Atomic structure of nanosystems from first-principles simulations and microscopy experiments

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EMIL AALTOSEN SÄÄTIÖ A?

Programme

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Sensing magnetic ordering, electric fields & isotopes at the atomic and nanometer level: A Glimpse into Electron Microscopy in the Quantum Information Era

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Scanning and transmission electron microscopes (S/TEM) are now ubiquitous in materials and biological sciences laboratories. They have radically enhanced our understanding of organic and inorganic matter with the successful development of aberration correctors [1,2], detectors with film-equivalent dynamical range [3], and more recently, with monochromators capable of achieving sub-10 meV energy resolution spectroscopy [4]. Here, I will present several examples demonstrating how we have exploited these capabilities and solved the pertinent experimental challenges to probe materials behavior at the nanometer and atomic scales. Specifically, I will show how by utilizing the phase of the electron probe one can reveal the magnetic order of complex-oxide materials at the atomic level [5]. I will also explain how the new generation of monochromators, combined with aberration-corrected STEM, can be used (i) as a primary thermometer (without requiring any previous knowledge of the sample) [6]; (ii) to study minute volumes of liquid water [7]; (iii) to detect site-specific isotopic labels in amino acids at the nanometer scale [8]. Additionally, I will show how one can detect the electric field of individual atomic columns of heavy and light elements, at the sub-Angstrom scale, by using an ultra-low noise SCMOS detector in the diffraction plane [9]. Lastly, I will discuss potentially relevant new challenges that electron microscopy will need to resolve as it enters the forthcoming quantum information era. Will it be possible to map orbitals and spins with atomic resolution and with single atom sensitivity? Can we detect a superconducting transition? Can we spectroscopically measure cryogenic temperatures with 10s of mK precision? Can we measure the specific heat and thermal conductivity of materials? Can we detect minute concentrations of isotopic elements and perform radiocarbon dating at the nanoscale? These questions will be addressed and further elaborated during the presentation [10].
References:

Probing Nanostructured Materials Atom by Atom: A High Resolution Aberration-Corrected Electron Microscopy Study

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Defects can have a profound effect on the macroscale physical, chemical, and electronic properties of nanostructures. They can lead to structural distortions, introduce extra states in the band gap and give rise to excess potential locally at buried interfaces. While defects and interfaces have been a well-studied subject for decades, little is known about their local atomic and chemical structure and the sub-Angstrom structural distortions within their vicinity. Using high-resolution aberration-corrected S/TEM imaging and spectroscopy, this talk will discuss our recent efforts on the determination of the defect chemistry and sub-Angstrom relaxation effects in nanostructures around dopants, grain boundaries, domain walls, and interfaces in the family of 2D crystals, complex oxides, and novel nanostructures.

Manipulation of single impurity atoms in 1-, 2-, and 3-dimensional nanostructures using focused electron irradiation

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Recent advances in transmission electron microscopy have made it possible to modify nanostructures with atomic precision. In recent years, progress has been made from occasional observations of Si-C bond inversion in graphene [1] towards controlled movement of Si impurities using the atomically focused electron beam of an aberration-corrected scanning transmission electron microscope [2,3]. We have now demonstrated that the same technique can be used to manipulate Si impurities in single-walled carbon nanotubes (SWCNT) [4]. Recently, it was shown that an electron beam can also be used to controllably position single bismuth dopant atoms in crystalline silicon [5]. Here we summarize our recent experimental results on the manipulation of single atomic impurities in graphene and SWCNTs. We further provide a comprehensive theoretical analysis of the mechanisms and energetics of atomic dynamics in 1-, 2- and 3-dimensional nanostructures obtained using density functional theory m olecular dynamics.

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Formation and Properties of Mirror Twin Grain Boundary Networks in Molybdenum Dichalcogenides

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Edges, defects, and dopants in 2D transition metal dichalcogenides have been shown to give rise to special chemical, electronic, and magnetic properties in these materials. To utilize the potential of these modifications a detailed understanding of their controlled formation and atomic scale properties is needed. In this talk we present our studies on the controlled formation of metallic mirror twin grain boundaries (MTBs) in MoSe2 [1] or MoTe2 [2] by incorporation of excess Mo into the lattice. Very high density of MTB networks can be obtained in MoTe2 that effectively metallizes the material and thus may act as a metallic contact patch [3]. Such line defects may also increase electrocatalytic properties for hydrogen evolution reactions [4]. On a more fundamental level, we show that these 1D metallic grain boundaries host one dimensional electron gas and we present the first angle resolved photoemission (ARPES) studies of such line defects. These studies show evide nce for the presence of Tomonaga-Luttinger Liquid behavior of 1D electron systems [5]. Finally, we show that other transition metals may also be incorporated into MoTe2 and the incorporation of vanadium induces room temperature ferromagnetic ordering and thus is an example of a 2D dilute ferromagnetic semiconductor [6].

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[6] PM Coelho, et al. , *Adv. Electr. Mat.* in press (2019).

Insight into 3D structure formation during atomic layer deposition

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M. A. Verheijen[1,2] A. A. Bol[1]

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Nanoscale deposition techniques are becoming increasingly more important for various applications as the scalability of the current technology reaches the obtainable limit. Two-dimensional, layered materials, such as transition metal dichalcogenides (TMDs), have re-emerged as an intense area of study for future thin film applications [1]. Atomic layer deposition (ALD) is one synthetic technique that permits angstrom-level control of thin films that also exhibits a high degree of conformality over large, diverse surfaces [2]. However, development of ALD is still ongoing and mitigating a transition from in-plane to out-of-plane growth in TMD thin films is important. With increased film thickness, out-of-plane, or 3D, structures appear in addition to lateral film growth, a consequence of several factors (e.g. plane orientation variation, competition between grains, etc.). These 3D structures can significantly affect the overall film properties [3]. Several studies have address ed a formation mechanism for 3D structures, however, a detailed mechanism has not yet been well defined [3,4,5]. WS_2 ALD films of various thicknesses were studied with high resolution scanning transmission electron microscopy (STEM) to understand the 3D structure formation mechanism. Fast Fourier transforms (FFTs) were analyzed from areas surrounding 3D structures to study grain orientations. The angular difference of crystallographically equivalent diffraction spots in the FFTs reveals the misorientation between grains; misorientation angles were measured with respect to the horizontal. The 3D structures were found to predominantly form at grain boundaries with low misorientation angles, low angle grain boundaries, with an average of about 5.6 degrees. These misorientation angles were then compared with other grain boundaries with no 3D structure present. Misorientation angles at grain boundaries with no 3D structures was substantially higher with an average difference of about 16.5 degrees illustrating the preference for 3D structures to form at low-angle grain boundaries. >From these data and accounting for higher defect mobility at high angle grain boundaries [6], we propose three general formation mechanisms for 3D structures during ALD: (1) a discontinuous, (2) a preferential, and (3) a concerted mechanism. Understanding the mechanisms behind 3D structure formation during ALD is an important step toward further controlling and manipulating thin films at the nanoscale for future applications.

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WSe_2/metal heterostructures investigated by Quasi-Particle Interference mapping, STM/STS, and ARPES

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WSe_2 is one of the semiconducting TMDs that has great potential in both spintronics and valleytronics. Interfacing it with various metallic substrates however can affect its electronic structure through a variety of effects, one of them being the rotation angle of the WSe_2 layer relative to the underlying substrate, which creates a scattering potential for its quasiparticles. Here we studied the electronic structure of WSe_2/metal heterostructures as a function of the thickness of the WSe_2 overlayer (i.e. monolayer and thicker), and rotation angle relative to the atomically flat metallic substrate, using a combination of Scanning Tunnelling Microscopy and Spectroscopy (STM/STS), quasi-particle interference (QPI), and ARPES. From these complementary techniques we could observe: (i) evidence of zone folding due to the Moire potential of the heterostructure, (ii) gap states due to hybridisation, and (iii) intervalley scattering forbidden in isolated (i.e. no t metal supported) WSe_2. Our analysis tries to formulate a unified understanding of these various experimental facts.

Catalysis at nanoscale from DFT calculations

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Catalytic processes are important for many areas of our daily lives. One of the main aspects is the processing and storage of energy in the form of chemical compounds, which is an alternative to energy storage using lithium-ion batteries. Another interesting application is the reduction of harmful gases such as CO generated in industrial processes. In this regard, there is an increasing interest in the study of catalytic processes at the nanoscale. The solution for many complex problems in the field of catalysis depends on the smart implementation of novel advanced nanomaterials. One of the promising directions is the utilization of hybrid nanomaterials, i.e. nanohybrids. Such hybrids, consisting of various nanostructures, have intensively been studied and successfully been used in many different areas because of the unique combination of properties. Primarily, the catalyst nanohybrid development is based on the right selection of a nanocarrier and a catalyst agent. While t he agents have a dominant role in the catalysis, the nanocarriers are also crucially important with respect to the material synthesis and following catalytic reactions. Hexagonal boron nitride (BN) is an attractive material due to its outstanding mechanical, chemical and physical properties. BN nanoparticles could be used as novel nanocarriers for different catalysts. Metallic nanoparticles supported by BN nanostructures demonstrated higher aggregative stability leading to superb catalytic properties. The catalytic activity of Ag nanoparticles (AgNPs) was under the spotlight for many years. In this study, the calculation of intermediate compound of methanol oxidation at Ag surface was made in order to investigate thermodynamic of this process [1] as well as CO oxidation thermodynamic and kinetic at Ag surface in Ag/BN hybrid structure [2]. In the area of photoinduced processes, the formation of a dipole on the interface of nanohybrid structures (Pt-Au-ZnO and Au-ZnO) as a co nsequenc e of the charge redistribution due to the difference in the electronegativity of the constituent parts of the interface leads to the increased of the efficiency at Toluidine blue photoreduction [3]. The inhomogeneity in the charge distribution in the defect region, as well as the contribution to the bottom of the conduction band from the embedding atoms, leads to a significant increase in the HER activity of the base plane of the 2D MoS_2 crystal [4]. The importance of the binding energy for HER activity is also shown for H2O dissociation on a carbon-coated Ni_3N (110) surface [5]. This result is in accordance with the experimentally observed enhancement of HER activities in Ni_3N@CQDs and suggests that the enhanced catalytic activity is largely governed by the more energy-favored water dissociation process. A set of factors such as binding energy, electronic structure, and charge distribution which is important for the explanation of catalysis processes at the nanosca le that can be obtained through DFT calculations will be discussed.

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Post-synthesis Introduction of Transition Metal Impurity into Molybdenum Dichalcogenides - Density Functional Study

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Introduction of impurities into a material, conventionally during its growth, is one of the promising ways to tune electronic and magnetic properties of bulk and nanomaterials as well. However, in two-dimensional materials, the impurities can be directly incorporated by depositing dopant atom at an elevated temperature, as demonstrated for $MoTe_2$ layer[1,2]. We have employed density functional calculations to find which transition metals are readily embedded into molybdenum dichalcogenides, instead of trivial clustering on the surface. Further, we rationalize the energetics and induced magnetic moment through atomic radii and the number of (s+d) electrons of TM atoms. Our results are in agreement with the available experimental data and should further guide the experiment.

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Single layer boron nitride: From templates to functionalized membranes

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Single layers of hexagonal boron nitride may be grown on transition metal surfaces by means of chemical vapour deposition of borazine ((HBNH)3). Using Rh [1] or Ru [2] as substrates leads to the formation of peculiar super-honeycomb structures, where in the case of Rh 13 BN units accommodate on 12 Rh unit cells. This 3.2 nm super-cell, first called 'nanomesh', houses two distinct electronic systems, on 'wires' where the BN is quasi freestanding and in 2nm 'pores' where the BN wets the Rh substrate [3]. This leads to a peculiar template function, where molecules may be selectively trapped in the 2 nm pores at room temperature. The super-honeycomb may act as a membrane beneath which hydrogen may be intercalated [4], also with electrochemical means [5,6]. The structures can be further functionalized with low energy ions, where single atoms may be implanted beneath the h-BN 'rainfly', in so called 'nanotents' [7]. The vacancy defects that are created in the course of the low energy ion irradiation process may be annealed and lead to the cut out of h-BN flakes formerly bound in the pores of the superhoneycomb [8]. Such systems are exfoliated and used as freestanding single layer membranes [9].

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Microscopic studies of grain boundaries in two-dimensional hexagonal boron nitride films

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Grain boundaries (GB) often play a vital role on determining the various properties of 2D materials, hexagonal boron nitride (hBN) is not an exception. Microstructures of GBs in hBN, owing to the directional B-N bonding, should possess additional freedom and thus are more complex comparing to that in graphene. In this talk, we will try to present a systematic TEM study of the GBs in CVD grown h-BN, and cover the following issues: I. The existence of overlapped GBs and their formation mechanism; II. A novel method to fabricate GBs with desired structures; III. Dynamics of GBs upon thermal excitation and beam irradiation.

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Dense storage of alkali metals between graphene and MoS2 bilayers: a computational study

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We study the intercalation of alkali metals, namely lithium and sodium, between graphene and MoS_2 sheets using density functional theory calculations with the van der Waals correction. The structures and energetics of a different number of alkali layers with closed packed structure have been investigated for various stacking sequences of bilayer graphene. The intercalation energies suggested that the AA stacking is more favorable for the single-layer intercalation but it has no considerable effect on multilayer storage. Our calculations showed that there is a clear correlation between the intercalation energy and the electron transfer between alkali atoms and layered material. While the higher values of charge transfer observed for the single layer intercalation, the charge transfer is noticeable only for the outer alkali layers in the multi-layer case. As a result, the intercalation energy reduces with increasing the number of the lithium and sodium layers but r educes f or potassium. In the case of lithium intercalation between MoS_2 bilayers, a 2H-1T phase transition was observed due to the significant charge transfer. The present study can shed light on the design of high storage alkali batteries using two-dimensional layered materials as reported recently [1].

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Wednesday 29.05.2019

13:50 – 14:20 *Coffee and pastry*

chair: Batzill
14:20 – 15:00 **Tautz**
Nanoscale Engineering at Surfaces
15:00 – 15:20 Hall
The 3x3 charge density wave in quasi-freestanding monolayer TaS2
15:20 – 15:40 Shawulienu
Epitaxial ferromagnetic VSe2 monolayers on superconducting NbSe2
15:40 – 16:00 Palotas
Scanning tunneling microscopy simulations based on the revised Chen's derivative rules

16:00 – 18:00 Coffee at posters

chair: Heine
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Integrating atomistic simulations with microscopy to probe defect dynamics in 2D materials
18:40 – 19:20 **Schiøtz**
Using Neural Networks to Identify Atoms in HRTEM Images
19:20 – 19:40 Kvashnin
Evolutionary prediction of 2D materials formation on substrates

20:00 – 21:30 *Dinner*

Nanoscale Engineering at Surfaces

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The increasing interest in quantum technologies puts tailor-made materials into the focus. In this context the term material is more and more understood in a wider sense to also include designer structures beyond a single crystalline phase. For example, such designer structures can be customized stacks of 2D materials as well as surface-supported nanostructures made by assembling individual atoms or molecules. A further challenge, apart from crafting the structures themselves, is studying their properties. Often, this requires the refinement of existing experimental methodology. In my talk, I will report on our recent work regarding tailor-made materials based on graphene and designer structures based on individual atoms and molecules. With increasing complexity, new properties and phenomena emerge, and the design of functional (quantum) devices becomes possible. As it turns out, even relatively simple designer structures show intriguing functionalities, including q uantum d ot behaviour, electrostatic potential sensing, and coherent single-electron field emission. On the analytic side, I will illustrate the power of several advanced experimental methodologies.

The 3x3 charge density wave in quasi-freestanding monolayer TaS2

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We report on the 3×3 charge density wave (CDW) in a quasi-freestanding monolayer of TaS_2, as grown by molecular beam epitaxy on graphene on Ir(111) [1]. Investigated by scanning tunnelling microscopy, the 3×3 periodicity of the CDW is visible at liquid helium temperatures, and allows analysis of spatial CDW amplitude variations and the influence of point and line defects. Performing low temperature scanning tunnelling spectroscopy (STS) reveals a decreased density of states at the Fermi energy, indicating partial gapping of the Fermi surface. We investigate the influence of the environment on the CDW state and In constant current STS maps, an energy dispersive standing wave pattern is found, which firstly illustrates the quasi-freestanding nature of the TaS_2 islands and secondly allows partial determination of the band structure, which is compared to data from angle resolved photoemission spectroscopy of the same system.

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Epitaxial ferromagnetic VSe2 monolayers on superconducting NbSe2

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Combination of magnetism and superconductivity has been predicted to result in a novel phase of matter called topological superconductivity. This has recently attracted intense interest due to the predicted boundary modes hosting Majorana fermions and their relevance to topological quantum computation. Topological superconductivity has been experimentally realized in 1D in both engineered nanowire systems and in chains of magnetic adatoms on an superconducting substrate [1,2]. Very recently, these concepts have been extended to 2D by studying the edge modes around magnetic islands on superconducting substrates [3-5]. However, this type of systems are sensitive to the atomic scale details of the coupling between the magnetic layer and the substrate and in some cases, require interface engineering using an atomically thin separation layer. This creates a big challenge in real device applications and there clearly is a need for more robust experimental systems for the realizat io n of 2D topological superconductivity.

We propose a new platform based on the recently discovered 2D monolayer van der Waals ferromagnet vanadium diselenide (VSe2) that can be grown directly on layered materials [6]. Here, we report the growth of monolayer VSe2 by molecular beam epitaxy (MBE) on superconducting niobium diselenide (NbSe2) substrate. We characterize the electronic and magnetic properties by low-temperature scanning tunneling microscopy (STM) and macroscopic magnetization measurements. The demonstration of the coexistence of ferromagnetism and superconductivity in a hybrid van der Waals heterostructure will provide opportunities for the investigation of novel quantum phases of matter and open new possibilities for real-life devices applications.

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Scanning tunneling microscopy simulations based on the revised Chen's derivative rules

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Chen's derivative rules for electron tunneling are revised [1] for the purpose of computationally efficient simulations of scanning tunneling microscopy (STM). The new features include (i) the weighting of tunneling matrix elements of different tip-orbital characters by an arbitrary energy-independent choice or based on first-principles data, (ii) arbitrary tip geometrical orientations enabling the consideration of asymmetric tips, and (iii) the possibility of quantitative analysis of tip-orbital interference contributions to the tunneling current. The model has initially been applied to two functionalized surfaces where quantum interference effects play an important role in the STM imaging and the Tersoff-Hamann model fails to describe the correct STM contrast under certain conditions: N-doped graphene [2] and a magnetic Mn_2H complex on the Ag(111) surface [3]. For both of these surface structures, the importance of interference between s and p_z tip orbit als is highlighted that cause a significant contrast change in the STM images [1]. Moreover, the revised Chen's method has recently been applied (i) to validate a newly proposed structural model for the magnetite Fe_3O_4(110) surface with two-fold oxygen vacancies [4], (ii) to study surface defects in the organic perovskite $CH_3NH_3PbBr_3$ [5], and (iii) to investigate ultrathin Mo-oxide structures on Au(111) [6].

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Integrating atomistic simulations with microscopy to probe defect dynamics in 2D materials

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In this talk, I will present some of our recent work on the use of machine learning (ML) to seamlessly bridge the electronic, atomistic and mesoscopic scales for materials modeling. Our automated ML framework aims to bridge the significant gulf that exists between the handful of research groups that develop new interatomic potential models (often requiring several years of effort) and the increasingly large user community from academia and industry that applies these models. Our ML approach showed marked success in developing force fields for a wide range of materials from metals, oxides, nitrides, hetero-interfaces to two-dimensional (2-D) material. This talk will also briefly discuss our ongoing efforts to integrate such cheap yet accurate atomistic models with AI techniques to perform inverse design and deep learning to improve spatiotemporal resolutions of microscopy and ultrafast X-ray imaging.

Using Neural Networks to Identify Atoms in HRTEM Images

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We have developed a methodology, where deep convolutional neural networks can be used to identify local structures in high resolution transmission electron microscopy (HRTEM) images. The methods are available as Python modules under an open source license [1, 2].

While conventional image processing and peak finding algorithms can be used to pinpoint the position of the atoms (within the uncertainty due to imaging effects) [3], the fact that contrast varies from image to image, and sometimes even inverts within a single micrograph makes such methods difficult to use. A neural network can act as an advanced filter, giving a clean signal for peak detection.

In most cases, using machine learning (ML) for image analysis is limited by the availability of high-quality pre-analyzed images that can be used for training the ML methods; acquiring the training data can be both time-consuming and expensive. In this case, we are in the fortunate situation that atomic-resolution HRTEM images can be reliably simulated, providing the training data at low cost. We have shown that it is possible to reliably identify the positions of the atoms in experimental micrographs of single sheets of defected graphene, and the atomic columns in micrographs of metallic nanoparticles, even when the signal-to-noise ratio is low due to the desire to limit beam exposure [3].

While a single HRTEM image contains sufficient information for the neural net to identify the positions of the atoms, more information can be extracted from a focal series. We have demonstrated, albeit in simulations only, that a set of three images taken at different defocus is sufficient to identify chemical species and vacancies in single sheets of molybdenum disulfide, and to count the number of atoms in atomic columns in gold nanoparticles [1], which has until now only been possible with STEM.

In conclusion, we find that deep learning is a promising tool within electron microscopy, which may both accelerate analysis of large amounts of microscopy data and enable analyses that would not otherwise be possible, such as counting the height of atomic columns in HRTEM images.

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Evolutionary prediction of 2D materials formation on substrates

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Successful synthesis of graphene opens a new possibility of formation of fundamentally new low-dimensional materials: ultrathin films with atomic thickness with unique physical properties. At the first stages 2D films were obtained by mechanical exfoliation from the crystals having layered structure (graphene, h-BN, MoS_2[1], etc.), while further two-dimensional materials with structure and properties having no analogues in 3D (as silicene[2], borophene[3], CuO[4], Fe[5], FeO[6], CoC[7] etc.) were synthesized. Important that there is a very limited set of methods for simulation of the formation process of nanostructures and can only partially describe the formation of nanostructures. Necessary conditions for obtaining the desired material during the growth process is the correctness definition of the main parameters: the type and composition of the substrate, the external conditions (temperature and pressure), the definition of the necessary parameters of the cells of the substrate and the desired material, as well as their symmetry. Here we presented an effective method for simulation of formation of two-dimensional materials with one and several layers thickness on substrates of different composition using Evolutionary algorithm USPEX. New expanded modules of the USPEX software allow to simulate the formation of low-dimensional nanostructures and predict the crystal structure of low-dimensional materials with random composition consisting of more than 2 types of atoms on different substrates depending on external parameters (temperature, pressure). Applied extended USPEX modulus simulation of the formation of 2D nanostructures with several layers thickness of a given composition (including NaCl, LiCl) on various substrates (including Cu, Ni, Ag, graphene, diamond) as well as the formation of novel 2D-CuO[3] layer in bilayered graphene nanopore were carried out. Obtained results has an excellent agreement with available experimental data. Authors acknowledge the financial support of the RSF according to the research project No. 18-73-10135.

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Thursday 30.05.2019

			chair: Sankaranarayanan
9:00	–	9:40	**Heine** Two-Dimensional Topological Polymers
9:40	–	10:20	**Persson** Structural and chemical tailoring of 2D MXenes
10:20	–	10:40	Ibragimova Theoretical study of two-dimensional titanium carbide MXenes functionalization process
10:40	–	11:20	*Coffee*
			chair: Tautz
11:20	–	12:00	**Booth** Synthesis and atomic scale patterning of 2D compounds
12:00	–	12:20	Krejčí NC-AFM recognition of molecular adsorption and on-surface reaction of Si and triple bond containing molecule
12:20	–	12:40	Alldritt Automated Structure Discovery in Atomic Force Microscopy
12:40	–	13:00	*Closing*
13:00	–	14:00	*Lunch*

Two-Dimensional Topological Polymers

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The discovery of graphene initiated an immense research effort in the field of two-dimensional (2D) crystals. Graphene shows extraordinary high stability, intriguing electronic, including topological, properties, and chemical inertness. Soon it was clear that 2D crystals can be formed from virtually all layered materials by top-down (exfoliation...), but also bottom-up (chemical vapor deposition...) approaches. The family of 2D materials contains a lot of remarkable phenomena, for example 2D semiconductors that get metallic when the number of layers is increased, 2D topological insulators, and 2D metals. It is somewhat less known that graphene represents also the prototype 2D polymer. 2D polymers (also 2D covalent-organic frameworks - 2D COFs) are a rather new family of synthetic 2D crystals where molecular units are stitched together with strong bonds. This offers a regular crystal lattice and thus materials comprising all collective phenomena that are known from solid state physics, however, with a much richer diversity due to the essentially infinite number of molecules that can be considered. A recent breakthrough was the discovery of chemical coupling reactions that achieve full conjugation between the constituting molecules, which is the precondition for the formation of 2D semiconductors with ballistic transport properties. For the 2D polymers I will to focus on structural diversity: while mathematically, 11 tilings are possible in two-dimensions (the so-called Kepler nets), nature offers much less structural diversity in crystalline 2D materials. By picking suitable molecular building units we can form lattices with structural topologies that impose, in turn, electronic topologies. One of the examples that I will highlight is the kagome structure, which produces both Dirac points and flat bands.

Structural and chemical tailoring of 2D MXenes

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MXenes constitute a family of two-dimensional transition metal carbides, carbonitrides and nitrides. MXenes are rapidly emerging as breakthrough materials in applications such as energy storage [1], water filtering, electromagnetic shielding[2], as catalysts for H2 evolution from water[3] and as astonishingly effective materials for capturing CO2. [4] Discovered in 2011, [5] the number of MXenes has expanded significantly and more than 20 different MXenes have been synthesized, with many more predicted from theoretical calculations. MXenes constitute an exceptional family of materials based on their availability for elemental alloying [1,6,7] and control of surface terminations, [4] which enables synthesis of a range of structures and chemistries. Consequently, the MXenes exhibit an unparalleled potential for tuning of the materials properties for a wide range of applications.

Using first principles calculations, theory guided synthesis, and characterization and tailoring by aberration corrected scanning transmission electron microscopy (STEM) in combination with X-ray photoelectron spectroscopy, we have explored some the range of structural and chemical modifications available in the MXene family.

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Theoretical study of two-dimensional titanium carbide MXenes functionalization process

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MXene phases are a new rapidly developing class of two-dimensional materials with suitable electronic, optical and mechanical properties for different applications [1]-[3]. These phases consist of transition metals such as Ti, Sc, Zr, Hf, V, Nb, Ta, Cr, Mo and carbon or nitrogen atoms, and can be produced through the etching of layered MAX phases. During the etching process, it is possible to terminate the surface by O, OH, and F functional groups in order to modify materials properties [4]-[6]. In this work, we accurately describe the surface distribution of functional groups and its interaction with titanium-based two-dimensional carbides in the solution through the use of different approaches. The free Gibbs energies of formation for the distinctly terminated surfaces have studied by combining DFT, phonon calculations and implicit solvation model. Our results indicate the formation of O, OH and F mixture, which coincides with experimental data [1]. Furthermore, DFT together with cluster expansion (CE), and Monte Carlo methods are employed to investigate the distribution of the functional groups on the surface. The proposed computational approach allows us to deeper understand a functionalization mechanism and introduce the range of experimental conditions for further tuning the MXenes properties.

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Synthesis and atomic scale patterning of 2D compounds

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Of the thousands of possible 2D materials [1], only a handful have been synthesised to date due to the need to develop and tailor precursors and recipes for each material. Here I will present recent progress on the synthesis of binary 2D compounds from simple elemental precursors and under otherwise identical conditions [2]. The atomically thin layers are epitaxially aligned to an underlying Au 111 surface, and show properties comparable to exfoliated materials in many cases. We have already synthesised over 30 distinct binary compounds in this way. I will also report on progress on the patterning of 2D materials at the nm- to atomic scale using standard lithography [3] and via in-situ environmental TEM techniques [4,5], including the role of encapsulating heterostructures, and perspectives for future patterning techniques based on these.

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NC-AFM recognition of molecular adsorption and on-surface reaction of Si and triple bond containing molecule

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In this work we are focusing on identification of reactants and products of Cu(111) mediated on-surface reaction. We used Non-Contact Atomic Force Microscopy (NC-AFM) experiments and simulations with microscope tip modified by CO molecule [1] for this purpose: The reactant is adorbed trimethelsilyl molecule. Since non-planar parts of this molecule are flexible, an enhanced model [2] of frequently used Probe Particle code [3,4] and extensive density functional theory (DFT) calculations were employed to recognise the atomistic model of the reactant, and to understand the experimentally measured contrast. The resolved model shows an unforeseen binding of small, partially aromatic molecule to the copper surface. The examined reaction was one-shot desilylative homocoupling performed for the first time on Cu(111) surface and which resulted in diacetylene linked anthracene oligomers. The NC-AFM force measurement combined with theoretical calculations revealed the chemical nature at the centre of products anthracene unit [5].

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Automated Structure Discovery in Atomic Force Microscopy

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While atomically-resolved non-contact atomic force microscopy images of molecules has developed since initial reports with flexible CO and Xe terminated tips [1,2], most experiments were limited to planar molecules, due to the challenge of interpreting AFM data from non-planar molecules. Further, the interpretation of adsorption geometry of a single molecule depends on tip termination and relaxation of the tip and the sample. It is possible to simulate AFM images using a simple mechanical model [3,4], but it still requires an extensive search for a similar molecular structure that matches the experimental data. Presented are results from a combined experimental and computational investigation that suggest a convolutional neural network (CNN) trained on simulated AFM data can learn an inverse mapping process easily and identify potential geometric configurations [5]. I will discuss the results of experiments performed on 1S-camphor on a Cu(111) surface and the associ ated com putational results which led to the understanding of the geometric configurations of this molecule. This process holds significant promise for applying high-resolution AFM to a variety of systems where understanding of the chemical structure of individual molecules can be a major breakthrough.

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Posters

Ilia Chepkasov

Atomic structure and electronic properties of few-atom alkali layers between two graphene and MoS2 sheets

Alexandru Ionut Chirita Mihaila

Quantifying the effect of in-plane vibrations for a 3D description of elastic electron scattering in transmission electron microscopy

Sergey Erohin

Nanostructuring few-layer graphene films by swift heavy ions for electronic application: tuning of electronic and transport properties

Somesh Chandra Ganguli

Magnetic field driven pseudogap in 2D $NbSe_2$

Sadegh Ghaderzadeh

Channeling effects in gold nanoclusters under He ion irradiation: a molecular dynamics study

Zineb Hamlati

Nanocrystalline and Amorphous FeAlSn and FeAlV Alloys Prepared by Mechanical Alloying

Konstantin Larionov

Prediction of novel 2D iron oxide films formation

Zhongpeng Lyu (lv)

Real-time study of phase transformation in anisotropic nanoparticles assembling by poor-solvent enrichment

Clifford Murray

Band bending in monolayer MoS_2 creating a one-dimensional hole gas

Tomasz Ossowski

Simulations of STM images of iron-oxides surfaces

Zheng-Ze Pan

Effects of Surface Modification on the Reactivity of Activated Carbon in Direct Carbon Fuel Cell

Pavel Sorokin

Electronic and magnetic properties of graphene/$Co_2Fe(Ge_{0.5}Ga_{0.5})$ Heusler alloy heterostructure

Camiel van Efferen

Layer dependent properties of quasi-freestanding 2H-TaS_2 investigated with STM and STS

Atomic structure and electronic properties of few-atom alkali layers between two graphene and MoS2 sheets

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Recent investigations of lithiation and delithiation of bilayer graphene showed that formation of a multilayer close-packed Li phase between graphene sheets is possible [1]. The formation of such a close-packed multilayer phase of lithium allows to increase the areal Li storage capacity. Sodium-ion batteries and potassium-ion batteries have also rapidlydeveloped. However, the formation of multilayer phases of sodium and potassium between the graphene layer has not previously been investigated. In this paper, using the density functional theory, we study the intercalation of sodium and potassium atoms intobilayer graphene with the main focus on the redistribution of electron density for different numbers of sodium and potassium layers. The electronic and structural properties close-packed multilayer phase of Li, K, Na between of molybdenum disulfide also was investigation.

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Quantifying the effect of in-plane vibrations for a 3D description of elastic electron scattering in transmission electron microscopy

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The atomic structure of materials is often studied using transmission electron microscopy. In addition to image formation, the energetic electrons impinging on the sample may also cause changes in the structure [1,2]. If momentum transfer from an electron scattering from the electrostatic potential of a nucleus leads to a kinetic energy transfer exceeding the displacement threshold energy of the atom, a defect is created. Recent studies have shown that the atom's vibration has a great influence on its displacement, since due to momentum conservation a moving atom can gain more energy than if it were static [3,4,5], activating dynamical process at lower electron energies. While those studies provide the most accurate description to date, a full three-dimensional description of the transferred energy including in-plane vibrations is needed to explain observed dynamic events of certain heteroatoms in graphene, such as pyridinic nitrogen[6]. In this work, we present t he general formalism for predicting the displacement cross section taking into account the atomic vibrations in all directions as well as the direction-dependant energy threshold. We apply this theory for the quantitative analysis of experimental data on the in-plane jumping of pyridinic nitrogen measured at two different electron energies.

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Nanostructuring few-layer graphene films by swift heavy ions for electronic application: tuning of electronic and transport properties

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Graphene, a two-dimensional (2D) carbon crystal with honeycomb structure was first isolated by the micromechanical cleavage of graphite in 2004. Beside the monolayer film, bilayered graphene attracts a specific attention due to its particular electronic properties. However like in the case of monolayer, the bilayered graphene is semimetal, therefore, the problem of the lack of a semiconductor band gap remains. A promising way to open a band gap in graphene or bigraphene is the making of periodical nanopores in the structure. It was predicted that these periodic arrays of holes in graphene lattice transform graphene from semimetal to semiconductor with a tunable band gap by means of the changing of the period and the size of the holes [1]. To create such kind of local structural modifications swift heavy ions (>1 MeV/nucleon) can be used. We have studied the morphology and electronic properties of single and few-layer graphene films nanostructured by the impacts of heavy high-energy ions [2]. It is found that ion irradiation leads to the formation of nano-sized pores, or antidots, with sizes ranging from 20 to 60 nm, in the upper one or two layers. The sizes of the pores proved to be roughly independent of the energy of the ions, whereas the areal density of the pores increased with ion dose. With increasing ion energy (>70 MeV), a profound reduction in the concentration of structural defects (by a factor of 2 - 5), relatively high mobility values of charge carriers (700 - 1200 cm2/V·s) and a transport band gap about 50 meV were observed in the nanostructured films. For high energy ions, structural modifications due to electronic stopping are normally most pronounced in the vicinity of the surface, whereas defects due to nuclear stopping mostly appear at the ends of ion trajectories or ranges, which are typically several micrometers. The interpretation of the experimental results through atomistic simulations requires proper treating of dynamic energy exchange between electronic and ionic subsystems in the irradiated system. To achieve this, we used a two-temperature molecular dynamics model in which atomic subsystem is described by classical molecular dynamics simulations, whereas electronic subsystem is characterized by local electronic temperature and treated as a continuum on a regular grid. Via this model we showed that even a single Xe atom with energy in the experimental range produces considerable amount of damage in graphene lattice, whereas high dose ion irradiation allows to propose a high probability of consecutive impacts of several ions into area already amorphized by previous ions, which increase average radius of the pore to match the experimental results. We also found that the formation of "welded" sheets due to interlayer covalent bonds at the edges and, hence, defect-free antidot arrays is likely at high ion energies (above 70 MeV).

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Magnetic field driven pseudogap in 2D $NbSe_2$

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There has been extensive study on 2-dimensional superconductivity over the past several decades. Superconductivity in several systems survive down to monolayer thickness. Several quantum phenomena such as Berezenskii-Kosterlitz-Thouless (BKT) transition, oscillation of superconducting transition temperature, superconductor-insulator transition (SIT) has been observed in the superconducting state in the 2-dimensional limit. Like reduced dimensionality and disorder, external magnetic field in a 2D superconductor also gives rise to several quantum phenomena such as superconductor-metal transition (SMT), SIT, quantum Griffiths singularity, vortex glass phase to electron-(or Bose) glass phase transition etc. Here we study the evolution of superconducting state of unit-cell thick dichalcogenide superconductor $NbSe_2$. From the evolution of superconducting spectra upon application of external out of plane magnetic field, we observe that the gap in the tunneling spectra continue s to persist till the highest possible applied field. This could be caused by the magnetic field driven superconductor to electron glass transition proposed in two dimensional superconductors.

Channeling effects in gold nanoclusters under He ion irradiation: a molecular dynamics study

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Ion channeling is a well-known effect in ion irradiation processes, which is a result of ion moving between the rows of atoms. It drastically affects the ion distribution, ion energy-loss and consequently the damage production in the target. Therefore one could derive the ion-channeling pattern out of the energy-loss behavior of ion-target interaction. Ion channeling effect is studied for a few pure element crystals and also for some compounds in a systematic way [1]. In this work, we focus on nano-structures which are of major importance, due to their high surface-to-volume ratio. Our results, for different gold cluster sizes, show that ion-channeling occurs not only in the principal low-index, but also in other directions in between. The strengths of different channels are specified, and their correlations with sputtering-yield and damage production is discussed.

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Nanocrystalline and Amorphous FeAlSn and FeAlV Alloys Prepared by Mechanical Alloying

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Objective of the work was to synthesize nanostructured FeAlSn and FeAlV alloys powder by mechanical alloying (MA). The work concentrated on synthesis, characterization, structural and microstructural properties of the alloys. Nanostructured FeAlSn and FeAlV intermetallics were prepared directly by MA in a high energy ball mill. To prevent oxidation phenomena, the mixed powder was sealed in a cylindrical vial under an argon atmosphere with stainless steel balls. Phase transformation, structural changes, morphology and particle size measurement during MA were investigated by X-ray diffraction (XRD), Mössbauer spectroscopy, Scanning electron microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDX) respectively. XRD and SEM studies revealed the alloying of elemental powders as well as transition to nanostructured alloy. A structural refinement of X-ray powder data on the mechanically alloyed products according to the Rietveld method has detailed the progressive dissolution of aluminium, tin and vanadium into the lattice of α-iron as a function of MA time. The complete formation of bcc-FeAlSn solid solution was observed after 12 h of milling. Crystallite size of 5nm was obtained after 24 hours of milling

Prediction of novel 2D iron oxide films formation

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Two-dimensional (2D) and quasi-2D materials have attracted increasing attention since the discovery of graphene. A short time ago it was reported [1] about comprehensive study of monolayer copper oxide clusters with untypical square lattice: theoretically observed atomic structures were claimed to be stable and correspond to available experimental data. Another remarkable report was devoted to two-dimensional iron in pores of graphene [2] that could also open new possibilities in the field of research and application of low-dimensional structures. Here we report a new material based on transition metal oxide FeO that supplements the results of 2D-CuO and extends the class of structures with uncommon two-dimensional square lattice [3]. Electronic and magnetic properties were investigated for FeO films of various thickness. Having based on the effect of graphitization of films of ionic compounds [4], the exfoliation effect of FeO films into layers with a square two-dimensional lattice was studied and the critical film thickness applicable for such transition was determined as well. The stability of the iron oxide monolayer in a free-standing state at 0 K and finite temperature as well as in heterostructure was considered in details. In search of a stable compound, structures based on the monolayer of FeO in graphene matrix were investigated. Analytical dependence of the edge energy on the type of interface was obtained which is in a good agreement with ab initio calculations. By means of Wulff construction, the optimal shape of the edges at the FeO/graphene interface was determined. The TEM images of the square lattice of iron oxide in the pores of graphene obtained during the simulation demonstrate good agreement with experiment [2] and let us to suppose that experimental samples could consist of 2D iron oxide. Thus, the obtained results on the structure of iron oxide and its promising antiferromagnetic and semiconducting properties expand the underinvestigated class of two-dimensional compounds with a square lattice and confirm the possibility of synthesizing structures based on it. The authors gratefully acknowledge the financial support of the Russian Science Foundation (Project identifier: 17-72-20223).

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Real-time study of phase transformation in anisotropic nanoparticles assembling by poor-solvent enrichment

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The interest in ordered materials obtained through the assembly of anisotropic nanoparticles with well-defined sizes and shapes has steadily increased in recent years.[1] Recent developments focus towards preparing functional nanoparticle assemblies with long-range translational order and atomic coherence that display collective optic, magnetic, or mechanical properties have fueled this interest.[2, 3] Controlling the structure and morphology of nanoparticle assemblies is a very crucial part for understanding and exploiting such collective properties. Although various methods were established for fabricating desirable assemblies, the formation and transformation mechanisms in the assemblies are still poorly understood. In this work, we study the in-situ assembly of iron oxide nanocubes by poor-solvent enrichment in levitating colloidal droplets using a combination of techniques covering several length scales from nanometer to millimeter.[4] Owing to a substrate-free technique, it is easy to directly obtain quantitative information from the time-resolved SAXS measurements without the need of complex approximations (e.g., grazing incidence measurements). After the superlattice formation in the drying droplet, a rapid and continuous transformation from tilted face-center-cubic (fcc) phase to perfect fcc phase was observed, which facilitated by excess surfactant and solvent polarity changing. Our results show that: (1) the formation of highly ordered superlattices is dominated by the evaporation-driven increase of the solvent polarity and particle concentration; (2) the later transformation of the resulting superlattice can be controllably induced by applying different growth parameters (e.g. s olvent systems, free ligand concentration). This study introduces an unconventional degree of freedom that can be utilized for tuning superlattice structures and raises new questions about the forces that control self-assembly.

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Band bending in monolayer MoS_2 creating a one-dimensional hole gas

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We epitaxially grow high-quality monolayer molybdenum disulfide (ML-MoS_2) on graphene on Ir(111) [1], which is close to freestanding on this substrate [2]. We probe its electronic structure with low temperature scanning tunnelling spectroscopy (STS).

Localised charge at defects - such as 4|4E-type mirror twin boundaries (MTBs), flake edges and certain point defects - is seen to cause a large upward bending of the bands in the surrounding ML-MoS_2 semiconductor. This nanometre-scale bending creates a potential well in the valence band, leading to a 1D confinement of the charge carriers (holes) perpendicular to the defect - a 1D hole gas is formed. We study this 1D hole gas with STS in the well-defined environment of the 4|4E MTB, and seek to understand and describe its behaviour with the help of density functional theory.

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Simulations of STM images of iron-oxides surfaces

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Simulated scanning tunneling microscopy images of different terminations of iron-oxide surfaces hematite (0001) and magnetite (111), are presented and compared with experiment [1]. Based on DFT+U calculations of α-Fe_2O_3(0001) and Fe_3O_4(111) surfaces the STM images are simulated within Chen approach [2] using Bskan code [3]. Different biases and tip-sample distances are considered as well as the role of tip type and its functionalization by different atoms or molecules are discussed. Good agreement is found between measured and simulated STM images for hematite surfaces, whereas for magnetite surfaces some discrepancies are observed.

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Effects of Surface Modification on the Reactivity of Activated Carbon in Direct Carbon Fuel Cell

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A direct carbon fuel cell (DCFC) is the only fuel cell type that converts the chemical energy stored in solid carbon, which could be obtained from coal and biomass, into electricity directly via an electrochemical route with a higher energy efficiency and less pollution than conventional coal-fired power plants [1,2]. In this work, the effect of the surface properties of carbon fuel on its electrochemical oxidation reactivity is investigated. Activated carbon (AC) is pre-treated with HNO_3 and NaOH, respectively, which both increase the oxygen content and decrease the graphitization degree of AC. The amount of hydroxyl groups on the surface of AC increases after the treatments with HNO_3 and NaOH, and then decreases during the subsequent heating process in an inert atmosphere. On the contrary, the carbonyl and quinone groups on the surface of the activated carbon remain stable during the heating process. The activated carbon treated with HNO_3 shows the highest reactivity towards oxidation and reverse Boudouard reactions due to its lowest graphitization degree and highest oxygen content. The performance of the cell supported by a 380-μm-thick yttria stabilized zirconia (YSZ) electrolyte layer with 50 wt.% $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ -50 wt.% Gd_2O_3 doped CeO_2 as the electrodes is investigated with various fuels. The cell with AC-HNO_3 as the fuel has exhibited a maximum power density of 128 mW cm^{-2} at 800 ^oC.

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Electronic and magnetic properties of graphene/$Co_2Fe(Ge_{0.5}Ga_{0.5})$ Heusler alloy heterostructure

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As a zero-gap semiconductor with a pin-hole free nature, graphene was proposed as an attractive low energy barrier for vertical spin-valves (SV) to solve the trade-off between MR ratio and low RA product usually observed in MgO-based vertical SV. So far, the MR ratio reported in graphene-spacer vertical SV is far below the application level due to the usage of conventional ferromagnetic electrodes (Ni, Co, Fe etc.) with low spin polarization. Utilizing high spin-polarized ferromagnetic electrodes such as full Heusler alloys is potential way to enhance the MR ratio in graphene-spacer SV, however, there is no precedent for success in the growth of graphene on Heusler alloy underlayer. Here, we report the realization of high-quality single-layer graphene (SLG) by in situ high vacuum CVD method on a magnetron-sputtered half-metallic Heusler alloy $Co_2Fe(Ge_{0.5}Ga_{0.5})$ (CFGG) underlayer. CFGG was selected in this work because of its the highest spin-polarization among the various types of Heusler alloys. So far, the largest MR ratio (82%@ room temperature and 285%@10 K) recorded in metal-based vertical SV was based on CFGG. The heterostructure of SLG/CFGG was carefully investigated by both experimental ways and density function theory (DFT) calculations. We quantitatively observed an enhanced magnetic moment at the interface of SLG/CFGG, which is well resembled by simulation with a superlattice model of FeGeGa-terminated SLG/CFGG interface. The weak chemical bonding between SLG and CFGG(001) attributes to a quasi-freestanding nature of SLG on CFGG(001) and vice versa. Combination of the advantage of graphene as low resistive spacer material for ve rtical S V and long-lifetime spin channel material for lateral SV, the features of high bulk spin-polarization and robust magnetic moments at the interface make the SLG/CFGG heterostructure to be an extremely promising building block for the further development of high-performance graphene-spintronic devices.

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Layer dependent properties of quasi-freestanding 2H-TaS_2 investigated with STM and STS

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We epitaxially grow quasi-freestanding TaS_2 multilayers on graphene on Ir(111) and investigate their thickness dependent properties. Using scanning tunnelling microscopy the monolayer is observed to be in the expected 3×3 charge density wave (CDW) phase, whereas the bilayer unexpectedly shows a 2×2 superstructure, which we prove to be of CDW nature. Furthermore, the moiré of Gr on Ir(111) is no longer visible through the bilayer. We probe the electronic structure with low temperature scanning tunnelling spectroscopy, and correspondingly find a CDW energy gap around the fermi level. The width of the gap is compared with its monolayer analogue. Supported by density functional theory calculations we disentangle contributions to the electronic structure stemming from intrinsic bilayer properties, stacking effects and possible intercalation.

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