphene [2] and carbon nanotubes [3]. The incorporation of nitrogen atoms results in noticeable knock-on damage already at 80 kV. In the case of substitutional N, damage is initiated by the displacement of carbon atoms neighboring the dopants, leading to the conversion of substitutional dopant sites into pyridinic ones.

Although such events are relatively rare at 80 kV, they become significant at higher voltages typically used in EELS studies. Correspondingly, we measured an energy loss spectrum time series at 100 kV that provides direct evidence for such conversions in N-SWCNTs, in good agreement with our theoretical prediction. Our improved understanding of the irradiation stability of these materials shows that structural changes cannot be neglected in their characterization using high-energy electrons.

[1] T. Susi et al., *ACS Nano* **6**, 8837 (2012).
[2] J. C. Meyer et al., *Nature Materials* **10**, 209 (2011).
[3] T. Susi et al., *Chemistry of Materials* **23**, 8837 (2012).

Inter- and intramolecular reaction mechanisms in nanocatalysed synthesis of N-CNTs

S. Taubert[1] K. Laasonen[1]

[1]Department of Chemistry, Aalto University

Chemical vapor deposition (CVD) is used to synthesize carbon nanotubes on transition metal nanoclusters. Similar methods can also be used to form graphene in metal surfaces. The detailed reaction mechanisms in the early stages of the CVD process are not well known. Nitrogen-doped carbon nanotubes (N-CNTs) can be used as metal-free electrodes for the oxygen-reduction reaction, as gas sensing devices, and the reactivity of the N-CNTs could enable functionalization. The early steps in the CVD synthesis of nitrogen-doped carbon nanotubes hava been studied previously using molecular dynamics methods at the density-functional tight-binding (DFTB) level [1]. Since every nitrogen atom affects the properties of the doped nanotube [2,3], it would be of importance to understand the formation mechanisms in detail. We have used Bader analysis to obtain the atomic charges of carbon and nitrogen containing fragments on the Fe_{55} nanocluster. The investigated structures were obtained as snapshots from the DFTB-MD trajectories and the structures were refined at the DFT level. Due to charge transfer from the iron cluster to the adatoms all fragments are negatively charged. The localization of atomic charges in the fragments can be utilized to explain the inter- and intramolecular reactions among the fragments.

[1] S. Taubert and K. Laasonen, *J. Phys. Chem. C* **116**, 18538-18549 (2012).
[2] P. Ayala, R. Arenal, *Carbon* **48**, 575-586 (2010).
[3] T. Susi, A. Kaskela, Z. Zhu, P. Ayala, R. Arenal, Y. Tian, P. Laiho, J. Mali, A. G. Nasibulin, H. Jiang, G. Lanzani, O. Stephan, K Laasonen, T. Pichler, A. Loiseau, and E. I. Kauppinen, *Chem. Mater.* **23**, 2201-2208 (2011).

Interaction of ductile crack with grain boundaries in BCC Fe and W: an atomistic study

D. Terentyev[1]

[1]SCK-CEN, Belgium Nuclear Research Centre.

The behaviour of crack propagation and blunting at different loading rates, temperature and crack geometry in two important BCC metals Fe and W has been studied by molecular dynamics under load mode I. Large scale atomistic simulations coupled with a special analysis have been performed to reveal conditions at which dislocations can be emitted from a semi-infinite crack in both FCC and BCC metals. Once the crack alone has been thoroughly characterized, we moved to the description of the interaction of the crack with grain boundaries (GB). Here, we considered pure tilt low- and high-angle grain boundaries. The results obtained clearly show the deflection of the crack propagation on low-angle GBs, and change from ductile to brittle behaviour in the case of high-angle GBs which do not allow for the dislocation passage

EPR and pNMR parameters in point-defected graphenes

J. Vähäkangas[1] J. Mare[1] P. Lantto[1] J. Vaara[1]

[1]NMR Research Group, Department of Physics, University of Oulu, Finland

Recently it has been observed that fluorine adatoms and irradiation defects (vacancies) in graphene carry permanent magnetic moments of one μ_B size causing spin-1/2 paramagnetism.[1] Electron paramagnetic resonance (EPR) is a highly sensitive spectroscopy technique for investigation of the electronic structure and molecular environment of the paramagnetic centers. In EPR, the $\mathbf{g}$-tensor parameterises the Zeeman interaction of the unpaired electrons. The hyperfine coupling tensor $\mathbf{A}$ between electronic and nuclear spins is responsible for fine structure of EPR spectra. These parameters offer the possibility to distinguish different defect structures. Further structural information can be gained by paramagnetic nuclear magnetic resonance (pNMR) spectroscopy in the form of chemical shifts. The pNMR shift can be calculated from the knowldege of $\mathbf{g}$ and $\mathbf{A}$ tensors.[2] Extraction of information from the EPR and pNMR spectra is greatly assisted by first-principles calculations of predictive quality. In this project this is done for a varying concentration of different chemisorbed adatoms and vacancies in graphene, graphane, and fluorographene.

[1] R.R. Nair, M. Sepioni, I-Ling Tsai, O. Lehtinen, J. Leinonen, A.V. Krasheninnikov, T. Thomsom, A.K. Geim and I.V. Grigorieva, *Nat. Phys.* **8**, 199 (2012).
[2] T.O. Pennanen and J. Vaara, *Phys. Rev. Lett.* **100**, 133002 (2008).

Formation of structures smaller than 100 nm by focused ion beam milling

A. Savenko[1] I. Yildiz[1] D. L. Lorenzen[2] Z. I. Balogh[2] P. Boggild[1]
[1]DTU Nanotech
[2]DTU Center of Electron Nanoscopy

Fabrication of small structures by FIB milling is limited by effects occurred in region of scattering of ions inside matter. For example 30 kV Ga ions produce defects in Si within 45 nm near the surface that includes implantation of ions, amorphisation and significant increase of temperature. These effects impose restrictions on minimal size of structures that can be produces. It also depends on the shape of structure (e.g. 1D or 2D, supported or not). When the size of the structure is comparable to ion penetration depth then the structure becomes unstable under ion beam irradiation and may shrink, be melted or bended. An example of description of small and thin structures behavior basing on simulations and experiments was given by Holmström [1]. FIB milling of sharp tips for AFM is one of the possible applications that is currently elaborated [2]. 200 nm thin suspended Si membranes are utilized for fabrication of AFM exchangeable tips by milling from the side. The smallest diameter of the tip that is currently obtained is 10 nm. Advanced strategy of FIB milling is used in order to eliminate influence of redeposition, drift of the beam and to preserve stability of structure. Further improvements are expected to be achieved by using additional methods (e.g. lower ion beam energies, wet etching). Study of these structures in TEM allows to understand better the changes in crystal structure and distinguish crystalline and amorphousized regions. It is known that thin membranes can be bended under ion beam irradiation [3]. Recently we have shown that 70 nm Si_xN_y membranes (strips) are bended upwards (towards the beam source) by FIB induced stress by 30 kV Ga ions [4]. Appropriate dose can result in controllable bending of the structures between 0 and 90 degrees. The basis of this effect is a joint influence of amorphisation and implantation in surface layer as well as transfer of atoms from top surface towards back surface. One of the targeted applications [2] is formation of the out-of-plane bended structures that are more easily accessible for manipulation and assembly. Additionally an experiment on fabrication of thin lamella films in single crystalline silicon by FIB for TEM study was done at different energies of Ga ions. It is shown that lower energies of ions can help to fabricate thinner lamellas with a thinner damaged layer on the surface.

[1] E. Holmström, *AIP Advances* **2**, 1-13 (2012).
[2] "Nanobits", EU FP7 project. www.nanobits-project.eu, - -, - (2010-2013).
[3] Y.R. Kim, *J. Appl. Phys.* **110**, 1-9 (2006).
[4] A. Savenko, *Microelectronic Engineering* **submitted**, - (2013).

From Gold nanotube to atomic section wire

R. Zoubkoff[1]
[1]CSMM, COMP, Department of Applied Physics, Aalto University

Using TB molecular dynamics we realize traction from gold nanowire to atomic section wire. We report the formation of gold nanotube (GNT). Similar to CNT, GNT correspond to a dense (111) plane rolled-up on itself that minimize the surface energy of the system. During the traction process we observed different GNT with various chirality and a radius decrease. For too small radius, the energetic cost to curve the plane was too expensive and lead to the formation of ribbons. At the final stage before breaking junction, we observed that ribbons formation permit to form long atomic section wire.

Ion irradiation response of graphene

E. H. Åhlgren[1] J. Kotakoski[1,2] O. Lehtinen[3] A. V. Krasheninnikov[1,4]

[1]University of Helsinki
[2]University of Vienna
[3]University of Ulm
[4]Aalto University

Defects in nanomaterials can have drastic effects on the properties of these materials. This allows, in principle, controlled modification of these materials for example with ion irradiation. While nanomaterials can have a different response to irradiation than their bulk counterparts, existing theories only occasionally apply in their case. Therefore, to answer the question of what are the specific defect production mechanisms in graphene under ion irradiation, we have studied ion irradiation of graphene using molecular dynamics simulations. We show that the defect types in freestanding graphene depend strongly on the energy of the specific ion, defects occurring at distinct energy ranges that differ from one defect to the next [1]. Our results also indicate, that with growing amount of defects, the membrane is stable, even with defect concentrations up to 35 ne on a Pt (111) surface to analyze the effect of the substrate to the defect production mechanisms in graphene under ion irradiation.

[1] E. H. Åhlgren, J. Kotakoski and A. V. Krasheninnikov, *Phys. Rev. B* **83**, 115424 (2011).

[2] E. H. Åhlgren, J. Kotakoski, O. Lehtinen and A. V. Krasheninnikov, *App. Phys. Lett.* **23**, 233108 (2012).

Participants

Gabriel Autes	Switzerland	gabriel.autes@epfl.ch
Konstantin Avchaciov	Finland	konstantin.avchachov@helsinki.fi
Richard Berndt	Germany	berndt@physik.uni-kiel.de
Carla Bittencourt	Belgium	carla.bittencourt@umons.ac.be
Torbjörn Björkman	Finland	torbjorn.bjorkman@aalto.fi
Alfredo Caro	Usa	caro@lanl.gov
Karel Carva	Czech Republic.	karel.carva@mff.cuni.cz
Marina Casartelli	Italy	marina.casartelli@unimi.it
Jian-Cheng Chen	Finland	jian-cheng.chen@aalto.fi
P. Andre Clayborne	Finland	penee.a.clayborne@jyu.fi
Flyura Djurabekova	Finland	flyura.djurabekova@helsinki.fi
Robert Drost	Finland	robert.drost@aalto.fi
Franz Eder	Austria	f.eder@univie.ac.at
Vladimir Falko	Uk	v.falko@lancaster.ac.uk
Weijia Fan	Finland	weijia.fan@aalto.fi
Gregor Fessler	Switzerland	gregor.fessler@unibas.ch
Alexandra Freidzon	Russia	freidzon.sanya@gmail.com
Julian D Gale	Australia	j.gale@curtin.edu.au
Claudia Gomes da Rocha	Finland	claudia.c.gomes-darocha@phys.jyu.fi
Fredric Gustaf Granberg	Finland	fredric.granberg@helsinki.fi
Irina Grigorieva	Uk	irina.grigorieva@manchester.ac.uk
Ari Harju	Finland	ari.harju@aalto.fi
Xiaohui Hu	China	huhuihui2005@sina.com
Hannes Jonsson	Finland	hj@hi.is
Volodymyr Khranovskyy	Sweden	volkh@ifm.liu.se
Andras Kis	Switzerland	andras.kis@epfl.ch
Hannu-Pekka Komsa	Finland	hannu-pekka.komsa@helsinki.fi
Jani Kotakoski	Austria	jani.kotakoski@iki.fi
John Landers	France	john.landers@grenoble.cnrs.fr
Markus Langer	Switzerland	markus.langer@unibas.ch
Ossi Lehtinen	Germany	ossi.lehtinen@uni-ulm.de
Jose Miguel Luque-Raigon	Finland	jose.luque.raigon@aalto.fi
Keith Mckenna	United Kingdom	keith.mckenna@york.ac.uk
Florian Mittendorfer	Austria	florian.mittendorfer@tuwien.ac.at
Tiziana Musso	Finland	tiziana.musso@aalto.fi
Heinz Christoph Neitzert	Italy	neitzert@unisa.it
Kai Nordlund	Finland	kai.nordlund@helsinki.fi
Riku Oja	Finland	riku.oja@aalto.fi
Ari Markus Ojanperä	Finland	ari.ojanpera@aalto.fi
Luiz Felipe Pereira	Germany	pereira@mpip-mainz.mpg.de

Patrick Philipp	Luxembourg	philipp@lippmann.lu
Bernhard Reischl	Finland	bernhard.reischl@aalto.fi
Jascha Repp	Germany	jascha.repp@physik.uni-regensburg.de
Tuomas Petteri Rossi	Finland	tuomas.rossi@aalto.fi
Burkhard Sachs	Germany	bsachs@physnet.uni-hamburg.de
Arto Sakko	Finland	arto.sakko@aalto.fi
Nino Samadashvili	Finland	nino.samadashvili@aalto.fi
Alexey Savenko	Denmark	ales@nanotech.dtu.dk
Alexander Schwarz	Germany	aschwarz@physent.uni-hamburg.de
Gotthard Seifert	Germany	gotthard.seifert@chemie.tu-dresden.de
Peter Spijker	Finland	peter.spijker@aalto.fi
Divya Srivastava	Finland	divya.srivastava@aalto.fi
Sebastian Standop	Germany	standop@ph2.uni-koeln.de
Toma Susi	Finland	toma.susi@aalto.fi
Ingmar Swart	the Netherlands	i.swart@uu.nl
Stefan Taubert	Finland	stefan.taubert@aalto.fi
Dmitry Terentyev	Belgium	dterenty@sckcen.be
Jarkko Vähäkangas	Finland	jarkko.vahakangas@oulu.fi
Alfred Weymouth	Germany	jay.weymouth@physik.uni-r.de
Izzet Yildiz	Denmark	izyi@nanotech.dtu.dk
Oleg Yazyev	Switzerland	oleg.yazyev@epfl.ch
Remi Zoubkoff	Finland	remi.zoubkoff@aalto.fi
Elina Harriet Åhlgren	Finland	harriet.ahlgren@helsinki.fi

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