Towards Reality in Nanoscale Materials IX

Nanoscale Materials for Warfare Agent Detection: Nanoscience for Security

13th – 16th February 2017 Levi, Finland



The NATO Science for Peace and Security Program

Organizers

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TRNM IX

Programme

	Monday		Tuesday		Wednesday		Thursday
8:40	Intro						
8:45	Capan						
	chair: Hoffmann		chair: Liljeroth		chair: Jelinek		chair: Facsko
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10:20	Blood	10:20	Valerius	10:20	Tagmatarchis	10:40	Coffee
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						11:20	Haluska
	chair: Hierold		chair: Charlier		chair: Kotakoski	11:20	Hofer
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12:20	Rio	12:20	Kralj	12:00	Remediakis	12:40	Legut
12:40	Debliquy	12:40	Jamroz	12:20	Rinaldi		
				12:40	Lajaunie	13:00	Lunch
13:00	Lunch	13:00	Lunch			16:40	Coffee
16:40	Coffee	16:40	Coffee	13:00	Lunch		
				16:40	Coffee		chair: Ottaviano
	chair: McKenna		chair: Jonsson			17:00	Bøggild
17:00	Kawai	17:00	McKenna		chair: Swager		
17:40	Gulans	17:40	van Dijken	17:00	Hierold	17:40	Closing
18:00	Schulz	18:00	Wolf	17:40	Kretschmer		
18:20	Jónsson	18:20	Büchner	18:00	Carva		
18:40	Granberg	18:40	Erbahar	18:20	Abergel		
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			Chemical Sensors for Explosives and CW Detection
9:40	-	10:20	Liljeroth
			Atomically precise graphene nanoribbons through on-surface synthesis
10:20	-	10:40	Blood
			Design and Implementation of the Chemical Warfare Agent Force Field
10:40	-	11:20	Coffee
			chair: Hierold
11:20	-	12:00	lelinek
			Exploring structural and electronic properties of helical molecules on surfaces.
12:00	-	12:20	Biel
			SPM fingerprints and electronic properties of point-like and extended defects in single-
12.20		12.40	
12.20	-	12.40	NU 1D and 2D networks of cuclo-paraphenulanes (CPPs) using covalent and self-assembly
			process by DFT
12:40	-	13:00	Debliquy
			Formaldehyde detection for indoor air quality
13:00	_	16:40	Lunch
16:40	-	17:00	Coffee
			chair: McKenna
17:00	-	17:40	Kawai
			On-surface chemical reaction and its product studied by high-resolution atomic force microscopy
17:40	-	18:00	Gulans
			Photoabsorption of adsorbed azobenzene monolayers: impact of graphene substrate
18:00	-	18:20	Schulz
			Elemental contrast in noncontact atomic force microscopy on a boron-nitride monolayer
18:20	-	18:40	Jónsson
			Semi-infinite solid approach to calculations of surface properties
18:40	-	19:00	Granberg
			Multiscale modelling of defect evolution in equiatomic multicomponent alloys

Chemical Sensors for Explosives and CW Detection

T. M. Swager¹

¹Massachusetts Institute of Technology

This lecture will detail the creation of ultrasensitive sensors based on electronically active conjugated polymers (CPs) and carbon nanotubes (CNTs). A central concept that a single nano- or molecular-wire spanning between two electrodes would create an exceptional sensor if binding of a molecule of interest to it would block all electronic transport. The use of molecular electronic circuits to give signal gain is not limited to electrical transport and CP-based fluorescent sensors can provide ultratrace detection of chemical vapors via amplification resulting from exciton migration. Nanowire networks of CNTs provide for a practical approximation to the single nanowire scheme and selectivity is generated by covalent and/or non-covalent binding selectors/receptors to the carbon nanotubes. Sensors for a variety of materials and cross-reactive sensor arrays will be described. Polar hydrogen bonding groups provide selectivity for nitro-groups and methods for responding to electrophilic chemical weapons will also be detailed.

- Yang, J.-S.; Swager, T. M. Porous Shape Persistent Fluorescent Polymer Films: An Approach to TNT Sensory Materials J. Am. Chem. Soc. 1998, 120, 5321-5322.
- [2] Schnorr, J. M.; van der Zwaag, D.; Walish, J. J.; Weizmann, Y.; Swager, T. M. Sensory Arrays of Covalently Functionalized Single-Walled Carbon Nanotubes for Explosive Detection Adv. Funct. Mater. 2013, 23, 5285-5291.
- [3] Wang, F.; Gu, H.; Swager, T. M. Carbon Nanotube/Polythiophene Chemiresistive Sensors for Chemical Warfare Agents J. Am. Chem. Soc. 2008, 130, 5392-5393.
- [4] Weis, J. G.; Swager, T. M. Thiophene-fused Tropones as Chemical Warfare Agent-Responsive Building Blocks ACS Macro Lett., 2015, 4, 138-142.
- [5] Belger, C.; Weis, J. G.; Ahmed, E.; Swager, T. M. Colorimetric Stimuli-Responsive Hydrogel Polymers for the Detection of Nerve Agents Macromolecules 2015, 48, 7990-7994.
- [6] Ishihara, S.; Azzarelli, J. M.; Swager T. M. Ultratrace Detection of Toxic Chemicals: Triggered Disassembly of Supramolecular Nanotube Wrappers J. Am. Chem. Soc. 2016, 138, 8221-8227.
- [7] Zhu, R.; Azzarelli, J. M.; Swager, T. M. Wireless Hazard Badges for Nerve Agent Simulants Angew. Chem. Int. Ed. 2016, 55, 9662-9666.

Atomically precise graphene nanoribbons through on-surface synthesis

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Graphene nanoribbons (GNRs) are a new class of materials that have promising applications in next-generation nanoelectronic, photonic and spintronic devices. GNRs have been predicted to show interesting electronic properties that depend strongly on their width and edge structure. However, the required precision cannot be achieved by top-down approaches, including e-beam lithography on a sheet of graphene or unzipping carbon nanotubes. Recently, bottom-up synthesis using molecular precursors has been shown to provide precise control over the width and edge geometry of GNRs [1]. By changing the monomer design, fabrication of a wide range of different GNRs can be achieved with engineered chemical and electronic properties.

In the typical picture of the on-surface synthesis, the substrate does not play a big role in the chemical reaction. Using low-temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM), I will show that the substrate is not always an innocent bystander in these reactions. On Au(111) surface, the prototypical precursor dibromo-bianthryl (DBBA) polymerizes via an Ullmann route to form straight GNRs with armchair edges. However, on Cu(111), the DBBA precursor forms chiral (3,1)GNRs. In contrast, dibromoperylene (DBP) precursors do form armchair GNRs via Ullmann coupling, in close analogy to recent results on Au(111). The reaction intermediates highlight the role of the precursor shape, molecule-molecule interactions and substrate reactivity as decisive factors in determining the reaction pathway [2]. Our findings help to realize new routes for previously unattainable covalently bonded nanostructures.

The armchair GNRs can be divided into three families based on their width N: GNRs with N=3m or N=3m+1, where m is an integer, are semiconducting. On the other hand, GNRs with a width of N=3m+2 are predicted to be nearly metallic with a very small bandgap. We have synthesized N=5 armchair GNRs and studied their electronic properties in detail using low-temperature scanning probe techniques [3]. Scanning tunneling spectroscopy demonstrates that N=5 ribbons show nearly metallic behavior with much smaller bandgap than the wider N=7 GNRs belonging to the N=3m+1 family. These narrow armchair GNRs with a small bandgap would form ideal molecular wires to be used as interconnects in molecular scale circuitry. In addition monocomponent GNRs, we have realized metal-semiconductor heterostructures by

joining armchair GNRs belonging to the metallic (5-atom wide) and semiconducting (7-atom wide) families through on-surface synthesis. These structures constitute the first steps towards enco ding more functionality into a single GNR for electronic applications.

- [1] L. Talirz, P. Ruffieux, R. Fasel, Adv. Mater. 28, 6222 (2016).
- [2] F. Schulz et al., *submitted* (2016).
- [3] A. Kimouche et al., *Nat. Commun.* **6**, 10177 (2015).

Design and Implementation of the Chemical Warfare Agent Force Field

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In recent months there have been continuing reports of chemical warfare agents (CWAs) being used in conflict situations in Syria.[1] How these chemicals react with the body is well understood, however it is less clear how they interact with porous materials they can encounter in the field, such as sand, brick, soil, etc. Molecular simulations are an ideal way to investigate these highly toxic chemicals at an atomistic level. To this end we present the Chemical Warfare Agent Force Field (CWAFF), which has been parameterised to describe the nerve agents GB, VX, and VM, as well as the vesicant HD.

CWAFF has been used to model agent behaviour in a variety of substrates chosen to mimic chemical functionalities of materials with which the agents could come into contact. In order to obtain a more comprehensive understanding of the sorption and diffusion of CWAs, both organic and inorganic host materials were chosen, with a variety of chemical moieties and pore sizes. CWAFF has been implemented with DL_POLY[2] for molecular dynamics simulations and RASPA[3] for Grand Canonical Monte Carlo simulations.

- Associated Press, *The Guardian* https://www.theguardian.com/world/2016/aug/25/assadregime-isis-chemical-attacks-syria-un-investigators (2016).
- [2] I. T. Todorov, W. Smith, K. Trachenko, M. T. Dove, M. R. S. Pinches, D. Tildesley, W. Smith, D. Rapaport, M. E. Tuckerman, B. J. Berne, G. J. Martyna, G. J. Martyna, M. E. Tuckerman, J. T. Douglas, M. L. Klein, H. C. Andersen, U. Essmann, L. Perera, M. L. Berkowtz, T. Darden, H. Lee, L. G. Pedersen, D. E. Shaw, X. L. Cao, Z. Y. Mo, I. T. Todorov, W. Smith, W. Smith, T. R. Forester, M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, M. C. Payne1, J. P. Ryckaert, G. Ciccotti, H. J. C. Berendsen, W. C. Swope, H. C. Andersen, P. H. Berens, K. R. Wilson, J. Tersoff, P. J. D. Lindan, M. J. Gillan, S. A. Adelman, J. Doll, J. A. Izaguirre, K. Trachenko, M. T. Dove, T. G. W. Geisler, I. T. Todorov, W. Smith, K. Trachenko, I. T. Todorov, M. Smith, I. T. Todorov, J. A. Purton, N. L. Allan, M. T. Dove, M. Berkowitz, J. , J. Mater. Chem. 16, 1911 (2006).
- [3] D. Dubbeldam, S. Calero, D. E. Ellis and R. Q. Snurr, Mol. Simul. 7022, 1-21 (2015).

Exploring structural and electronic properties of helical molecules on surfaces.

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Molecules with helical structure fascinate chemists for many years due to their nonplanar structure, which introduces inherently chirality and it exhibits interesting optical and electronic properties. We will present two different studies of helicene molecules on metal surfaces to explore: i) chirality transfer driven by on-surface reaction and ii) their mechanical response to an external field. In the first case, we will demonstrate that transfer chirality from a homochiral helical precursor to enantiofacially adsorbed prochiral products through a cascade of stereoconservative on-surface reactions is possible [1]. Detailed molecular structure of intermediates and final products of the chemical reactions, including their chirality, are identified by means of high-resolution SPM images supported by extensive theoretical DFT-based analysis. In the second case, we will report simultaneous tunneling current and force through helicene molecules deposited on Ag(111) surface. We will show that simultaneous AFM/STM measurements together with DFT calculations reveals strong piezoelectric effect detected on a single molecule on metal surface.

[1] O. Stetsovych et al, , Nature Chemistry 10.1038/nchem.2662 (2016).

SPM fingerprints and electronic properties of point-like and extended defects in single-layer MoS_2

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Defects, commonly created during the growth process in two-dimensional (2D) materials, can dramatically modify the performance of 2D-based devices. In the case of MoS_2 , a transition metal dichalcogenide (TMD) semiconductor with a direct gap of 1.8 eV [1] with promising applications in nanoelectronics, many of these defects have already been observed, of both the point-like [2] and extended kinds [3]. However, with the exception of the S monovacancy, a detailed characterization of their electronic, magnetic and transport features is still lacking.

A valuable tool for identifying the properties of such defects is Scanning Probe Microscopy (SPM). However, the interpretation of the images produced via this technique is not always straightforward and often requires the help of atomic-scale simulations to provide a correct understanding of the sample under study.

In this work, we present an *ab initio* study of the most common point-like defects observed in monolayer MoS_2 . The investigation of several types of grain boundaries that may appear in polycrystalline MoS_2 has been addressed as well. We analyze the electronic and transport features of the selected defects [4,5] and supply their simulated images for both the Scanning Tunneling (ST) [6] and Atomic Force (AF) [7] Microscopy techniques.

We expect our work to provide a valuable tool for experimentalists and to help improve the understanding of the electronic and transport properties of defected MoS_2 monolayers.

- K.F. Mak et al., Physical Review Letters 105, 136805 (2010).
- [2] J. Hong et al., Nature Communications 6, 6293 (2015).
- [3] Y.L. Huang et al., Nature Communications 6, 6298 (2015).
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- [5] C. Gonzalez, Y. Dappe and B. Biel, (in preparation).
- [6] C. Gonzalez, B. Biel and Y. Dappe, Nanotechnology 27, 105702 (2016).
- [7] C. Gonzalez, Y. Dappe and B. Biel, The Journal of Physical Chemistry C 120, 17115 (2016).

1D and 2D networks of cyclo-paraphenylenes (CPPs) using covalent and self-assembly process by DFT

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Cycloparaphenylenes (CPPs) represent the shortest possible segment of (n,n) armchair carbon nanotubes (CNTs), and as such may represent a new route to producing chirally selected carbon nanotubes [1] [2]. Current approaches for this envisage controlling synthesis of uniform-diameter single chirality CNTs using CPPs as templates, which has met with limited success [3]. At the same time complexes of fullerenes with CPPs have been reported, highlighting a high size selectivity of the CPPs to the specific fullerene.

In the current study we explore a new approach, namely using covalent- and non-covalent self-assembly of either functionalized CPPs, or CPP-C₆₀ hybrid systems, to create new types of poly-CPP-nanotubes. These new materials, while also adopting a controlled chirality tubular morphology, show distinctly different chemical, mechanical, electronic and optical behavior to conventional carbon nanotubes.

The first of these families involves chemical cross-linking between neighbouring CPPs using fullerenes as alignment templates. The resultant poly-CPP-nanotubes share some properties with conjugated polymers, notably the ability to add functionality and control electronic properties through functionalisation control. The second family using self-assembly stacking between C₆₀ and different sizes of [6]-, [8]-, [10]-CPPs to form 1D and 2D networks. While the study is driven by our theoretical modelling, we successfully demonstrate via a joint experimental-theoretical study the first steps towards their production, namely trapping of 2CPP rings around a fullerene dimer (C₅₉N)₂ [4].

- A.-F. Tran-Van, E. Huxol, J. M. Basler, M. Neuburger, J.-J. Adjizian, C. P. Ewels and H. A. Wegner, Org. Lett. 16, 1594-1597 (2014).
- [2] J. Rio, D. Erbahar, M. Rayson, P. Briddon and C. P. Ewels, *Phys. Chem. Chem. Phys.* 18, 23257-23263 (2016).
- [3] H. Omachi, T. Nakayama, E. Takahashi, Y. Segawa and K. Itami, *Nat. Chem.* 5, 572-576 (2013).
- [4] J. Rio, S. Ahles, C. Ewels, D. Jacquemin, N. Tagmatarchis, H. A. Wegner, in preparation . (2017).

Formaldehyde detection for indoor air quality

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Volatile Organic Compounds in indoor air have become these last years the subject of a big concern. The main emission sources are: furniture, paintings, varnishes, wood protection, construction materials, etc. In particular, formaldehyde is now considered by the authorities as one of the priority pollutants because of its carcinogenic [1] character and because of the multiplication of sources in our close environment. The World Health Organization (WHO) guideline for indoor air formaldehyde concentration is 80 ppb (0.1 mg/m3) [2]. Methods based on air sample collection and lab measurements are available and are the most used methods [3]. They are accurate and reliable but these methods are expensive, are not real time and some statistics issues are raised because of that. That is why, it is important to detect and measure formaldehyde in real time, in situ and with a low cost equipment. Devices based on chemical sensors are a good solution as these systems can be very sensitive, low cost and easily integrated in common electronics to build portable systems [4]. Different sensing technologies exist and we will focus on electrochemical systems exploiting organic or inorganic semiconductor materials. These sensors are based on the monitoring of the conductivity changes of a semiconducting sensitive coating due to a reversible doping by the adsorbed gases. This paper will shortly present a overview of the existing sensors for formaldehyde detection and new sensors based on metal oxides and on the use of molecularly imprinted polymers. Metal oxide gas sensors are well known for their high sensitivity allowing detection in the ppb concentration range and their stability. The main drawback is that they generally need to be heated to temperatures in the range 150-350°C. In order to reduce the power consumption, the area of the sensitive layer is miniaturized using MEMS technology. Our sensor with an area of 200x200 μ m2 consumes a power of 15mW when it operates continuously. The concentration range for formaldehyde is 10-2000 ppb. Molecularly imprinted polymers (MIP) are polymers that are synthesized incorporating the target molecule we want to detect as a template. Functional monomers form a complex around the template and are linked afterwards to form a polymer constituted of a series of "cages" trapping the template. Once the synthesis is complete, the template molecule is extracted, leaving a molecular cavity imprinted in the polymer matrix that allows the polymer to selectively recognize the target molecule [5]. These elements are cheap, easy to synthesize and can be adapted to any kind of surface. Using conducting polymers for building MIPs allows to get semiconductor gas sensors working at room temperature with a good selectivity. We succeeded in preparing sensors based on polypyrrole deposited by electropolymerization detecting formaldehyde in the range [100 ppb-20 ppm].

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On-surface chemical reaction and its product studied by high-resolution atomic force microscopy

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Since the first direct observation of the chemical structure of pentacene, atomic force microscopy (AFM) became a powerful tool for surface chemistry [1]. Such high-resolution imaging technique is quite beneficial to identify structures of molecules condensed by the C-H···F hydrogen bonding [2], halogen bonding [3], and two-dimensional metal organic framework [4] and of the doped graphene nanoribbons [5] and novel aromatic compounds [6] synthesized by on-surface chemical reaction. Furthermore, the synthesized products as polyfluorene [7] and graphene nanoribbon [8] can be used for measurement of the mechanical properties, in which the effect of the commensurability and incommensurability plays a role in friction during lifting and sliding the objects.

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Photoabsorption of adsorbed azobenzene monolayers: impact of graphene substrate

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We use density-functional theory and many-body perturbation theory to study the impact of the graphene substrate on the photo-absorption properties of *trans*- and *cis*-azobenzene monolayers. The molecules are weakly bound to graphene, and their orbitals are essentially not hybridized with bands of the substrate. Yet graphene remarkably modulates the absorption spectra of the adsorbates. Firstly, it influences excitation energies via (i) substrate polarization reducing the band-gap of azobenzene and (ii) enhanced dielectric screening, which weakens the attractive interaction between electrons and holes. Secondly, graphene activates intermolecular excitations, which are dark in the isolated monolayers. Our results demonstrate that the photoisomerization process of weakly adsorbed azobenzene undergoes notable changes on the carbonbased substrate compared to the isolated monolayers.

Elemental contrast in noncontact atomic force microscopy on a boron-nitride monolayer

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Elemental contrast with atomic resolution is a key aspect of cutting-edge microscopy, enabling materials research at the nanoscale. Transmission electron microscopy (TEM) offers chemical sensitivity through different modes, most strikingly as Z-contrast and via atomically resolved electron energy loss spectroscopy (EELS) in scanning TEM [1]. However, due to the high-energy electron beam, TEM is not suitable for more sensitive structures such as small organic molecules. A less destructive alternative might be noncontact atomic force microscopy (nc-AFM). Though not yet capable of chemical fingerprinting as powerful as EELS, elemental contrast is one of the most-studied topics in nc-AFM. In a seminal contribution, Sugimoto et al. identified different atomic species in a surface alloy by comparing the maximum attractive forces on different lattice sites in $\Delta f(z)$ spectroscopy [2]. Measurements of the local contact potential difference (LCPD) in Kelvin probe force microscopy, either via an AC modulation of the tip-sample voltage or through $\Delta f(V)$ spectroscopy, is another avenue that achieved chemical resolution, in particular on ionic systems [3-5]. Here, we employ nc-AFM with CO-functionalized tips [6] to investigate the atomic-scale contrast on a monolayer of hexagonal boron nitride (hBN) on Ir(111) [7]. hBN constitutes an interesting model system, as it is a mostly covalently bonded insulator with a nearest-neighbour distance of only ~ 145 pm. Yet constantheight maps of both frequency shift and local contact potential difference reveal strong contrast between the boron and nitrogen sub-lattices. nc-AFM simulations based on the density functional theory-optimized hBN/Ir(111) geometry allow us to match the two distinct atomic sites with the different elements and shine light on the origin of the atomic-scale contrast. Our combination of constant-height images and atomically resolved LCPD maps offers a robust method to identify different chemical species in nc-AFM.

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Semi-infinite solid approach to calculations of surface properties

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A method for carrying out electronic density functional theory calculations of surface properties using a semi-infinite solid model and a fixed chemical potential of electrons is presented along with various applications to metal and semiconductor surfaces. A Green function approach [1] is used to simulate a system consisting of two regions: (A) the bulk solid represented by a minimal unit cell and subject to periodic boundary conditions in three dimensions, and (B) a surface region represented by a few atomic layers subject to periodic boundary conditions in two dimensions with a free surface on one side but matched to region (A) on the other side. Not only is this a more accurate description of a solid surface but the computational effort is also an order of magnitude smaller than with the commonly used slab model. The semi-infinite solid approach has been implemented in the ATK software using atomic basis sets. Results of calculations demonstrate fast and system atic convergence of, for example, work function and band gap with the number of layers in region (B), while results of slab calculations show erratic convergence or even lack of convergence with the number of layers in a slab. This new methodology opens up new possibilities for simulating the properties of thin films and nanostructures on surfaces where the coupling to the substrate is properly taken into account.

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Multiscale modelling of defect evolution in equiatomic multicomponent alloys

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High entropy alloys, and a sub category of them, equiatomic multicomponent alloys, have shown both good mechanical and corrosion resistant properties, desired in future nuclear power plant concepts. The alloys have good mechanical properties both at cryogenic temperatures as well as at high temperatures. But to use them in environments where radiation is present, it is crucial to know their radiation response. In recent studies it have been found, both computationally and experimentally, that they also show a reduction in accumulated defects, compared to their elemental materials [1,3]. It was found that one key mechanisms of this reduction was the mobility of dislocations [1,2,3]. The results show that the binary NiFe and the ternary NiCoCr and NiCoFe all show better response to irradiation damage, compared to pure Ni and binary NiCo. Simulations of dislocation mobility show that the dislocations can easily move in Ni and NiCo, whereas the other alloys show a lower mobility and a higher onset stress. One of the key questions regarding especially nuclear power plants is the long time evolution of the materials, when the expected lifetime of modern power plant are over 50 years. To answer this question, we have started to use a multiscale approach to the problem, to assess the defect annealing and evolution over longer timescales. The defect production is simulated with Molecular Dynamics (MD), which can capture the picosecond primary damage production, and then use a Self Evolving Atomistic Kinetic Monte Carlo (SEAKMC) method to assess the long time evolution. These two methods will be used consecutively after each other, first to produce the correct damage (with MD) and then anneal it at timescales proportional to experimental ones (with SEAKMC).

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Tuesday 14.02.2017

			chair: Liljeroth
9:00	-	9:40	Hofmann
			Crystal growth of 2D materials: from model systems to integrated manufacturing
9:40	-	10:20	Kotakoski
			Atomic-level manipulation of two-dimensional materials through electron and ion irra- diation
10:20	_	10:40	Valerius
			Epitaxially grown h-BN on Ir(111) ,Äì A one atomic thick layer under ion irradiation
10:40	-	11:20	Coffee
			chair: Charlier
11:20	-	12:00	Haigh
			Understanding nanoparticle catalysts and 'beyond-graphene' heterostructures using advanced analytical scanning transmission electron microscopy
12:00	-	12:20	Komsa
			Structural changes in two-dimensional materials under electron beam
12:20	-	12:40	Kralj
			Direct visual observation of 2D transition metal dichalcogenide growth
12:40	-	13:00	Jamroz
			Short-range ordering effects in binary and ternary B-C-N two-dimensional hexagonal structures in the presence of defects
13:00	_	16:40	Lunch
16:40	-	17:00	Coffee
			chair: Jonsson
17:00	-	17:40	McKenna
			Effect of polaronic charge transfer on band alignment at the Cu/TiO $_2$ interface
17:40	-	18:00	van Dijken
			Resistive Switching in All-Oxide Ferroelectric Tunnel Junctions with Ionic Interfaces
18:00	-	18:20	Wolf
			Fluorine clusters at CeO2(111) - A DFT+U and Monte Carlo study
18:20	-	18:40	Büchner
			A Chemically Saturated 2D SiO $_2$ Sheet - Preparation, Structure and Transfer
18:40	-	19:00	Erbahar
			Selective statistical analysis of MD simulations for vibrational spectroscopy modelling

Crystal growth of 2D materials: from model systems to integrated manufacturing

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The commercial potential of 2D materials hinges on the development of growth and process techniques that are scalable and allow an adequate level of structural control. Chemical vapor deposition (CVD) can uniquely serve the demand for integrated manufacturing of electronic-grade large-area 2D material films as well as potentially allows the direct growth of vertical, stacked or unique in-plane 2D heterostructures. Understanding the underlying crystal growth mechanisms is a current bottleneck and key future enabler. This talk will review our current understanding of graphene and h-BN CVD based on model catalyst systems, including results from a range of in-situ characterization methods such as environmental scanning and transmission electron microscopy, high-pressure X-ray photoelectron spectroscopy, X-ray diffraction and scanning tunneling microscopy [1-3]. We will outline the potential of direct CVD of various 2D heterostructures as well as current challenges for integrated manufacturing and industrial device integration of these 2D materials [4,5].

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Atomic-level manipulation of two-dimensional materials through electron and ion irradiation

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Despite the great promise of two-dimensional materials due to their exciting properties, they are not always directly suitable for applications. One way to tune the material properties is to manipulate the atomic structure using particle irradiation. However, as one might expect, this is challenging to do in the case of extremely thin materials, where careful control over the irradiation energy and solid understanding of the underlying atomic-scale phenomena are required.

Despite the challenges, electron and ion irradiation have recently evolved into powerful techniques to manipulation the atomic structure of two-dimensional materials. At the same time, the recent advancements in aberration-corrected transmission electron microscopy both provide means to directly image the manipulated structures but also to fine tune them by inducing local structural changes and even to move defects and impurity atoms.

In this presentation, I will describe the advances in manipulating graphene with electron irradiation (e.g., Ref. [1]) and overview our latest progress in using ion irradiation at a large energy scale to implant foreign atoms into graphene [2], moving impurity atoms and defects at will (e.g., Refs. [3,4]), creating nanopores into graphene [5] and MoS2, patterning graphene with gratings and two-dimensional amorphized areas [6,7] as well as other recent results.

If time allows, I will also describe our new experimental setup (to be finished in 2017) combining low-energy ion irradiation line in the same vacuum as a state-of-the-art aberration-corrected scanning transmission electron miroscope fitted for in situ manipulation during imaging.

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Epitaxially grown h-BN on Ir(111) A one atomic thick layer under ion irradiation

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Chemical vapor deposition of $B_3N_3H_6$ molecules on Ir(111) results in a well aligned monolayer of hexagonal boron nitride (h-BN) which forms an incommensurate (11.7 x 11.7) moiré on (10.7 x 10.7) substrate unit cells. The center of each unit cell provides a chemisorbed valley area, where h-BN is hybridized with the Ir substrate. Exposing such a monolayer of h-BN on Ir(111) at room temperature to low energy Xe⁺ irradiation causes amorphization of the 2D layer, as evidenced by low energy electron diffraction. The recovery process is followed up to 1550 K using scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). Surprisingly, upon annealing the h-BN layer and the moiré recover to good perfection, except of blisters formed due to aggregation of implanted noble gas species, as well as vacancy clusters and larger vacancy islands resulting from sputtering. With STM we image through the h-BN blister lid and find a superstructure corresponding in lattice parameter to what we expect for a crystalline, pressurized Xe. The blisters survive annealing to 1550 K, a temperature where pristine h-BN on Ir(111) is already decomposed. They transform to a triangular shape, driven by the energetic preference of boron terminated edges. The extraordinary stability of Xe-filled triangular, boron-terminated h-BN blisters is confirmed by dedicated DFT calculations. The vacancy clusters form an ordered array of holes in the h-BN layer (a nanomesh), precisely at the locations of the valleys, as there h-BN edges bind strongest to the substrate. Such a nanomesh membrane could be well suited for water purification applications. Finally, we report on experiments investigating the chemical reactivity of the valley region by deposition of metallic and non-metallic elemental species, in order to determine the suitability of the h-BN layer on Ir(111) as a template for aggregation of clusters, providing opportunities for nano-catalysis or nano-magnetism.

Understanding nanoparticle catalysts and 'beyond-graphene' heterostructures using advanced analytical scanning transmission electron microscopy

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The current generation of aberration corrected scanning transmission electron microscope (STEM) instruments optimized for high spatial resolution energy dispersive x-ray (EDX) spectroscopy provide exciting opportunities for structural and elemental analysis of nanoscale objects. Here I will discuss recent example applications from our studies of nanoparticle catalysts and 2D device heterostructures where these analytical capabilities have provided new insights to interpret the optical, electronic and catalytic properties of such systems.

The emerging area of 2D materials has attracted a great deal of attention in recent years. Like graphene, these materials can be exfoliated to single atom thickness and can then be layered together to create new van der Waals crystals with bespoke properties. We have been developing methods for investigating the structure of these novel materials at the atomic scale. I will present work demonstrating that cross sectional STEM-EDX spectrum imaging can be used to reveal the internal atomic structure of van der Waals heterostructure devices[1,2]. For example, we have studied light emitting diode (LED) devices, produced by mechanical exfoliation and subsequent stacking of 13 different 2D crystals, including four MoS2 monolayer quantum wells3. Using cross sectional STEM spectrum imaging we reveal that the crystal interfaces of such devices are atomically flat and provide detailed structural information to help to explain the photoluminescence results obtained. Other 2D crystal het erostructures will also be discussed including those incorporating air sensitive 2D crystals, such as black phosphorus and NbSe2, which are fabricated under an argon atmosphere to preserve the structure of the material.[4] Recent results where heterostructures containing atomically engineered nanoscale channels have been used to study water transport will also be discussed.[5]

Most (S)TEM imaging and analysis gives only a 2D projection of the structure in vacuum. I will discuss the application of elementally sensitive STEM EDX electron tomography to provide a route to understanding the full 3D morphology and chemistry with nanometre resolution.[6] I will also discuss current progress and using customised modification of an in situ STEM holder system has allowed us to perform high spatial resolution STEM-EDX spectrum imaging during in-situ gas and liquid phase experiments and at elevated temperature.[7]

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- [3] Withers et al, Nature Materials 14, 301 (2015).
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- [7] Lewis et al, Chemical Communications 50, 10019 (2014).

Structural changes in two-dimensional materials under electron beam

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During electron microscope imaging, the beam of electrons with relativistic energies can not only cause unintentional damage, but also lead to possibly useful structural modifications that may further be controlled with nanoscale resolution.

In my talk, I will cover two examples of such modifications from our recent work. First, we have observed structural evolution of layered tin chalcogenides from SnS₂ to SnS, as well the corresponding selenides, upon sputtering of large number of chalcogen atoms [1]. First-principles calculations are used to propose how the transformation proceeds in the atomic level. A dependence of the layer orientation of the resulting SnS is rationalized by a transformation pathway in which vacancies group into ordered S-vacancy lines, which convert via a Sn₂S₃ intermediate to SnS. Absence of a stable Sn₂Se₃ intermediate precludes this pathway for the selenides, hence SnSe₂ always transforms into basal plane oriented SnSe.

Second, electron microscopy imaging of monolayer of black phosphorus has proven challenging due to the material's sensitivity to the impacts from the energetic electrons. To aid in understanding the response of this material to the beam and design imaging conditions, we performed computational study of initial damage processes and evaluated the relevant cross sections [2]. We also considered the stability of the sample edges, as well as the vacancy and adatom dynamics.

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Direct visual observation of 2D transition metal dichalcogenide growth

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Mono- and few-layer transition metal dichalcogenides (TMDs) attract increasing attention due to their interesting semiconducting and optoelectronic properties and corresponding advantages over semimetallic graphene [1]. Typical preparation methods of high-quality samples are mechanical exfoliation and chemical vapor deposition (CVD). Work with TMDs is made easy by the fact that on SiO2 covered silicon, monolayer and few layer samples are clearly visible due to interference effects [2]. In this work we show that this effect persists at typical CVD growth temperatures of 700–900 degrees C and flakes are still visible if external illumination is stronger than the black body radiation. We designed miniaturized CVD system with optical access for real time microscopy that enables observation of TMDs during growth. This makes possible direct observation and measurement of nucleation and growth rates, morphology evolution, in situ etching and changes during cooling, which leads to guicker and easier optimization of growth conditions and recipes. Grown MoS2 and WS2 single layers, and vertically stacked bilayer heterostructures are further characterized by atomic force microscopy, Raman spectroscopy and photoluminescence emission to confirm their thickness and quality.

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Short-range ordering effects in binary and ternary B-C-N two-dimensional hexagonal structures in the presence of defects

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Boron and Nitrogen doped graphene layers constitute very important class of materials, mostly because B and N are natural dopants for carbon systems (pand n-type, respectively). At higher concentration of dopants, one should actually consider such systems as binary or ternary alloys. A fundamental issue for any alloy is the degree of ordering among its constituent atoms and to quantify the alloy position between its extreme phases (completely random alloy or perfectly ordered crystal). In our previous studies, it has been shown that binary $B_x C_{1-x}$ and $N_x C_{1-x}$ layered alloys constituting ideal honeycomb lattice exhibit (at least for the dopant concentration x ranging from 0 to 0.5, and temperatures up to 1500 K) rather pronounced short range order and deviate strongly from the random alloys. For ternary $B_x C_{1-x-y} N_y$ alloys, we observed formation of boron nitride domains surrounded by pristine graphene areas, which also indicates presence of short range ordering phenomena. Furthermore, we started investigating behavior of abovementioned structures containing typical for graphene internal defects, such as single and multiple vacancies, 5-7 Stone-Wales defects, grain boundaries. We extent our studies also to the systems with reduced periodicity just considering the alloyed nano-ribbons and platelets. In the present communication, we report the detailed studies of short range order in binary $B_x C_{1-x}$, and $N_x C_{1-x}$ alloys, and of ternary $B_x C_{1-x-y} N_y$ layered graphene based alloys containing defects and having full or reduced periodicity. Through the studies of energetics of the system, we determine first the thermodynamic equilibrium morphology of the studied systems and then we analyze short-range ordering, as quantified by the Warren-Cowley short-range order parameters. We focus on parameters corresponding to first, second, third and fourth coordination shell for each atom, that allow us to draw conclusions on the trends not only for nearest neighbors but also further relations within the lattice. This comprehensive analysis covers relevant range temperatures and is based on Monte Carlo (MC) calculations within the NVT ensemble employing Metropolis algorithm and Valence Force Field (VFF) approach to calculate the total energies of the of the system. We use Te rsoff like potentials for C, N, and B atoms with Matsunaga's parameterization [1]. We have also implemented into the computational algorithm the conjugate-gradient method to determine the equilibrium geometry. This turns out to be essential for systems containing edges and defects. To get reasonable statistics, we perform few dozen of Monte Carlo runs for each concentration of elements and temperature (with up to $2 \cdot 10^5$ MC steps per run), and perform simulations for temperatures up to 1500 K. Generally, the simulations for defected structures confirm the existence of the short range order in alloys (at least up to 1500 K) and the finding that the mixed C-N and B-N bonds are favorable for all dopant concentrations up to 50 %. A number of noteworthy effects in the defects' area is observed, and suggests that breaking the lattice symmetry disturbs locally distribution of species, and additionally this may impact concentrations of atoms in the whole alloy structure.

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Effect of polaronic charge transfer on band alignment at the Cu/TiO $_2$ interface

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We present a first principles investigation into the electronic properties of an extended interface between rutile TiO_2 and Cu. We show that owing to the highly polarizable nature of TiO_2 , the interface is unstable to the spontaneous formation of small electron polarons at the interface. The resulting dipole leads to an increase in the conduction band offset by 0.4 eV and the presence of a band of occupied states related to Ti d states 1.4 eV below the Fermi energy. This effect should be expected more generally at interfaces between highly polarizable oxides and metals but is missed by standard first principles approaches. Given the ubiquitous nature of such interfaces, this previously overlooked effect may have important implications for diverse applications across science and technology.

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Resistive Switching in All-Oxide Ferroelectric Tunnel Junctions with Ionic Interfaces

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Ferroelectric tunnel junctions have opened up promising routes towards energyefficient data storage applications and memristive devices [1]. Polarization reversal in a ferroelectric tunnel barrier can change the electrical resistance of a junction, a phenomenon known as tunneling electroresistance (TER). On the other hand, redox-based effects such as the migration of oxygen vacancies can cause large resistive switching in transi-tion metal oxides [2]. Here, we demonstrate nearly identical switching behavior in nominally symmetric tunnel junctions that are comprised of two La2/3Sr1/3MnO3 (LSMO) electrodes separated by a ferroelectric PbZr0.2Ti0.8O3 (PZT) or BaTiO3 (BTO) tunnel barrier, or a paraelectric SrTiO3 (STO) tunnel barrier [3]. Giant changes in electrical resistance with RH/RL ratios of up to 10^6 are measured on 20 nm LSMO/2.5 nm barrier/20 nm LSMO junctions, whereas the effect is substantially reduced for thicker barriers. The invariance of resistive switching with barrier material and its anomalous dependence on tunnel barrier thickness strongly point towards a redox-based effect that is not noticeably influenced by ferroelectric polarization in the barrier. From transmission electron microscopy measurements, it can be found that the bottom LSMO/barrier interface is atomically sharp, but that the top barrier/LSMO interface extends over three unit cells. Current-voltage characteristic and data fits based on models for direct tunneling and Fowler-Nordheim tunneling indicate that the redox-based mechanism leads to the formation of an insulating layer in the LSMO bottom electrode when a positive bias voltage is applied to the top electrode. This conclusion is independently verified by in-plane elect rical transport measurements on Hall bar structures. The following physical picture emerges from the experimental data: At positive bias voltage, oxygen vacancies migrate into the bottom LSMO electrode. This changes the valency of the Mn ions and enhances the electrical resistance. If enough oxygen vacancies migrate into the bottom electrode, a thin layer of LSMO next to the barrier becomes insulating, which leads to a giant increase of the junction resistance. Under negative bias voltage, the oxygen vacancies migrate back and the low resistance state is re-established. A similar sequence of events does not take place at the top LSMO/barrier interface because oxygen vacancy migration is hampered by structural roughness and atomic mixing. Electric-field induced oxygen migration is reduced for thicker tunnel barriers and this limits the resistive switching effect.

Fluorine clusters at CeO2(111) - A DFT+U and Monte Carlo study

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STM experiments on CeO2(111) reveal depressions in the surface oxygen sublattice which are observed to form clusters of various shapes and sizes [1]. While these depressions were assumed to be oxygen vacancies, subsequent DFT calculations have indicated that clusters of oxygen vacancies are energetically unstable [2-4]. Recently, we showed theoretically that fluorine impurities should appear almost identical to oxygen vacancies in STM experiments, but that their properties are more in line with those of the defects observed in experiments [5]. Here, I will present the results of a further investigation into the distribution of F impurity clusters at CeO2(111), using a combination of DFT+U calculations, and Monte Carlo sampling based on a simple but accurate pair potential which was fitted to the DFT results. The distribution is characterised in terms of the number of clusters of a certain size, and also on their topology, i.e. whether they are compact or open/linea r. Our results compare favourably with the experiments, and also exhibit some interesting physics in their own right.

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A Chemically Saturated 2D SiO_2 Sheet - Preparation, Structure and Transfer

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Two-dimensional (2D) materials hold immense potential for creating technological solutions at the nanoscale. But in order to be utilized successfully, 2D materials need to be stable under realistic conditions, as opposed to ultrahigh vacuum and low-temperature environments. Recently, a 2D SiO₂ sheet was prepared, which has an atomically flat surface and is fully chemically saturated.[1] The tetrahedral bulding blocks form complex networks with either hexagonal or amorphous topologies.

Scanning tunneling spectroscopy and density functional theory show that the 2D silica sheet has a band gap upwards of 6.5 eV, [2,3] which makes it a promising insulator that can complement conducting and semiconducting 2D materials in heterostacks. The key aspect in making 2D silica accessible for device building is sufficient material stability. We investigate the stability of 2D silica by imaging in a liquid-environment atomic force microscope.[4] Highresolution real space data reveal the same network structure that is observed in ultrahigh vacuum, highlighting the stability of this thin film.

Furthermore, we demonstrate a polymer-based transfer of the 2D silica film, characterized with scanning tunneling microscopy, low energy electron diffraction, and Auger electron spectroscopy.[5] During a transfer from the growth substrate Ru(0001) to a new Pt(111) substrate, the nanosheet maintains its morphology without any signs of damage. Characterization using environmental scanning electron microscopy shows that the silica sheet is transferred at the millimeter scale.

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Selective statistical analysis of MD simulations for vibrational spectroscopy modelling

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Infrared and Raman spectroscopy are amongst the most important characterization methods in the domain of nanoscience and nanotechnology. As the analysis of raw data requires careful decomposition of the output signal, modelling plays a crucial role identifying the various physical processes that contribute to the spectrum. The most used *ab initio* modelling techniques like DFT are limited by the computer time required to solve for systems with number of atoms having an order of magnitude of 2 or more.

We present an alternative approach based on the selective statistical analysis of molecular dynamics simulations to model the vibrational spectroscopy of nanostructures. We demonstrate this approach —besides having the obvious advantage regarding the calculation time and system size over *ab initio* methods— is also more relevant and applicable to realistic scenarios especially when one has to deal with systems prone to a lot of parameters like stress, distortion, charging, etc.

We adopt this approach to calculate the radial breathing mode frequencies of cycloparaphenylenes of various sizes and compare our results with DFT values and experimental observations. We also demonstrate a case where the anomaly at Raman response of a carbon nanotube under lateral stress can be succesfully elucidated using our approach.

Wednesday 15.02.2017

			chair: Jelinek
9:00	-	9:40	Charlier
			Electronic and optical properties of strained graphene and borophene
9:40	-	10:20	Facsko
			Nanomembranes Modified by Highly Charged Ions
10:20	_	10:40	Tagmatarchis
			Functionalization of exfoliated graphene with electron donors
10:40	-	11:20	Coffee
			chair: Kotakoski
11:20	-	12:00	Rosenwaks
			Electrostatically Formed Nanowires: a Novel Platform for Sensors, and Other Elec- tronic Devices
11:20	-	12:00	Djurabekova
			Formation Mechanism of Fe Nanocubes by Magnetron Sputtering Inert Gas Conden- sation
12:00	-	12:20	Remediakis
			Electronic structure of metal nanoparticles and metallic edges of 2D materials
12:20	-	12:40	Rinaldi
			Toxicity assessment of anatase and rutile titanium dioxide nanoparticles: The role of degradation in different pH conditions and light exposure.
12:40	-	13:00	Lajaunie
			Revisiting EELS Characterization and its Coupling with Raman Spectroscopy: Chemi- cal Inhomogeneities at the Nanoscale of DLC and Nanodiamond Thin Films
13.00	_	16.40	Lunch
16.40	_	17.00	Coffee
10.10	-	17.00	Conce
			chair: Swager
17:00	-	17:40	Hierold
			Device Architectures for Single Walled CNT Sensors and NO2 Measurement Results
17:40	-	18:00	Kretschmer
			Phase Transitions in Two-Dimensional Transition Metal Dichalcogenides under Elec- tron Beam
18:00	-	18:20	Carva
			The role of native defects and magnetic dopants in topological insulators $Bi_2 Te_3$ and $Bi_2 Se_3$
18:20	-	18:40	Abergel
			Topologically protected electronic transport in graphene, Älboron nitride heterostruc- tures
18.40	_	20.40	Posters
21.00	_	23:00	Dinner

Electronic and optical properties of strained graphene and borophene

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When passing an optical medium in the presence of a magnetic field, the polarization of light can be rotated either when reflected at the surface (Kerr effect) or when transmitted through the material (Faraday rotation). This phenomenon is known as a direct consequence of the optical Hall effect arising from the light-charge carrier interaction in solid state systems subjected to an external magnetic field, in analogy with the conventional Hall effect. The optical Hall effect has been explored in many thin films and also more recently in 2D materials. Here, an alternative approach based on strain engineering is proposed to achieve an optical Hall conductivity in graphene without magnetic field [1]. Indeed, strain induces lattice symmetry breaking and hence can result in a finite optical Hall conductivity. First-principles calculations also predict this strain-induced optical Hall effect in other 2D materials. Combining with the possibility of tuning the light energy and polarization, the strain amplitude and direction, and the nature of the optical medium, large ranges of positive and negative optical Hall conductivities are predicted, thus opening the way to use these atomistic thin materials in novel specific opto-electro-mechanical devices. Borophene, a recently synthesized two-dimensional monolayer of boron atoms, is expected to exhibit anisotropic metallic character with relatively high electronic velocities [2]. At the same time, very low optical conductivities in the infrared-visible light region have been reported. Based on its promising electronic transport properties and a priori high transparency, borophene could become a genuine LEGO piece in the 2D materials assembling game. Such early suggested properties demands for an in depth investigation of borophene electronic structure. Moreover, borophene is naturally degraded in ambient conditions and it is therefore important to assess the mechanisms and the effects of oxidation on borophene layers. Optical and electronic properties of pristine and oxidized borophene have been investigated using first-principles techniques [3]. Optical response of the oxidized layer is found to be strongly modified suggesting that optical measurements can serve as an efficie nt probe for borophene surface contamination.

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Nanomembranes Modified by Highly Charged Ions

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Smart membranes play a key role in different sensor applications, e.g. for drug and explosive detection. By tailoring the structure and properties of these membranes physical-chemical functionality can be added to the sensor. One way of modifying membranes is by particle irradiation with electrons or ions. Specifically, highly charged ions (HCI) carry a large amount of potential energy (the stored ionization energy) which is released when interacting with the membrane creating nanopores by a single HCI impact. In order to be able to control the ion induced modification, e.g. defining the pore size, the energy deposition in the membranes has to be determined.

For the interaction of HCl with thin membranes this is particularly interesting because the HCls are still in a pre-equilibrium interaction regime for thicknesses below a few nm. Within 1 nm thick carbon nano membranes (CNMs) for instance, holes are produced by the passage of highly charged Xe^{q+} ions only above a threshold in the potential energy of the HCl which depends on the kinetic energy [1]. In order to study the stopping force of the HCls in the membrane we examined the charge state and the energy loss of the Xe^{q+} ions after their passage through the CNM. Surprisingly, two distinct exit charge distributions were observed [2]. While some of the ions pass the membrane with almost no charge loss, other ions lose most of their charge. Apparently, the observed charge distribution reflects two different impact parameter regimes. The different impact parameter regimes are also connected to different energy losses: ions with large impact parameters are not stopped, w hereas ions in close collisions exhibit high stopping force which is strongly dependent on the incident charge state.

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Functionalization of exfoliated graphene with electron donors

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The rise of graphite exfoliation, pumping up graphene's chemistry, brings significant impact toward the preparation of novel hybrid materials combining the exceptional electronic properties of graphene sheets with those of photoinduced charge transfer phenomena from organic chromophores or semiconducting quantum dots interacting with the carbon nanostructure. Applications based on such charge transfer processes demand both defect-free graphene sheetsand chemical procedures for the covalent grafting or supramolecular decoration of the electron donors onto the sp2-honeycomb lattice of graphene.[1] Covalent chemistry of graphene leads to strong interactions between the electron donor and the graphitic skeleton, however, introduces defects at the anchoring sites, thus acting as insulators.[2, 3] On the other hand, when supramolecular interactions are utilized to integrate the electron donor moieties to graphene, the resulted ensembles although may suffer from weaker - interactions and the subsequent release of the donor units to the solution, [4] the extended aromatic lattice of graphene sheets remains intact and undisrupted, as no bond formation takes place, thus allowing for ballistic transport of charges with negligible loss of energy. Herein, the preparation and the photophysical properties evaluation of graphene-based ensembles, in which graphene sheets supramolecularly interact with porphyrins[4, 5], oligothiophenes[6], perylene diimides[7] and CdS quantum dots[8], will be presented.

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Electrostatically Formed Nanowires: a Novel Platform for Sensors, and Other Electronic Devices

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We present a new paradigm in nanowire based devices termed Electrostatically Formed Nanowires (EFN). The EFN is composed of a nanowire-like conducting channel that is not physically fabricated, but electrostatically formed post fabrication. The conductive channel is a doped silicon region surrounded by four gates: a back gate, two lateral junction gates, and a top dielectric that functions as a molecular gate. The size and shape of the EFN is defined and tuned by controlling the bias applied to the surrounding gates. We demonstrate the use of EFN for sensing of various gases including Ethanol, Acetone, and various n-alcohols and n-alkanes.[1] By electrically tuning the EFN diameter for a particular concentration range, the sensitivity as well as the overall dynamic range over which the sensor operates is highly enhanced; this tunable sensitivity is attributed to the nanowire size and shape controlled electrically.[2] It is also found, that in addition to polar target molecules, the EFN sensor is also capable of detecting non-polar alkanes, without any explicit additional surface treatment. The underlying mechanism responsible for the observed phenomena is attributed to interplay between the alcohol/alkane-silicon oxide interaction, induced surface EFN electric field and inherent molecular properties of our target species. We also demonstrate the application of the EFN to temperature sensing, multiple state transistors and other novel electronic devices.

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Formation Mechanism of Fe Nanocubes by Magnetron Sputtering Inert Gas Condensation

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Why do iron nanocubes form during condensation process instead of usual spherical or close-to-spherical shapes? It is counter-intuitive from the surface minimization considerations. We address this question by applying the combination of three different techniques: experiment, Molecular Dynamics and Kinetic Monte Carlo simulations. By these method we study kinetics of the formation mechanism of iron nanocubes. Our experiments as well as computer simulations indicate that the cubic shape of iron nanoparticles is explained by the difference in the kinetic growth modes of (100) and (110) surfaces, rather than the surface formation energetics. Our results are in good agreement between the different methods, showing that the final shape is defined by condensation temperature in combination with deposition rate. We present also the full deposition rate-temperature diagram of iron nanocluster shapes as well as an analytical model predicting the temperature and deposition rate evolution in nanoparticles. Combined together, the diagram and the model can be used to tune the desired final shape of the grown iron nanoparticles.

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Electronic structure of metal nanoparticles and metallic edges of 2D materials

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Gold nanoparticles and two-dimensional materials are among the most widelyused components of modern advanced materials. We present recent results from Density-Functional Theory (DFT) simulations for the quantum confinement and localization of electrons in such nanostructures. In all cases, we employ the free-software packes GPAW and ASE.

The equilibrium shape of nanoparticles can be calculated from first-principles with the use of the Wulff theorem and surface energies obtained from DFT calculations. The resulting shapes agree very well with microscopy images. Clean Au nanoparticles have truncated octahedral shape, while nanoparticles in CO ga have an almost spherical shape. As a general rule, stronger interactions between the nanoparticle and its host material result in higher sphericity [1]. Single-electron states are found in these nanoparticles by solving the well-known "particle-in-a-box" problem of quantum mechanics. The boundary condition is that the wavefunction is zero outside the nanoparticle. Apart from the well-known size-dependence of electron excitation energies, we find a strong shape-dependence for these quantum confinement levels. Therefore, the energy spectrum of a nanoparticle could be used as an indirect probe of its shape [2].

A similar analysis leads to new findings for the well-known problem of metallic edges on two-dimensional semiconductors. MoS_2 is found to possess metallic edges. Electrons are localized within 0.5 nm of the zigzag edge, and the energy of these states lies in the middle of the gap of the single-layer [3]. We repeat this calculation for different transition metal dichalcogenides, with different edge terminations and reconstructions, modeled by nanoribbons of variable width. In all cases, we find the same type of edge states that have k-dispersion and are truly metallic. We discuss the Fermi level pinning between the metallic phase at the edge and the semiconducting phase at the interior of the nanostructures.

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Toxicity assessment of anatase and rutile titanium dioxide nanoparticles: The role of degradation in different pH conditions and light exposure.

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Recently, development in nanotechnology has promoted the use of nanomaterials in many different fields. On other hand, increasing in the use of nanomaterials has led to release of these materials to the environment. Therefore, before employing these materials in biological and environmental and living systems, they should be evaluated in terms of biocompatibility and distribution. Although the toxic effects of nanomaterials on living organisms, human health and the environment have been studied by some researchers [1], however, there are too much uncertainty about the effects and mechanisms of toxicity of nanomaterials. The study of nanomaterial impacts on environment, health and safety (nanoEHS) has been largely predicated on the assumption that exposure and hazard can be predicted from and associated to physical-chemical properties of nanomaterials. Titanium dioxide nanoparticles (TiO_2NPs), in the two crystalline forms, rutile and anatase, have been widely used in many industrial fields, especially in cosmetics, and, more recently, in solar energy applications [2]. Therefore, a lot of details about their safety issues have been discussed by the scientific community. Many studies have led to a general agreement about TiO_2NPs toxicity, in particular for anatase form, but no mechanism details have been proved yet. In our study, data confirm the different toxic potential of rutile and anatase TiO_2NPs in two cell lines up to 5 nM nanoparticles concentration [3]. Moreover, we evaluated the role of titanium ions released by TiO_2NPs in different conditions, at pH = 4.5 (the typical lysosomal compartment pH) and at pH = 5.5 (the skin physiological pH) in conditions of darkness and light, to mimic the dermal exposure of cosmetics. Anatase nanoparticles were proner to degradation both in the acidic conditions and at skin pH. Our study demonstrates that pH and sunlight are dominant factors to induce oxidative stress, TiO_2NPs degradation and toxicity effects.

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Revisiting EELS Characterization and its Coupling with Raman Spectroscopy: Chemical Inhomogeneities at the Nanoscale of DLC and Nanodiamond Thin Films

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The long-term stability of the properties of hydrogenated amorphous carbon (a:C-H) thin films makes them very promising materials for numerous applications, including coatings for spatial applications [1]. For improving their performances, a full understanding of their local chemistry is highly required. Fifteen years ago, according to the seminal work of Ferrari et al., [2] EELS was the most used technique to get such kind of quantitative information on these materials. Nowadays, the complexity of the physics phenomena behind EELS is well known [3], but this technique is regarded as time-consuming and difficult to interpret properly. Other optical techniques, such as Raman spectroscopy, are now clearly favored by the scientific community. However, these macroscopic techniques still lack the high spatial resolution. This limitation can be overcome by STEM-EELS, which offers the possibility of getting direct chemical information at the local (atomic) scale.

In this contribution, we will revisit the procedures to extract proper and reliably quantitative chemical information from EELS spectra. In addition, the coupling of multi-wavelength Raman and EELS spectroscopies to obtain a wealth of chemical information will be discussed. Our results provide a complete combination of C-hybridization, spatial elemental analyses and structural defects studies for shedding light on these complex materials. In particular, we will show how the deposition process induces a gradient of sp² ratio in the thin films and how this gradient is modified as a function of the annealing time [4]. In addition, recent results on nanocrystalline and microcrystalline CVD diamond films will be presented [5]. Surprisingly, strong in-depth inhomogeneities of the local chemistry has been highlighted and the evolution of the morphology, nanostructure and composition of the films, as a function of methane in excess of hydrogen, will be discussed.

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Device Architectures for Single Walled CNT Sensors and NO2 Measurement Results

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We report on the concept of applying single walled carbon nanotube field effect transistors (SWNT FETs) as functional building blocks in gas sensors. Advances in the device architecture, fabrication processes as well as better understanding of the behavior of SWNT FETs has enabled the vision of using individual-tube devices directly for NO2 gas sensors [1]. Significant progress has been made in understanding the sources of drift and hysteresis, and techniques have been introduced to counteract. Reducing the presence of process residues and dielectrics close to the SWNT to the best possible level leads to the suppression of hysteresis and significant improvement in the noise performance [2, 3, 4] as well as improvement in the cross-sensitivity to humidity [5]. Suspended devices are also attractive for self-heated, ultra-low-power architectures [6].

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Phase Transitions in Two-Dimensional Transition Metal Dichalcogenides under Electron Beam

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Recently a phase transition from the hexagonal 1H to trigonal distorted 1T'phase in two-dimensional (2D) MoS_2 has been induced by electron irradiation [1]. Using density functional theory calculations, we study the energetics of these stable and metastable phases when electric charge, mechanical strain and vacancies are present. Based on the results of our calculations, we propose an explanation for this phenomenon which is likely promoted by charge redistribution in the monolayer combined with vacancy formation due to electron beam and associated mechanical strain in the sample. We further show that this mechanism can be extended to other 2D transition metal dichalcogenides.

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The role of native defects and magnetic dopants in topological insulators $Bi_2 Te_3$ and $Bi_2 Se_3$

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Magnetic doping is a way to add novel functionality to topological insulators [1], as well as a test of stability of topological properties. We calculate on ab initio level electronic structure of Bi2Te3 and Bi2Se3 doped by Mn at different possible positions in the lattice and also in the presence of native antisites. This provides for the first time a comprehensive map of possible behavior affecting strongly the bulk resistivity, carrier concentration and magnetism [2]. Density of states calculations reveal in which case the Fermi level lies at low conducting impurity Mn peak and which effects shift it. This allows us to tune the bulk resistivity, and also help to uncover the location of Mn atoms. Concentration dependence of resistivity exhibits significant difference between substitutional or interstitial Mn position, the resistivity for pure substitutional doping is significantly higher. Calculations indicate that at least two of the considered defects have to be present simultaneously in order to explain the observations, and the role of interstitials may be more important than expected. Exchange interactions between the Mn magnetic moments in bulk Mn-doped Bi2Se3 and Bi2Te3 have been calculated using ab initio methods. From these ferromagnetic Curie temperature and other magnetic magnetic properties are systematically studied by means of atomistic Monte Carlo simulations. Curie temperatures are shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [2].

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^[1] Y. S. Hor et al., *Phys. Rev. B* 81, 195203 (2010).

Topologically protected electronic transport in graphene-boron nitride heterostructures

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Graphene nanoribbons have been suggested for use as nanoscale conducting wires which could connect devices in an integrated circuit. Implementing this would be highly advantageous for fabrication of such circuits. However, lattice scale disorder was shown to be prohibitively detrimental to the transport properties of such nanoribbons. In this talk, we show that topological protection generated by lateral heterostructures of graphene with hexagonal boron nitride can circumvent this difficulty, and the transport through such heterostructures is remarkably robust against all the common forms of lattice scale disorder created by contemporary fabrication techniques. This reopens the possibility of utilizing graphene ribbons as chip-scale conducting wires.

[1] D.S.L. Abergel, arXiv preprint 1609.01608 (2016).

Thursday 16.02.2017

10:00	-	10:40	chair: Facsko Ottaviano Response to oxidising and reducing gases of 2D materials: Graphene oxide, ${\sf MOS}_2$ and ${\sf WS}_2$
10:40	-	11:20	Coffee
			chair: Haigh
11:20	-	12:00	Haluska
			Improved contacts for individual SWCNT based CNFETs
11:20	-	12:00	Hofer
			Isotope analysis in the transmission electron microscope
12:00	-	12:20	Flores-Livas
			Emergence of superconductivity in doped H ₂ O ice
12:20	-	12:40	Umek
			Tunning Titanium Oxynitride Nanoribbons Conductivity Properties: Synthesis and Characterization
12:40	-	13:00	Legut
			Importance of the electron correlations and spin-orbit coupling for lattice dynamics of \ensuremath{UC}
13:00	_	16:40	Lunch
16:40	-	17:00	Coffee
			chair: Ottaviano
17:00	_	17:40	Bøggild
			Perfect and imperfect graphene for gas sensing
17:40	_	17:50	Closing

Response to oxidising and reducing gases of 2D materials: Graphene oxide, MOS_2 and WS_2

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2D materials are inherently "all-surface-materials", therefore they offer the ultimate surface/mass ratio among low dimensional materials. For this reason they are excellent candidates for the fabrication of gas sensing devices. In this paper we review the gas sensing response of various 2D materials (graphene oxide [1,2], chemically exfoliated MoS₂ [3], WS₂ [4] and phosphorene [5]. The gas sensing response, is discussed on the basis of a thorough study of the morphological and chemical properties of the 2D materials used.

[1] S. Prezioso et al., J. Phys. Chem. C 117, 10683 (2013).

[2] M. Donarelli et al., 2D materials 2, 035018 (2015).

[3] M. Donarelli et al. , Sensors & actuators 207, 602 (2015).

- [4] F. Perrozzi et al. , *unpublished.* —, (2017).
- [5] M. Donarelli et al., 2D materials 3, 025002 (2016).

Improved contacts for individual SWCNT based CNFETs

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This talk will focus on a novel fabrication flow for field-effect transistors with individual SWCNT channels (CNFETs) having electrical contacts with long lifetime and narrow distribution of device on-resistances. The approach is based on combination of a sacrificial layer protecting as-grown SWCNTs during CN-FETs fabrication process, plasma oxidation to remove photo or e-beam resist residuals from contact areas, and deposition of optimized thickness of the Cr adhesion layer prior to noble metal deposition for electrical contacts. As grown SWCNTs are covered by Al2O3 sacrificial layer deposited by atomic layer deposition (ALD) to prohibit their direct contact to resist [1] and to protect them from oxygen plasma impact during further processing. Al2O3 layers thicker than 18 nm protect SWCNT sufficiently from the impact of one minute applied 100 W oxygen plasma as we proved by CNFET electrical measurements and SWCNT Raman spectroscopy. The sacrificial alumina layer is then removed by hot H3PO4 prior to formation of electrical contacts. We have shown [1,2] that utilization of this protective/sacrificial layer greatly improves the cleanliness of nanotube surfaces in respect to resist residuals without detectable change of their original properties. The median on-resistance for alumina passivated, Pd/Au-contacted CNFETs reached 190 kOhm which is nearly 3x lower value than the one of CNFETs prepared without using sacrificial layer and oxygen plasma [2]. Imortantly, the inter-quartile dispersions of the CNFETs on-resistance were narrowed from 2050 to 247 kOhm. We observed long lifetime of devices prepared by this fabrication approach (longer as 90 days) even for non-passivated CNFETs using Cr layer thinner than 2 nm in Cr/Au contacts [3].

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[2] W. Liu, et al., Phys. Status Solidi B 1-7, xxx (2016).

[3] W. Liu, et al., Nanotechnology 27, 015201 (2016).

Isotope analysis in the transmission electron microscope

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Recent advances in aberration-corrected scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy have allowed the identity and bonding of individual atoms to be determined in two-dimensional materials such as graphene. However, discerning the isotopes of a particular element has not yet been possible. Isotopes of carbon, in particular, have proven invaluable for archeology through radiocarbon dating, and in materials science, isotope labeling is a powerful tool for understanding chemical vapor deposition.

Here we differentiate between two isotopes of the same element by quantifying how likely the energetic imaging electrons are to eject atoms. Our technique rests on a crucial difference between electrons and photons when used as a microscopy probe: due to their finite mass, electrons can transfer significant amounts of momentum. When the transferred energy is comparable to the energy required to eject an atom from the material when probing pristine or doped single-layer graphene with 60-100 keV electrons, atomic vibrations need to be included for the correct description of the process. We measure the displacement probability in graphene grown from either 12 C or 13 C and describe the process using a quantum mechanical model of lattice vibrations coupled with density functional theory simulations. We then test our spatial resolution in a mixed sample by ejecting individual atoms from nanoscale areas spanning an interface region that is far from atomically sharp, mappi ng the isotope concentration with a precision better than 20%.

Although these results were achieved with graphene, our technique should work for any low-dimensional material, including hexagonal boron nitride and transition metal dichalcogenides such as MoS_2 . This could potentially extend to van der Waals heterostructures of a few layers or other thin crystalline materials, provided a difference in the displacement probability of an atomic species can be uniquely determined.

[1] Susi, Hofer et al., Nat. Commun. 7, 13040 (2016).

Emergence of superconductivity in doped H₂O ice

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In my talk I will show that for realistic levels of doping, the covalent phase X of ice becomes superconducting with a critical temperatures of about 60 K under pressure. The throughout of the investigation points out to the possibility of achieving high-temperature superconductivity in hydrides under pressure by inducing metallization of otherwise insulating phases through doping, a path previously used to render standard semiconductors superconducting at ambient pressure. We have taken H₂O as testbed, one of the most abundant and wellstudied substances in the universe, and identify nitrogen as the most likely and promising substitution/dopant. Furthermore, I will discuss a possible path to reach the synthesis of the nitrogen doped ice-X and the superconducting state, which consists in starting from a similar synthesis to what is used to obtain H_2+H_2O clathrates, and then induce defect oxygen vacancies at moderate pressures. In view of the vast number of hydrides that are strongly covalent bonded, but that remain insulating up to rather large pressures, our results open a series of new possibilities in the quest for the so dreamed room-temperature superconductor.

Tunning Titanium Oxynitride Nanoribbons Conductivity Properties: Synthesis and Characterization

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Transition metal oxynitrides are important functional materials for a wide spectrum of applications such as photocatalysts, pigments, dielectric and magnetic materials. They can combine the properties of transition metal oxides and nitrides, and are typically prepared thermally by nitridation of metal oxide where nitrogen or ammonia gases are used as a nitrogen source. The substitution of oxide anions with nitride ones in metal oxides enables the fine tuning of oxynitride properties.

In our work, this paradigm was applied to formation of titanium oxynitride (Ti(O,N)) nanoribbons, transformed from hydrogen titanate (H2Ti3O7) nanoribbons by heating in a dynamic ammonia atmosphere. The effect of reaction conditions, NH3(g) flow and reaction time, on magnetic properties, resistivity and morphology of the prepared samples was investigated. Structural and morphological properties of the products were characterized with X-ray diffraction and electron microscopy techniques (TEM, SEM, HRTEM). Elemental composition was determined by means of X-ray photoelectron spectroscopy. Magnetic properties of the products were measured with a SQUID magnetometer, while the temperature dependence of the resistivity of individual nanoribbons was measured with a four point method.

The transformation of H2Ti3O7 to Ti(O,N) proceeds in two stages, first H2Ti3O7 transforms to TiO2 and in the second stage the nitridation stage é TiO2 converts to Ti(O,N). As revealed by SEM images the nanoribbon shape stays preserved but the nanoribbons became porous. The appearance of porosity could be a consequence of the Kirkendall effect. The nitrogen content, which determines the chemical disorder through random O/N occupancy and ion vacancies in the Ti(O,N) composition, increases with the reaction time. The presence of disorder has paramount effect on resistivity of Ti(O,N) nanoribbons.

Atypically for metals, the resistivity increases with decreasing temperature due to the weak localization effects. From this state, superconductivity develops below considerably or completely suppressed critical temperatures, depending on the disorder strength. Our results thus establish the remarkable versatility of anion exchange for tuning of the electronic properties of Ti(O,N) nanoribbons and suggest that similar strategies may be applied to a vast number of nanostructures. (1)

 M. Sluban, P. Umek, Z. Jaglicic, J. Buh, P. Smitek, A. Mrzel, C. Bittencourt, P. Guttmann, M.-H. Delville, D. Mihailovc, D. Arcon, ACS Nano 9, 10133 (2015).

Importance of the electron correlations and spin-orbit coupling for lattice dynamics of UC

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Uranium monocarbide, a potential fuel material for the generation IV reactors, is investigated within density functional theory. Its electronic, magnetic, elastic, and phonon properties are analyzed and discussed in terms of spin-orbit interaction and localized versus itinerant behavior of the 5f electrons. The localization of the 5f states is tuned by varying the local Coulomb repulsion interaction parameter. We demonstrate that the theoretical electronic structure, elastic constants, phonon dispersions, and their densities of states can reproduce accurately the results of x-ray photoemission and bremsstrahlung isochromat measurements as well as inelastic neutron scattering experiments only when the 5f states experience the spin-orbit interaction and simultaneously remain partially localized. The partial localization of the 5f electrons could be represented by a moderate value of the on-site Coulomb interaction parameter of about 2 eV. The results of the pres ent studies indicate that both strong electron correlations and spin-orbit effects are crucial for realistic theoretical description of the ground-state properties of uranium carbide. [1] We compare the novel material to the at presence used most common nuclear fuel material, UO_2 oxide. Here are calculations show that considering the exchange and electron correlations effects the generalized gradient approximations was succesfully in descrption of the phonon dispersion spectrum, thermal expansion, and heat capacity w.r.t to the recorded data.[2] For both materials the so-called direct method, based on the quasiharmonic approximation, was used. To study the pressure dependence of the phonon frequencies of UO_2 we calculate phonon dispersions for several lattice constants. Our computed phonon spectra demonstrate the opening of a gap between the optical and acoustic modes induced by pressure. Taking into account the phonon contribution to the total free energy of UO_2 it s thermal expansion coefficient and heat capacity have been computed from first-principles. Both quantities are in good agreement with available experimental data for temperatures up to about 500 K.

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[2] Y. Yun et al. , J. Nucl. Mater. 426, 109 (2012).

Perfect and imperfect graphene for gas sensing

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For many graphene and 2D material applications (such as electronics), imperfections are systematically hunted down and eliminated, through meticulous materials selection and synthesis, careful assembly of van der Waals heterostructures, and highly optimised cleaning procedures and device processing. Our recent "hot pickup" method allows batch fabrication of clean van der Waals heterostructures with a great flexibility in device architecture, including ultradense patterning with moderate performance penalty. For gas sensing, "defects" and "contamination" may play a beneficial role as active binding sites and functionalisation. Nanopatterning has been demonstrated to significantly improve the detection limit of chemiresistive graphene sensors, and may also provide a key to obtaining selectivity between different gas species. Graphene patterned by block copolymer lithography was used to achieve ppt-level detection limit for NO2 gas. While disorder seems to have a bene ficial effect, the need for reproducibility, selectivity and control in real applications, as well as the need for understanding the sensing mechanisms better, suggests that the ability of making perfect graphene devices, may be still be a key issue for graphene based gas sensing.

Posters

Abdul Wajid Awan Electrical properties of CVD Molybdenum disulfide Ekaterina Baibuz Electric field effect on the growth mechanism of nano-tips on metal surfaces Alexander Bakaev Trapping of hydrogen and helium at dislocations in tungsten: an ab initio study Ionathan Bean Atomic structure and electronic properties of MgO grain boundaries in tunnelling magnetoresistive devices Carla Bittencourt Wireless Connected Carbon Nanotubes Sensors Chris Ewels Functionalising transition metal dichalcogenide monolayers: towards gas detection Valentin Freilikher Total disorder as an alternative to perfect periodicity Christoffer John Patrik Fridlund Formation of Meta-Stable SiO_x by Ion Beam Mixing for Self-Assembly of a Si Nanodot Seyed Arsalan Hashemi Petrudi Phonon in single-layer transition metal trichalcogenides Eero Holmstrom Adsorption of H₂O onto SrTiO₃ from DFT, hybrid-functional DFT, and MP2 Anne Holtsch Analysis of local variations of the electronic properties of mono- and bilayer graphene/HOPG Anne Holtsch Analysis of Atomic Moiré patterns on Graphene/Rh(111) Stefan Hummel Mechanical and Electrical Study of 2D materials by novel Dual-Probe Atomic force- /Scanning tunneling microscope Sampo Inkinen In-situ TEM Observation of Oxygen Vacancy Driven Structural and Resistive Phase Transitions in La_{2/3}Sr_{1/3}MnO₃ Federico Iori Engineering SrTiO3/LaAlO3 heterostructures thickness: an ab initio study Marc Jäger Describing MoS2 Nanoclusters with Classical Potentials Elvar Örn Jónsson Self-interaction corrected energy functionals and Pipek-Mezey orbital localization Shawulienu Kezilebieke Local Electronic Structure of a Magnetic Dimer Impurity in a Superconductor Byung-Hyun Kim Multiscale modelling of CeO₂ nano-interfaces Franciszek Krok Formation of hexagonal gold nanostructures during self-assembling on Ge(001) surface

Artem Kuklin
Theoretical Prediction of One-Atom-Thick Hexagonal CrN: Electronic Structure and Magnetic Properties
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A general computational method for electron emission and thermal effects in field emitting nanotips
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Nanoripples production on a-Si surfaces under Ar irradiation
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Study of carbon nanostructures generated by gamma irradiation of graphene flakes on nickel
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Usage of carbon nanotubes
Mildred Quintana
Graphene processing towards applications
Isaac Tamblyn
First principles training sets and atomistic potentials for boron-nitride nanostructures
Dmitry Terentyev
Carbon-vacancy complexes controlling nano-scale irradiation damage in iron and steels
Camilla Tossi
Conversion of light for the production of fuels using cell factories
Henrique Vazquez Muinos
Creating nanoporous graphene with swift heavy ions
David Visontai
Controlling Josephson current with topological states in bilayer graphene
Lide Yao
In-Situ Transmission Electron Microscopy of Functional Materials
Junle Zhao
Multi-step growth and emission mechanism in matrix assembly cluster source
Shengqiang Zhou
Colossal Enhancement in Magnetic Moment of Ferrimagnetic NiCo2O4 via Strain-Doping

Electrical properties of CVD Molybdenum disulfide

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Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS2oS2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.8eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS2oS2 on SiO22 /Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS2oS2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectro scopy techniques, respectively, which confirm that the thickness of the CVD grown MoS2oS2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

Electric field effect on the growth mechanism of nano-tips on metal surfaces

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Surface evolution of metals operated under the electric field is particularly interesting to the wide range of applications. Recent experiments showed that femtosecond laser irradiation of a sharp tungsten tip exposed to strong DC electric field leads to gradual and reproducible surface modifications[1]. Asymmetric surface faceting mainly on the laser-exposed side along with the formation of a few nanometers high nano-tip were observed. A metallic nano-tip with sharpness of a few nanometers, can be highly beneficial for many applications such as electron diffraction, microscopy, and holography. Therefore, investigation of the influence of electric field on surface evolution of metals may be an important input for finding technological solutions of nano-tip fabrication process.

The growth of nano-tips under intense fields is also of potential importance to the particle accelerator community. Strong rf-field, such as planned to use in the Compact Linear Collider (CLIC) at CERN, Switzerland [2], may induce the formation of nano-tips on the surface of copper accelerating structures. Shortlived nano-tips are believed to cause vacuum arcs, which significantly decrease the efficiency of the accelerator.

In order to research the mechanism of nano-tip growth, the long time scale atomic diffusion should be taken into account. We have recently developed a Kinetic Monte Carlo (KMC) model of surface diffusion for fcc and bcc metals[3]. This KMC model has to be parameterized for a material under study in terms of migration energy barriers and attempt frequencies for all possible diffusion jumps. In order to extend the KMC model with electric field, its effect on the energy barriers of the migrating atoms should be researched.

In this work, we used DFT nudged elastic band (NEB) simulations to find the minimum energy paths of the diffusion processes on W surface under electric field. We also used DFT calculations to find dipole moments and polarisabilities of adatoms on W and Cu surfaces. The KMC model was used to simulate the nano-tip growth on faceted W surface under electric field.

^[1] H. Yanagisawa, V. Zadin et al., APL Photonics 1, 091305 (2016).

^[2] V. Jansson, E. Baibuz, F. Djurabekova, Nanotechnology 27, 265708 (2016).

^[3] CLIC and Boland, MJ and Felzmann, U and Giansiracusa, PJ and Lucas, TG and Rassool, RP and Balazs, C and Charles, TK and Afanaciev, K and Emeliantchik, I and others, CERN Yellow Reports 4, 0 (2016).
Trapping of hydrogen and helium at dislocations in tungsten: an ab initio study

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Retention of plasma gas components such as hydrogen (H) isotopes and helium (He) is one of the limiting factors in selection of plasma facing materials for future thermonuclear fusion devices. Tungsten (W) is one of the promising candidates for such materials and was chosen for the divertor armor for International Thermonuclear Experimental Reactor (ITER) and the first wall material for design of demonstrational fusion power plant DEMO. For the analytical estimation of accumulation of H/He components in tungsten, it is important to understand the relevant physical mechanisms of their trapping in the material and thoroughly parameterize them numerically. Experiments involving high flux plasma exposure of tungsten at the temperature below 500 K conclude on the significant amount of retained hydrogen, which unlike helium, does not agglomerate in the form of clusters in the bulk defect-free material. The observed hydrogen isotope trapping and deep diffusion is conventionally attributed to the trapping at the natural lattice defects such as dislocations and grain boundaries. Computational assessment of trapping strength and capacity of the dislocations is the subject of this work. Here, the electronic structure calculations using density functional theory (DFT) are done to evaluate the affinity of hydrogen and helium to the screw and edge dislocations. For this, we calculate the interaction energy map around the dislocation core for hydrogen and helium atoms. The energetically favorable positions are rationalized on the basis of charge density distribution and local stress concentration. The results obtained help to refine the input parameters of macro-scale models of retention of plasma components, such as mean field rate theory methods. The additional molecular statics simulations are also performed to analyze whether the contemporary atomistic models using the recently developed interatomic potentials for W-H-He system can grasp adequately the interaction of H and He with dislocations.

Atomic structure and electronic properties of MgO grain boundaries in tunnelling magnetoresistive devices

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Polycrystalline metal oxides find diverse applications in areas such as nanoelectronics, photovoltaics and catalysis. Although grain boundary defects are ubiquitous their structure and electronic properties are very poorly understood since it is extremely challenging to probe the structure of buried interfaces directly. In this paper we combine novel plan-view high-resolution transmission electron microscopy and first principles calculations to provide atomic level understanding of the structure and properties of grain boundaries in the barrier layer of a magnetic tunnel junction. We show that the highly [001] textured MgO films contain numerous tilt grain boundaries. First principles calculations reveal how these grain boundaries are associated with locally reduced band gaps (by up to 3 eV). Using a simple model we show how the shunting a proportion of the tunnelling current through grain boundaries imposes limits on the maximum magnetoresistance that can be achi eved in devices.

Wireless Connected Carbon Nanotubes Sensors

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There is a growing interest in the development of smart global systems of wireless, distributed sensors that can be deployed and then operated with no human intervention. However, there are still important technological barriers related to sensor performance and power consumption that limit the implementation of such systems. Taking the example of carbon nanostructures, we show that nanotechnology could help overcome these barriers. Oxygen plasma treatment has been used to functionalize, in a controlled way, the outer walls of multiwalled carbon nanotubes fine tuning their sensing properties towards nitrogen dioxide. This treatment respects the integrity of carbon nanotubes but gives rise to carbonyl groups grafted at their sidewalls, which greatly enhance the room-temperature sensitivity and selectivity of the nanomaterial to nitrogen dioxide. Sensing at near room-temperature reduces power consumption. The detection mechanism of nitrogen dioxide in the presence of ambient moisture is discussed in light of computational modelling, compositional characterisation and gas sensing tests [1]. The optimized nanomaterial has been used to develop a semi-passive radio frequency identification tag with the capability of sensing nitrogen dioxide in the environment. The tag, which is read by a low-cost commercially available ultra-wideband radar, is normally in sleep mode and includes a wake-up circuit, so power consumption is minimised. This wireless sensor is able to reproducibly detect nitrogen dioxide concentrations from 10 ppm to 100 ppm, with a mean relative error of 0.29%.

 P. Clément, A. Ramos, A. Lazaro, L. Molina-Luna, C. Bittencourt, D. Girbau, E. Llobet, Sens. Act. B: Chem. 208, 444 (2015).

Functionalising transition metal dichalcogenide monolayers: towards gas detection

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We explore through a combination of DFT modelling and experimental synthesis and characterisation different covalent and physisorption strategies for functionalising transition metal dichalcogenide monolayers (MoS_2 , WS_2 , ...). We demonstrate differences in behaviour, notably preferential edge-site functionalisation for covalent attachment, and basal-plane stacking for polyaromatic physisorbed species. Such species significantly modify TMD behaviour under laser irradiation, and point the way towards chemical modification of TMDs for advanced gas detection.

This work is performed in collaboration between the IMN Nantes, National Hellenic Research Institute in Athens, and Instituto de Nanociencia de Aragón, Zaragoza, within the framework of the H2020 ITN network No 642742 "Enabling Excellence". For more details see eetraining.wordpress.com

Total disorder as an alternative to perfect periodicity

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Creation of new optical tunable elements is nowadays an important area of research and nanotechnology. Photonic crystals are promising candidates for this purpose. However, even small random deviations from periodicity could affect significantly their optical characteristics. Considerable effort and creativity have therefore been invested to develop highly periodic dielectric systems. Alternatively, for many applications it may be possible to utilize disordered samples as tunable narrow-line resonant elements. In this talk, we will give a brief introduction to the physics of the light transport in random media, and will present the results of the most recent theoretical and experimental studies of the quasi-normal states (resonances) in one-and two-dimensional disordered structures. We will show how the unique spectral properties of these structures could be harnessed to create and couple resonant micro-cavities, control light transport and spontaneous emission, etc .

Formation of Meta-Stable $\text{SiO}_{\rm x}$ by Ion Beam Mixing for Self-Assembly of a Si Nanodot

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The ever-expanding "Internet of Things" requires more power efficient components and devices to keep up with the need of the users. Single electron transistors (SET) are promising for this purpose, with very low energy consumptions. Nanometer-sized quantum dots are needed for the SET to work at room temperature. A reliable method of producing the needed nanodots, is through controlled self-assembly during phase-separation in restricted volumes of meta-stable SiO_x.

Here, we present a comprehensive computer simulation model on the formation of SiO_x restricted volumes by ion beam mixing of Si into a thin SiO_2 layer embedded in Si. Systems with both one and two interfaces to the adjacent Si layers have been used in the simulations. Atomic cascades, initiated subsequently by thousands of energetic Si⁺ ions in a volume of approximately 15x15x7 nm³, are needed to provide sufficient mixing of Si recoil atoms into SiO₂, for self-assembly of the 2-3 nm wide quantum dots.

The formation of the meta-stable SiO_x volume was simulated with an accelerated molecular dynamics (MD) method. The interactions of the Si⁺ ions with the Si and O atoms were handled by splining a universal ZBL potential to a Munetoh potential. The system was connected to a heat bath by having a Berendsen thermostat controlling the border atoms during the cascades. The intermixing of Si into SiO₂ layer from both interfaces due to forward- and back-scattering during development of atomic cascades was analyzed in detail (only forward-scattering in the single interface system). The resulting concentration profiles of SiO_x from our MD model was used for phase-separation simulations by kMC model.

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Phonon in single-layer transition metal trichalcogenides

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We investigate the phonon dispersion relations, Raman and Infrared (IR) spectra of two dimensional (2D) MPX3 (M = Zn, Cd, Mn and X = S, Se) transition metal chalcogenophosphates. We also discuss the character tables of all materials in detail to present more information about the behavior of active modes.

Adsorption of H_2O onto $SrTiO_3$ from DFT, hybrid-functional DFT, and MP2

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For the past two decades, the standard quantum-mechanical approach to modeling adsorption of molecules onto surfaces has been density functional theory (DFT). At the same time, it has become clear that the result of a DFT calculation of such an adsorption process can be very sensitive to how the computation is set up, i.e., the choice of exchange-correlation functional, dispersion correction, and other ingredients such as a Hubbard +U correction for systems containing transition metals. Choosing the adsorption of water onto the prototypical metal-oxide photocatalyst SrTiO₃ as an example, we use DFT, hybrid-functional DFT, and the wavefunction-based MP2 method to break beyond the DFT-based paradigm. Through our results, we assess the accuracy of semi-local and non-local DFT and established dispersion corrections to these in describing the water-metal-oxide interaction. In addition, we probe general implications for the first-principles modeling of surface reacti vity.

Analysis of local variations of the electronic properties of mono- and bilayer graphene/HOPG

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Cleaving a HOPG bulk material can occasionally result in formation of graphene. Compared to other substrates HOPG has the advantage that occurring Moiré patterns solely have their origin in rotation of the graphene lattice with respect to the HOPG lattice orientation. We investigate the topography of the Moiré superstructure by scanning tunnelling measurement (STM) and changes of the electronic properties of graphene induced by the Moiré pattern and variation in amount of graphene layers using scanning tunnelling spectroscopy (STS). The formation of a Moiré pattern goes along with corrugation of the graphene sheet. This is the case for monolayer graphene (rotation with respect to the substrate) and bilayer graphene (rotation of both layers with respect to each other). STM measurements of bilayer graphene where both layers are aligned without rotation but the system itself is rotated towards the substrate do not show any corrugation. A possible Moiré pattern in the lower layer does not permeate to the top layer leading to the conclusion that the occurrence of a Moiré pattern is an effect restricted to the topmost graphene layer. Scanning tunnelling spectroscopy shows that the hopg substrate strongly influence the electronic properties of the graphene layer. In a monolayer graphene with corrugation due to a Moiré pattern the distance of the graphene layer to the substrate adjusts the size of a band gap opening. For small distance the monolayer can behave bilayer-like. With increasing distance the size of the band gap decreases. STS on bilayer graphene reveals that the HOPG surface layer have to be assumed as an additional graphene-like layer for low bias voltages. For higher bias voltages the graphene/HOPG system is dominated by the HOPG contributions.

Analysis of Atomic Moiré patterns on Graphene/Rh(111)

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Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate superstructures that originate from the different lattice parameters of the graphene and the substrate. The resulting vertical corrugation of the graphene within a Moiré unit cell is the consequence of strain and electronic interaction between graphene and the Rh(111). Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. The lattice constant of the superstructure depends on the rotation angle of the graphene layer with respect to the Rh(111) substrate. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. Scanning tunnelling spectroscopy measurements reveal a dependency of the local density of states on the hybridization of π orbitals of the graphene with the d band of Rh(111). This results in characteristic spectroscopic fingerprints of the individual symmetry points.

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Mechanical and Electrical Study of 2D materials by novel Dual-Probe Atomic force- /Scanning tunneling microscope

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Scanning probe microscopy (SPM) techniques are one of the most important experimental methods within the field of Surface- and Nanosciences. Since one can, in principle, obtain topographic information and spectroscopic data with atomic resolution at the same time, SPM techniques are also an invaluable tool within the relatively new field of low-dimensional materials. However, when dealing with suspended 2D materials (e.g. graphene, MoS_2 , etc.), interpretation of the measured data is very complicated, since the tip sample interaction is also changing the topography of the membrane. In this work, I will show recent results of a novel type of Dual-Probe AFM (Atomic force microscope)/STM (Scanning tunneling microscope) measurement, where the two probes approach a suspended membrane from opposite sides. Having the STM tip in tunneling distance to the membrane, we were able to investigate its dynamical response as a function of the position of the cantilever of the AFM. This provides insight into the interaction of the tip and the membrane . Additionally, we observed local deformations of 2D materials caused by an approaching STM tip, while performing AFM measurements on the same site. Furthermore, operating the device in STM/STM mode, we can explore electrical properties of suspended membranes and perform transport measurements at arbitrarily close distances of the two probes.

In-situ TEM Observation of Oxygen Vacancy Driven Structural and Resistive Phase Transitions in $La_{2/3}Sr_{1/3}MnO_3$

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Oxygen defects can have a profound effect on the physical properties of transition metal oxides. Electric-field driven migration of oxygen vacancies provides a viable mechanism for the formation, rupture and reconstruction of conducting filaments in insulating oxides, an effect that is used in nanoscale resistive switching devices [1,2]. In complex oxides where magnetic, ferroelectric and superconducting phases emerge from strong correlations between localized transition metal valence electrons, oxygen vacancies can radically alter a plurality of intrinsic properties via valence changes and structural phase transitions [3]. The ability to reversibly control the concentration and profile of oxygen vacancies in oxide nanostructures would thus open up comprehensive prospects for new functional ionic devices. Advancements in this direction require experimental techniques that allow for simultaneous measurements of oxygen vacancy dynamics, atomic-scale structural effects and macroscopic physical properties. Here, we use nanoprobing *in-situ* transmission electron microscopy (TEM) to demonstrate reversible switching between three distinctive resistance states in an epitaxial La_{2/3}Sr_{1/3}MnO₃ film. Simultaneous high-resolution imaging and resistance probing indicate that the switching events are caused by fast and uniform growth of new structural phases. Reversible migration of oxygen vacancies within the manganite film and between the film and Nb-doped SrTiO3 substrate, driven by combined effects of Joule heating and bias voltage, triggers the structural and resistive transitions. Our findings open prospects for ionotronic devices based on dynamic control of physical properties in complex oxide nanostructures.

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Engineering SrTiO3/LaAlO3 heterostructures thickness: an ab initio study

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The possibility to achieve conducting and superconducting properties at the interface between two bulk insulator oxides as SrTiO3 (STO) and LaAlO3 (LAO) in 2004 [1] has wide opened the route toward the discovery and control of broad functional emerging properties in different oxides heterostructures. Nonetheless the STO/LAO system still present not clarified questions concerning the possibility to control the presence of the 2DEG at the interface. In this work we present our theoretical results supported by experimental measurements concerning the possibility to tune the critical thickness of the LAO topmost layer through the deposition of a metallic capping layer at the surface. Our ab initio Density Functional Theory calculations show how different metallic contact can lead to a reduction of the LAO critical thickness of 4 u.c. still preserving the 2D electronic gas at the interface.

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Describing MoS2 Nanoclusters with Classical Potentials

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 MoS_2 has recently gained research interest in various fields. This inexpensive material is used currently mainly as a lubricant and for the hydrodesulfurisation reaction, but is gaining attention for other catalytic reactions, especially hydrogen evolution. Recent studies of single-layer MoS_2 have shown that its electronic band structure can be fine-tuned on the nanoscale [1]. Remarkable metallic properties occur at edges of triangularly to hexagonally shaped nanoclusters which are likely to be the active site for the hydrogen evolution reaction [1,2,3]. In this poster presentation, it will be shown how to simulate MoS_2 nanoclusters with a classical Stillinger-Weber potential. Trends on electronic energy and structure of MoS_2 with respect to different sizes and shapes will be presented.

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Self-interaction corrected energy functionals and Pipek-Mezey orbital localization

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While Kohn-Sham density functional theory (KS-DFT) has been extremely successful and is now widely used in the studies of molecules and condensed matter it has several shortcomings. This is due to the self-interaction error (SIE) inherent to practical implementations of the method. This, for example, makes the description of energy levels in semi-conductors, defect states in crystals, and magnetic states of metallic nanoclusters problematic. The Perdew-Zunger self-interaction correction (PZ-SIC) [1] implemented in a fully variational and self-consistent way using complex orbitals [2] has recently been found to be successful where commonly used exchange-correlation functionals fail. Accurate band-gap estimates for semi-conductors and insulators have been obtained which are in good agreement with GW calculations [3]. Furthermore, PZ-SIC calculations of localized defect states in crystals [4], charge-localized states in molecules [5] and magnetic states of metallic n anoclusters have been found to be in good agreement with experimental results while even hybrid functional KS-DFT calculations were in error.

The set of orbitals produced by conventional KS-DFT calculations (canonical orbitals, COs) typically extend over the whole system, making the analysis of the bonding and geometrical arrangement of atoms difficult. By defining a unitary rotation on the set of COs to produce localized orbitals (LOs) the properties of the system stay the same, but chemical bonding and geometry can be more readily rationalized. Recently [2] a generalization of the Pipek Mezey orbital localization was presented and shown to produce a clear separation of σ and π type orbitals while being a simple and an efficient post processing tool. This method has been extended to the condensed matter case where it is shown to produce as localized orbitals as the maximally localized Wannier functions (MLWFs), while maintaining clear σ and π bond separation and hence conforms to chemical intuition [5], while MLWFs produce mixed bonding orbitals ('banana'-shaped).

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Local Electronic Structure of a Magnetic Dimer Impurity in a Superconductor

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Magnetic impurities have a dramatic effect on superconductivity by breaking the time-reversal symmetry and inducing low energy bound states within the superconducting gap[1-3]. More interestingly, coupling between the individual magnetic impurities and superconducting substrate is essential for the formation of Majorana modes which have been detected in ferromagnetic chains of Fe atoms on a Pb(110) surface[4]. Therefore, it is important to have a fundamental understanding of the low energy bound states, their spatial extension, and the coupling between such states. Here, we demonstrate how a single cobalt phthalocyanine (CoPC) molecule modifies 2D superconducting states and the bound state within the gap extends spatially over nanometer from its magnetic center. The spatially extended states allow us to study the magnetic coupling between the impurities using a low-temperature scanning tunneling microscopy and spectroscopy. Our experimental work is supported by theo retical estimates of the coupling between magnetic impurities on the 2D superconductor. This work provides fundamental understanding of coupled bound states, which form the basis of the proposed exotic quantum states such as topological superconductivity in 2D magnetic lattices. These phenomena in artificial materials will allow the design and fabrication of new topological quantum devices.

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Multiscale modelling of \mbox{CeO}_2 nano-interfaces

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Ceria (CeO₂, cerium oxide) is a reducible oxide with a unique oxygen chemistry which makes it useful in many different technological applications, including the three-way catalyst, solid oxide fuel cells and chemical sensors. [1] In most cases, ceria is present in the form of applomerated nanoparticles, [2-4] containing specific interfaces. In this work, we address the nano-interface formation and its subsequent effect on important redox processes, in particular those related to the increased oxygen storage capacity found for small ceria nanoparticles (with d<5nm). [5] To allow for a systematic investigation of a manifold of different interfaces, we here applied a multiscale simulation approach combining three different levels of theory. At first, for the construction and examination of the initial geometry of various interface structures, we used molecular dynamics simulations with a reactive force field (ReaxFF). [6] This step was followed by the use of self-consistent charge density functional based tight binding (SCC-DFTB) calculations for geometry optimizations of the most stable interface geometries. In final, we used the density functional theory (DFT) for a detailed analysis of the chemistry of common defects at the nano-interface.

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Formation of hexagonal gold nanostructures during self-assembling on Ge(001) surface

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Nano sized gold has become an important material in various fields of science and technology such as nanoelectronics, catalysis, nanophotonics and medicine, where control over the size and crystallography of the structures is desired to tailor the functionality. The hexagonal closed packed (hcp) structure of gold is a very unusual form only recently chemically synthesized by Huang et al. [1] in form of graphene-supported thin sheets and nanowires of a few nm in thickness [2] and theoretically studied by Wang et al. [3]. The understanding of electrical as well as physical properties of the system is of great importance and strongly linked to their atomic structure. In the presentation, we will report on thermally-induced nanostructures formation after deposition of thin film of Au on reconstructed Ge(001) in UHV. It has been found that there exists preferential Au island orientation along crystallographic direction of the substrate surface as provided by diffraction methods (EBSD). For an annealing temperature close to the eutectic temperature of Au/Ge system (640 K), change in size and shape of the Au nanoislands is observed as well as the apparition of the hexagonal phase of gold, indicating eutectic melting of the system. TEM measurements of Au/Ge(001) sample cross sections revealed that the nanoislands created upon annealing at T<640 K are on top of the Ge(001) surface, while for T>640 K part of the island is buried beneath the substrate surface, which confirms the eutectic AuGe melting. The chemical composition of the Au/Ge interface was uncovered using quantitative atomically resolved HAADF-STEM and indicate the absence of alloyin g. The crystallographic structure of the Au islands and the presence of hexagonal gold as well as the Au/Ge interface were studied by quantitative atomically resolved HAADF-STEM and their structure was determined.

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Theoretical Prediction of One-Atom-Thick Hexagonal CrN: Electronic Structure and Magnetic Properties

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The family of 2D materials is rapidly increasing since the discovery of graphene [1]. Each new material brings interesting properties, which are usually different from their bulk analogues. Many theoretically predicted 2D materials with honeycomb structure, which are non-layered in bulk, were confirmed in experimental reports where graphitic thin ZnO [2], GaN [3] and stanene [4] were fabricated through different experimental techniques. Thin films of transition metal nitrides (TMNs) may provide one more possibility to obtain low-dimensional materials with unique spin-related properties because unpaired d-electrons are responsible for the formation of spin-depended surface electronic states. Transition metal mononitrides are known as advantage class of compounds. They have, relatively, high hardness, melting point, interesting optical, electronic, catalytic, and magnetic properties. In contrast to the most of one-atom thick 2D lattices like graphene, h-BN, transition metals dichalcogenides, etc. the TMN monolayers might be magnetic due to the presence of unpaired d-electrons. Therefore, no magnetic substrates or no doping with any atoms is necessary to induce spin injection into low-dimensional non-magnetic fragments for spin-related applications [5,6]. Using first principle calculations, we predict the existence of graphene-like hexagonal chromium nitride (h-CrN) with almost flat atomically thin structure. The results of the geometry search and phonon calculation of h-CrN indicate the possibility to create a 2D chromium nitride monolayer of (111) crystallographic orientation. The electronic structure calculations reveal that freestanding h-CrN has 100% spin-polarized half-metallic nature with possible ferromagnetic ordering. At HSE06 hybrid functional level of theory, the DOS of h-CrN displays the similar shape with the same band gap of spin-down (3.9 eV). As a possible way to stabilization and synthesis, deposition of h-CrN on 2D $MoSe_2$ or on MoS_2 is designed due to the guite good match of their crystalline lattice with h-CrN. The formation of composites keeps half-metallic properties and leads to reducing of spin-down band gaps up to 1.43 and 1.71 eV for energetically favorable h-CrN/MoSe₂ and h-CrN/MoS₂ configurations, respectively. It was also found that the electronic density at the Fermi level of $h-CrN/MoS_2$ heterostructure is much higher one of the freestanding h-CrNsheet. The h-CrN may be considered as a potential new fundamental 2D material with promising magnetic properties.

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A general computational method for electron emission and thermal effects in field emitting nanotips

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Electron emission from nanometric size emitters becomes of increasing interest due to its involvement to sharp electron sources, carbon nanotubes, vacuum breakdown phenomena and various other vacuum nanoelectronics applications. The most commonly used theoretical tools for the calculation of electron emission are still nowadays the Fowler-Nordheim and the Richardson-Laue-Dushman equations although it has been shown since the 1990's that they are inadequate for nanometrically sharp emitters or in the intermediate thermalfield regime.

In this paper we develop a computational method for the calculation of emission currents and Nottingham heat, which automatically distinguishes among different emission regimes, and implements the appropriate calculation method for each. Our method covers all electron emission regimes (thermal, field and intermediate), aiming to maximize the calculation accuracy while minimizing the computational time.

As an example, we implemented it in atomistic simulations of the thermal evolution of Cu nanotips under strong electric fields and found that the predicted behaviour of such nanotips by the developed technique differs significantly from estimations obtained based on the Fowler-Nordheim equation. Finally, we show that our tool can be also successfully applied in the analysis of experimental current-voltage data.

Our method has been implemented in an open-source computational tool, which is publicly available in https://github.com/AndKyr/GETELEC/. This tool can be used for either fast and simple calculation of emission currents or as a library for complex simulations of phenomena that involve electron emission.

MHDA-Functionalized carbon nanotubes for detecting non-aromatic VOCs and warfare agents

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The chemical modification of multiwalled carbon nanotubes (MWCNTs) is reported as a way to improve sensitivity and response time of gas sensors for detecting alcohols, acetone and warfare agents simulants such as DMMP [1,2]. We have developed sensors employing MWCNTs decorated with gold nanoparticles and modified with a 16-mercaptohexadecanoic acid (MHDA) monolayer. Morphological and compositional analysis by Transmission Electron Microscopy (TEM), Fourier Transform Infra-red Spectroscopy (FTIR) and X-ray photoelectron spectroscopy were performed to characterize the gold nanoparticles and to check the bonding of the thiol monolayer. The detection of aromatic and non-aromatic volatiles and DMMP vapors by MWCNT/Au and MWCNT/Au/MHDA shows that the presence of the self-assembled layer increases sensitivity and selectivity towards nonaromatics. Furthermore, it ameliorates response dynamics, and significantly reduces nitrogen dioxide and moisture cross-sensitivity.

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Nanoripples production on a-Si surfaces under Ar irradiation

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Ion beams are frequently used in industry for composition control of different materials as well as thin film deposition. It was noticed that low- and mediumenergy ions at high fluencies produce nanoripples and quantum dots on the irradiated surfaces. In the present work we focus our attention on the study of irradiation of amorphous silicon (a-Si) and germanium (a-Ge) with 1 keV Ar ions under different angles, taking into special consideration the angles close to grazing incidence.

This study has been carried out with Molecular Dynamics (MD), measuring the stress generated in the simulation cell as well as the total displacement of the particles which compound the cell, following the previous work on this matter [1]. The MD results are subsequently fed into a numerical module that allows the prediction of the ripple wavelength, which can be directly compared with experimental observations.

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Straining free-standing 2D materials in a TEM

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During the last decade, research on two-dimensional (2D) materials, epitomized by graphene and MoS_2 , has spawned a number of suggested applications including stretchable electronics. Theoretical calculations have shown a maximum strain for graphene up to 20% and about 10% for MoS_2 . However, measuring the intrinsic properties of 2D materials is difficult due to their delicacy.

We demonstrate here a simple method to strain freestanding 2D materials in situ in a transmission electron microscope (TEM). Our graphene and MoS_2 samples are grown through chemical vapor deposition and suspended on a substrate of perforated carbon films on gold TEM grids. The grids are glued onto a stretching holder and strained with small incremental steps to avoid breaking the membrane during the experiment.

We measure the deformation of the membranes from the diffraction pattern at each step. The change in the position of the diffraction spots allows us to estimate the applied uniaxial strain and to calculate the Poisson's ratio for both materials. Until now, the maximum uniaxial strain we have reached is approximately 1.5% – at larger strains the support film breaks. This problem may be overcome by using different substrates.

At higher strains our technique should allow the direct study of crack formation and propagation at the atomic level. These can then be correlated with the grain boundaries and their junctions in polycrystalline samples. Moreover, strain is also expected to have an influence on the formation and migration of point defects, which we can introduce with the electron beam during the experiment.

Molybdenum carbide and superconducting nitride nanowires: facile synthesis, transport measurements and their use as transparent electrodes

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We demonstrate a new and effective method of producing gram quantities of molybdenum carbide [1] and single-phase superconducting δ -MoN nanowires [2] from bundled Mo₆S_yI_z (8.2 $\leq y + z \leq 10$) nanowire templates in the presence of mixture of hydrogen/ethane and ammonia gas, respectively. By controlling the reaction conditions during the carburization, we can modify the ratio between MoC and Mo₂C carbide phases in nanowires and produce a new hybrid inorganic/organic nanomaterial composed of molybdenum carbide nanowires densely covered with carbon nanofibres. We used the same approach on nanowire networks and demonstrate a new use of molybdenum carbide and nitride in the form of nanowire networks as transparent electrodes. The sheet resistance of such robust and air-stable electrodes is around 1000 Ω /sg at room temperature and their optical transmittance between 93~% and 95~% in the range of 200 - 900 nm. The electrodes are thus suitable for electro-optic applications, especially where high transparency in the UV region is required. Measurements of four-contact resistance on single molybdenum nitride wires with diameters above 100 nm in a magnetic field are used to determine the critical field. We show that switching between different metastable superconducting states in δ -MoN nanowires can be very effectively manipulated by introducing small amplitude electrical noise. Furthermore, we show that deterministic switching between metastable superconducting states with different numbers of phase-slip centres can be achieved in both directions with small electrical current pulse perturbations of appropriate polarity [3].

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Buckyball Sandwiches

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Two-dimensional (2D) materials have considerably expanded the field of materials science in the last decade. Very recently various 2D materials have been assembled into vertical van der Waals heterostacks, and it has also been proposed to combine them with other low- dimensional structures to create new materials with possibly hybridized properties. In this contribution we demonstrate the first direct images of a suspended 0D/2D heterostructure incorporating C_{60} molecules between two graphene layers in a buckyball sandwich structure [1]. We demonstrate clean and ordered C_{60} islands with thicknesses down to one molecule, shielded by the graphene layers from the microscope vacuum and partially protected from radiation damage during scanning transmission electron microscopy imaging. The demonstrated sandwich structure serves as a 2D nanoscale reaction chamber allowing the molecular structure and dynamics to be analyzed at atomic resolution.

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Study of carbon nanostructures generated by gamma irradiation of graphene flakes on nickel

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Carbon nanostructures are widely studied in last twenty years in connection with their unique electronic, magnetic and mechanical properties [1]. Special attention is directed on the graphite single layers (graphene) because of their extremely high electron mobility and transparency in wide range of wavelengths [1, 2]. Stability and transformation of the graphene layers under different radiation exposures are important directions of research. The presented work considers formation of various nanostructures from the graphene layers synthesized on Ni film under gamma irradiation. The graphene layers were synthesized by the vacuum thermal treatment at 700-900 C for 2-20 min of sandwich a-Si_{1-X}C_X/Ni structure deposited on SiO2 film with thickness about 200 nm. The a-Si_{1-X}C_X was deposited on oxidized Si wafer by RF magnetron sputtering of the polycrystalline SiC target in Ar ambience, and the Ni film by DC magnetron sputtering of Ni target without withdrawing of the wafer from a chamber [3]. Fabricated structures were subjected by gamma irradiation with doses up to 5×10^6 Rad (Si) in vacuum and air. The graphene surface morphology and distribution of electrical potential were studied by optical microscopy (Axioscop 2 MAT, Carl Zeiss) in standard and differential interference contrast (DIC) mode, AFM and scanning Kelvin probe force microscopy (SKPFM, NanoScope IIIa Dimension 3000). Structure of graphene layers was studied by micro-Raman spectroscopy (mRS, triple Raman spectrometer T-64000 Horiba Jobin-Yvon, and excitation by the 514 nm line of an Ar-Kr ion laser). To identify the origin of the structures generated under irradiation the graphene surface was examined additionally by scanning electron microscopy (SEM) combined with local high resolution Auger electron spectroscopy (JAMP-9500 F). Employed technique results in a synthesis of the graphene flakes with size about 20x20 m which cover about 80% of the Ni surface. Raman spectroscopy shows that the flakes possess different thickness and different deffectiveness in central and edge parts. The gamma irradiation in vacuum does not lead to any changes in structure of the graphene flakes up to dose of $5 imes 10^6$ Rad. However the radiation in air with dose of 5×10^5 Rad results in formation of new structures such as domes with height about 100 nm and stars with rays size about 10-15 μ m. Results of the SKPFM and Auger electron spectroscopy (AES) attest on location of these structures on surface of multilayer graphene. The mRS and AES show that the structures compose of carbon. The rays are probably carbon tubes with diameters about 100-120 nm. The domes have a surface potential considerable lower than graphene layer that assumes either formation strained graphene structure or incorpo ration in the graphene layer any inclusions in these places. Also doublet behavior of Raman G band is observed for scanning of the dome structures that can be explained by strained layers formation during the gamma-irradiation of the graphene flakes. A nature of synthesis of such carbon structures under the irradiation is discussed.

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Graphene processing towards applications

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Several methods have been established for graphene preparation. However, most of them remain as demonstration techniques, mainly for basic research, and for providing proof of concept devices. Instead, the recent progress in making stable graphene dispersions allows the production of graphene sheets on a more preparative scale and permits the manipulation of the layers by chemical reactions. Thus, chemically manipulated graphene samples can be easily incorporated into new functional materials or can be modified for the formation of other carbon nanostructures. In this work, I will show our recent efforts toward 1) producing graphene stable dispersions [1]; 2) ultrasonic approaches performed in graphene dispersions that modify its chemical [2], and structural properties [3,4], i.e. MWNTs production by rolling up a graphene sheet; and finally 3) an applications where functionalized graphenes are used for photodynamic therapy [5].

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First principles training sets and atomistic potentials for boron-nitride nanostructures

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Boron nitride nanotubes are a promising material for nanoscale reinforcement of composites. An analog of the more familiar carbon nanotube family, boron nitride nanotubes exhibit exceptional structural, mechanical, and thermal properties. They are optically transparent and have high thermal stability, suggesting a wide range of opportunities for structural reinforcement of materials including glass, ceramics, and metals.

Theoretical modeling can play an important role in determining the optimal approach to integrating nanotubes into a supporting matrix. The most promising composites (with respect to mechanical load transfer) involve covalent functionalization of the supporting nanotubes. Developing accurate, atomistic scale models of such nanoscale interfaces embedded within composites is challenging, however, due to the mismatch of length scales involved. Typical nanotube diameters range from 5-50 nm, with a length as large as a micron (i.e. a relevant lengthscale for structural reinforcement). Unlike their carbon-based counterparts, well tested and transferable interatomic force fields are not common for BNNT. In light of this, we have developed an extensive training database of BN rich materials, under conditions relevant for BNNT synthesis and composites based on extensive first principles molecular dynamics simulations. Using this data, we have produced an artificial neural network poten tial capable of reproducing the accuracy of first principles data at significantly reduced computational cost, allowing for accurate simulation at the much larger length scales needed for composite design.

Carbon-vacancy complexes controlling nano-scale irradiation damage in iron and steels

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Ab initio techniques was applied to compute energetic stability of Carbonvacancy complexes and positron life time in BCC Fe. Positron lifetime is found to be tremendously sensitive to local Carbon-vacancy, Carbon-Carbon and vacancy-vacancy arrangements. Depending on C-V multiplicity, a certain complex is indistinguishable or to be detected as a single or clusterized vacancy by positron annihilation spectroscopy. Combining ab intio database for the life time and energetics of C-V clusters, rate theory cluster dynamics calculations were performed to model annealing of Fe-C alloys after electron irradiation in the conditions identical to experiment. Analysis of the lifetime spectrum and results of rate theory calculations allows one to qualitatively explain and accurately reproduce the experimental data if di-Carbon-vacancy complex is considered to be mobile. The migration energy of 1.1 eV is drawn from the best fit to experimental data.

Conversion of light for the production of fuels using cell factories

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Sunlight can promote water electrolysis in order to obtain hydrogen gas, which in turn can be paired with CO_2 to produce hydrocarbons. Phototrophic microbes, instead, can combine light and carbon dioxide in a wide range of organic compounds with a high product selectivity but exploiting only a small portion of the solar spectrum[1][2]. A third and interesting combination is microbial electrosynthesis, the capture of sunlight-generated electrons by microbes in order to drive the conversion of carbon dioxide to organic compounds[3]. The critical points in this type of processes are the low reactivity of CO₂, product selectivity, poor interaction between the electrical and biological components, and finally the necessity to tailor which fractions of the solar spectrum will be used by the device: UV light can be harmful to microbes, and some wavelengths might need to be converted in order to exploit as much light as possible. We aim to overcome these limitations by creating new optoelectronic nanotech materials (using nanostructured III-V semiconductors and plasmonic nanoparticles), engineering new microbial species, and finding a way to interface the two systems. A similar scope is being successfully pursued by a research team in Harvard, where CO_2 reduction and water electrolysis were achieved thanks to the interface between a biocompatible electrode and a strain of Ralstonia Eutropha[4].

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Creating nanoporous graphene with swift heavy ions

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We examine swift heavy ion-induced defect production in suspended single layer graphene using Raman spectroscopy and a two temperature molecular dynamics model that couples the ionic and electronic subsystems. We show that an increase in the electronic stopping power of the ion results in an increase in the size of the pore-type defects, with a defect formation threshold at 1.22-1.48 keV/layer. We also report calculations of the specific electronic heat capacity of graphene with different chemical potentials and discuss the electronic thermal conductivity of graphene at high electronic temperatures, suggesting a value in the range of 1 Wm $^{-1}$ 1 K $^{-1}$ 1. These results indicate that swift heavy ions can create nanopores in graphene, and that their size can be tuned between 1-4 nm diameter by choosing a suitable stopping power.

Controlling Josephson current with topological states in bilayer graphene

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We present a numerical, tight-binding calculation of dc Josephson current in long bilayer graphene (BG) junction using four, parallel doping gates (two below and two above the scattering region) with superconducting electrodes. As it was shown experimentally by Li et al[1]. this setup is suitable to electronically control the band gap and generate a topological state TS in the low energy regime of BG. In our calculations we show that in case the TS extends in the whole width of the system it couples the edge states from the opposite sides, which causes the electrons to scatter and the current to decrease. The presence of the TS lowers the critical current by an order of magnitude and the current-phi relation is clearly distinguishable from the setup where there is no TS. This behavior can be clearly observed in all the samples, which are wide enough so that the wavefunctions of edge states do not overlap. We investigate also the robustness of this effect against disorder and magnetic field. The Josephson current is calculated by the EQUUS code, developed by the Eötvös Quantum Transport Group [2]

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In-Situ Transmission Electron Microscopy of Functional Materials

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One of most exciting developments in nanomaterials characterization is the commercialization of aberration corrected TEMs and STEMs [1,2]. By correcting for spherical aberrations, these techniques allow for the imaging of atomic positions with a precision of a few picometers. Together with the integration of energy dispersive X-ray spectroscopy (EDS) and electron energy loss spectroscopy (EELS), the structural and elemental composition of nanomaterials can be determined at the atomic level. Recently, another exciting development in TEM has emerged, namely the use of special specimen holders for in-situ TEM measurements under various heating, cooling, and electrical bias conditions [3]. The combination of in-situ TEM/STEM imaging and EDS/EELS analysis is extremely powerful as it allows for real-time studies on nanoscale dynamical processes and their direct impact on macroscopic material properties. In the Nanomicroscopy Center at Aalto University, we have established a new platform for in-situ TEM characterization. Here, we review some recent experimental results, including (1) the observation of electron beam-induced structural phase transitions in epitaxial manganite films [4], (2) in-situ spectroscopy of electricfield controlled oxygen ion migration in metal/oxide heterostructures [5], and (3) simultaneous real-time analysis of resistive and structural phase transitions in complex oxide nanostructures. We also present an outlook on the development of a combined optical/electrical probing holder for in-situ TEM measurements on perovskite solar cells. The new setup will be used to address reliability and durability issues of this promising new type of solar cell by simultaneous characterization of ion migration, ionic polarization, ferroelectricity, etc., at high spatial resolution. Realization of this measurement technique will be a major step in the field of in-situ TEM with direct implications for the development of perovskite sola r cells and other opto-electronic devices. The project is financially supported by the Key Project Funding by the Academy of Finland, 2016.

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Multi-step growth and emission mechanism in matrix assembly cluster source

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To enable the industrial use of nanoclusters, their production rate must meet certain industrial demands. This imposes severe technological requirements, such as of high level of controllability and huge amount of nanocluster (at least, 1 g/hour versus 1 mg/hour in existing experimental equipment) are not easy to achieve on a nanoscale. A new type of cluster beam source, "Matrix Assembly Cluster Source", is introduced as a potential setup to scale up the production rate of cluster to industrial level [1]. The method is based on Ar sputtering Ar solid matrix with embedded metal nanoclusters. In this work, we study the growth and emission mechanism of Ag nanocluster in solid Ar matrix by combination of experiment and computational methods. The molecular dynamics simulations indicate that the growth mechanism can be described as "thermal spike enhanced clustering". The emission mechanism is shown to be a combination of "interface boiling" and "spring force effect". An analytical model is developed to describe the size-dependent cluster emission, which would lead to more precise control of nanoclusters in experiments without losing production rate and applications. The results of the current work obtained by different methods are in a good agreement.

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Colossal Enhancement in Magnetic Moment of Ferrimagnetic NiCo2O4 via Strain-Doping

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Strain doping has emerged as a powerful technique for efficient control of single axis lattice expansion to fine tune and modulates the inaccessible complex correlated phases in the oxide thin films. We report the fine tuning of the magnetic moment and insulator-metal transition in the ferrimagnetic NiCo2O4 inverse-spinel oxide by creating oxygen deficiencies employing high energy He-ion irradiation. Application of the uniaxial tensile strain, less than 1%, can effectively tune the oxygen vacancy driving the system in the colossal increase of the magnetic moment by two-factors in magnitude. This magnetic moment shows scaling with the He-ion irradiation fluence. Our results corroborates well with the X-ray absorption spectroscopic data which shows the peak-height changes and energy shifts of Co-L2,3 and Ni-L2,3 edge driven by the oxygen content from its typical crystal environment via He-ion ir radiation, useful for designing new functionalities in other spinel oxide thin films.

Participants

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