

51st Heyrovský Discussion

1D and 2D Materials

Book of Abstracts



May 27th – May 31st, 2018

The 51st Heyrovský Discussion 2018 was held at the Conference centre in chateau Třešť in town Třešť in the Czech Republic, from May 27th to May 31st, 2018.

Sponsors



51st Heyrovský Discussion

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Organizers

**Martin Kalbáč, Otakar Frank
and Jana Kalbáčová Vejpravová**

May 27th – May 31st, 2018

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PROGRAMME

Sunday, May 27th			
14:00	Registration in the entrance hall of the J. Heyrovský Institute		
15:00	Departure of a special bus from the J. Heyrovský Institute (Dolejškova 3, Prague 8 – Kobylisy)		
17:00	Arrival at the Castle Třešť, Registration		
19:00	Welcome buffet		
Monday, May 28th			
7:00-			
9:00	Breakfast		
9:00	Morning session:		
	Opening of the Discussion		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:05-10:05	M. Kalbáč	S. Reich	Surface- and tip-enhanced Raman scattering on carbon nanostructures
10:05-10:25		V. Valeš	Enhanced Raman scattering on functionalized graphene substrates
10:25-10:45		S. Heeg	Carbon nanotube chirality determines properties of encapsulated long linear carbon chains
10:45	Coffee break		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
11:05-11:45	S. Reich	<u>K. Bolotin</u>	Excitons in two-dimensional semiconductors “talking” to their environment
11:45-12:05		M. Hulman	Spectroscopy of horizontally and vertically aligned thin MoS ₂ films
12:05-12:25		F. Karlický	Fluorographane C ₂ FH: stable and wide band gap insulator with huge excitonic effect
12:25	Lunch		
14:30	Afternoon session:		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
14:30-15:10	K. Bolotin	<u>S. Berciaud</u>	Charge and energy transfer in two-dimensional heterostructures
15:10-15:30		A. López-Ortega	Plasmon Induced Magneto-Optical Enhancement in Metallic Ag/FeCo Core/Shell Nanoparticles Synthesized by Colloidal Chemistry
15:30-15:50		H. Tarábková	Electrochemically Controlled Winding and Unwinding of HOPG Supported Carbon Nanoscroll

15:50 Coffee break + Posters			
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
16:20-17:00	U. Wurstbauer	<u>A. Ciesielski</u>	2D materials: preparation, functionalization and application in sensing
17:00-17:20		P. Kovaříček	Chemistry on and with graphene: Introducing Selectivity, Functionality and Motion
17:20-17:40		J. Plšek	Fluorinated Graphene on Copper – Reactivity Driven by Support Phase Orientation and Decomposition under Heat Treatment
17:40-18:00		K. Drogowska	Effect of hydrogenation on the particular layer in isotopically labelled Turbostratic- and Bernal stacked bilayer graphene
18:30 Dinner followed by beer degustatin + Posters			

Tuesday, May 29th			
7:00-9:00 Breakfast			
9:00	Morning session:		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	A. Grüneis	<u>J. Kotakoski</u>	Atomic-Scale Defect-Engineering of 2D Materials with Electron and Ion Beam
9:40-10:00		N. Bendiab	Defects and interlayer coupling in in van der Waals heterostructures
10:00-10:20		M. Dopita	X-ray Scattering on Highly Perturbed Carbon Nanomaterials
10:20 Coffee break			
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:50-11:30	J. Kotakoski	<u>A. Krashennikov</u>	Electron Irradiation-Induced Defects and Phase Transformations in Two-Dimensional Transition Metal Dichalcogenides
11:30-12:10		<u>U. Wurstbauer</u>	In-situ spectroelectrochemistry of catalytically active sites in molybdenum dicalcogenide mono- and fewlayers for HER
12:10 Lunch			

14:00	Afternoon session:		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	
14:00-14:40	J. Kalbáčová Vejpravová	<u>A. Gómez Roca</u>	Magnetoplasmonic Heterostructures for Theranostic Applications
14:40-15:00		J. Honolka	Single 3d transition metal atoms on multi-layer graphene systems: electronic configurations, bonding mechanisms and role of the substrate
15:00-15:20		J. Červenka	Electronic detection of DNA on graphene
15:20-15:40		A. Poryvai	Multi-responsive nanocomposites based on liquid crystals
16:10	Departure for Jihlava Brewery for tour and dinner		
22:00	Return from Jihlava Brewery		
Wednesday, May 30th			
7:00-9:00	Breakfast		
9:00	Morning session:		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	A. Krasheninnikov	<u>A. Grüneis</u>	Resonance Raman spectrum of epitaxial graphene doped towards the Lifshitz transition
9:40-10:00		P. Janda	Quasi-2D Liquid Nanofoam on Water-Immersed Solid Surface
10:00-10:20		H. Shiozawa	Physical properties of metal-organic frameworks doped with TCNQ
10:20	Coffee break		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:50-11:30	R. Korytar	<u>O. Fenwick</u>	Thermoelectric properties of thin films
11:30-11:50		J. Kunc	Back-gated epitaxial graphene on SiC
11:50-12:10		V. Skákalová	Graphitization of diamond through different routes
12:10	Lunch		
14:30	Departure to Telč (Castle tour and general sightseeing)		
17:30	Departure from Telč		
19:30	Conference Dinner back in Třešť		

Thursday, May 31st			
7:00-9:00 Breakfast			
9:00	Morning session:		
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	O. Fenwick	<u>J. Parthenios</u>	Controllable synthesis of highly crystalline single and few layer MoS ₂ and the role of growth-induced strain
9:40-10:00		V. Guerra	Graphene as substrate for selective self-assembly of 2-D materials for optoelectronic applications
10:00 Coffee break			
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:30-11:10	J. Parthenios	<u>R. Korytár</u>	Transport and incommensurate quantum-size oscillations in oligoacene molecular wires
11:10-11:30		O. Frank	2D-3D Interfaces from the Topography Standpoint
11:30-11:50		T. Verhagen	Mastering the topography of graphene
11:50 Lunch			
13:30 Departure for Prague			

Monday, May 28th

Surface- and tip-enhanced Raman scattering on carbon nanostructures

Stephanie Reich

Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

Surface-enhanced Raman scattering (SERS) describes the giant enhancement of the Raman cross section close to a metal surface. SERS can detect single molecules by optical spectroscopy. Its variant, tip-enhanced scattering (TERS) increases the resolution of Raman imaging down to the molecular limit. Despite the wide-spread use of plasmon-enhanced Raman spectroscopy in imaging and materials characterization its fundamental principles remain debated. The dominant mechanism for SERS is thought to be plasmonic enhancement; the large Raman cross section is explained as an enhancement by the localized surface plasmons of metal nanoparticles.

In this talk I will discuss our research on SERS and TERS of carbon nanostructures – graphene, carbon nanotubes, and nanotubes filled endohedrally with organic molecules. I will highlight how SERS allows us to study strain, doping, and optical selection rules on a nanoscale level. At the same time, carbon nanostructures are shown to be an ideal test bed to study the fundamentals of SERS and to quantify the plasmonic contribution to the Raman enhancement. I will also present first results on hyperspectral tip-enhanced Raman scattering that maps optical transitions in real space with nanoscale resolution.

Enhanced Raman scattering on functionalized graphene substrates

Václav Valeš^a, Petr Kovaříček^a, Michaela Fridrichová^a, Xiang Ji, Xi Ling^b, Jing Kong^b, Mildred S Dresselhaus^b, Martin Kalbáč^a

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The concept of graphene-enhanced Raman scattering (GERS) was proposed and experimentally demonstrated in 2010. It was observed that molecules in very low concentrations exhibit a significant Raman signal in vicinity of graphene layer. In addition, the photoluminescence of molecules placed on graphene is quenched. A theoretical work by Barros et al. brought more insight by suggesting conditions for GERS enhancement.

In our work we used functionalized graphene to experimentally probe the theoretical GERS conditions with Rhodamine 6G (R6G) molecules by assuming the change of the Fermi level of graphene due to its functionalization. We showed that the photoluminescence of R6G was quenched also with functionalized graphene. By comparing multiple R6G Raman modes on differently functionalized graphene layers we were able to qualitatively validate the theoretical GERS conditions. Furthermore, we studied how the degree of functionalization, specifically fluorination, affects the GERS effect by inducing sp³ defects in graphene. We found that high fluorination degree leads to loss of the GERS effect, however it can be restored upon fluorine removal.

References

- [1] V. Valeš, P. Kovaříček, X. Ji, X. Ling, J. Kong, M. S. Dresselhaus, and M. Kalbáč, "Quenching of photoluminescence of Rhodamine 6G molecules on functionalized graphene," *Phys. status solidi B* 253, 2347–2350 (2016).
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Carbon nanotube chirality determines properties of encapsulated long linear carbon chains

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Long linear carbon chains encapsulated inside carbon nanotubes are a very close realization of carbyne, the truly one-dimensional allotrope of carbon at the one-atom cross section limit [1]. The local environment inside a nanotube, characterized by its chirality, strongly affects the encapsulated chains through interactions such as van-der-Waals forces, charge transfer or dielectric screening [2]. However, while the electronic and vibronic properties of the encapsulated chain are governed by its nanotube host, the correspondence between the tube's chirality and the properties of the encapsulated chain has not been investigated experimentally.

Here we study individual pairs of double-walled carbon nanotubes and encapsulated linear carbon chains by tip-enhanced Raman scattering (TERS) [3]. We observe that the radial breathing mode (RBM) of the inner nanotube correlates with the frequency of the carbon chain's Raman mode (C-mode) revealing that the nanotube chirality determines the vibronic and electronic properties of the encapsulated carbon chain. As a general trend, the Raman shift and the band gap of the encapsulated long linear carbon chains increases for larger inner carbon nanotube diameters as shown in Figure 1. No length dependence of the chain's Raman mode frequency is evident for the long linear carbon chains investigated, suggesting that they can be viewed as a close to perfect representation of carbyne.

Our results provide the missing link that connects the properties of the encapsulated long linear carbon chains with the structure of the host nanotube, and identifies parameters for tuning the electronic and vibronic properties of carbyne for device applications. nanotubes are a very close realization of carbyne, the truly one-dimensional allotrope of carbon at the one-atom cross section limit [1].

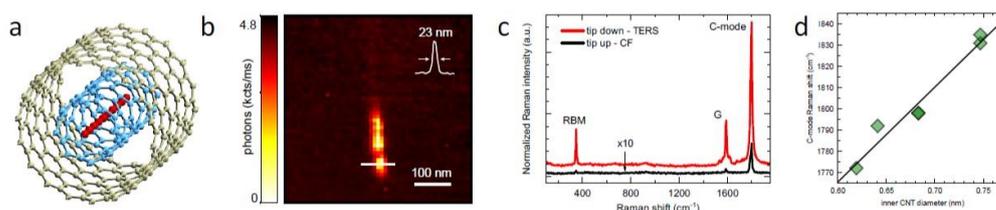


Figure 1: (a) Schematic of linear carbon chain (red) encapsulated inside double-walled carbon nanotube (blue/yellow). (b) TERS image of the chain's Raman mode (C-mode). (c) Confocal (black) and tip-enhanced Raman spectrum (red) of the chain shown in (b). The RBM of the inner carbon nanotube is in resonance with the excitation at 633nm. (d) Raman shift of the long linear carbon chain's C-mode depends linearly on the diameter of the inner carbon nanotube. All panels are adapted from [3].

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- [1] L. Shi *et al.* Nature Materials **15**(6), 634 (2016).
- [2] M. Wank *et al.*, Physical Review B, **94**(19), 195422 (2016).
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Excitons in two-dimensional semiconductors “talking” to their environment

Kirill Bolotin

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Every atom in two-dimensional semiconductors from the group of Transition Metal Dichalcogenides (TMDs) belongs to the surface. Because of that, TMDs are strongly affected by their microenvironment. In this talk we show that excitons, bound electron/hole pairs, in TMDs can serve as exquisite probes of the physical and chemical properties of that microenvironment.

First, we show that TMD excitons are strongly screened by nearby dielectrics. In suspended TMD, the behavior of pristine material is approached. We also examine frequency-dependent screening of excitons in TMD and show that the frequency-dependent dielectric function of the environment can be effectively “sampled” by examining spectral shifts and intensity redistribution between neutral, charged, and defect-bound excitons. Second, we examine near-field energy transfer between TMDs and nanoscale quantum emitters (semiconductor quantum dots or dye molecules) near it. We show that such energy transfer is very efficient, and that its rate can be controlled through electrical gating. Finally, we examine binding of excitons in TMDs to charged molecules on their surface. We demonstrate new molecule-specific excitonic species produced by such binding.

Spectroscopy of horizontally and vertically aligned thin MoS₂ films

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One of the most used methods for growing very thin films of MoS₂ is sulfurisation of predeposited Mo layers. We grew MoS₂ films on various substrates sulfurising Mo layers with different thickness. AFM measurements showed that our MoS₂ films are nanocrystalline with the grains as large as 40 nm randomly oriented with respect to each other. We further characterised the thin films by grazing incidence wide-angle X-ray scattering (GIWAXS). The most intense (002) diffraction observed defines the *c*-direction perpendicular to the individual MoS₂ layers. We have seen from the GIWAXS measurements that the angle between the *c*-direction and the substrate has two prominent values of 0 and 90°. This corresponds to the MoS₂ layers aligned parallel and perpendicular to the substrate, respectively. In agreement with previous reports [1], the alignment depends only on the thickness of the initial Mo layer and neither the details of the growth procedure nor the substrate have a significant impact on it. We may consider our samples as powder-like MoS₂ thin films.

In this contribution, we focus more on consequences the layer alignment has on optical properties of thin MoS₂ film. We measured parallel and crossed polarised Raman spectra. The intensity ratio of the two strongest Raman modes at ~ 384 and 408 cm⁻¹ does not depend for any polarisation on the layer thickness as long as the layer alignment is maintained. On the other hand, the intensity ratio does depend on the MoS₂ layer alignment. For crossed polarisation, it is much higher for parallel MoS₂ alignment compared to the perpendicular one. This way, we may decouple the impact of the layer thickness and alignment on the intensity of the MoS₂ Raman lines. As a consequence, it enables us to determine unambiguously the layer alignment only from Raman measurements. We also calculated the intensity ratio for different polarisations. A reasonable qualitative agreement with measurements was obtained.

References

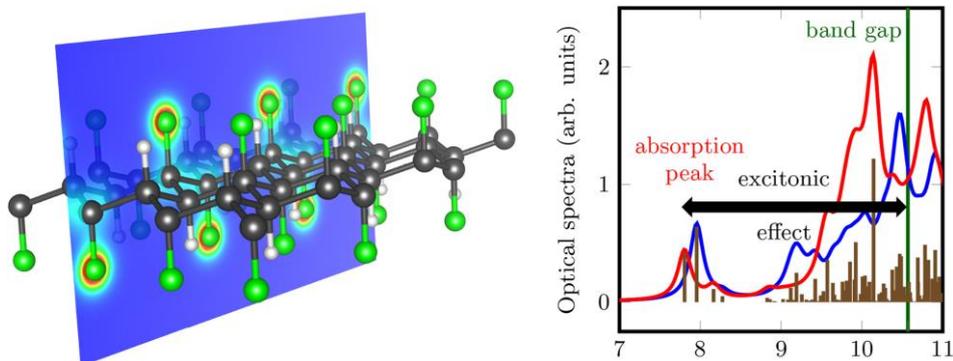
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Fluorographane C₂FH: stable and wide band gap insulator with huge excitonic effect

František Karlický, Josef Turoň

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2D materials derived from graphene by attachment of hydrogen and halogens have attracted considerable interest because of their potential applications [1]. We present structural, vibrational, electronic and optical properties of recently prepared [2] fully fluorinated and hydrogenated graphene, called fluorographane. We consider 1:1 ratio of F and H adatoms and we carefully investigate possible structural conformers in C₂FH stoichiometric material. We show that all conformers are dynamically stable and homogeneous structures with F and H atoms on both sides of carbon honeycomb structure are more stable than the Janus structures with F atoms on one side and all H atoms on the other [3]. While the main structural and vibrational features are roughly similar for various conformers, electronic and optical properties are very sensitive to local structure (namely specific combinations of F and H adatoms on the graphene surface) and differ significantly. Our highly accurate results based on many-body methods (GW and BSE) indicate that homogeneous fluorographane has unusually wide indirect electronic band gap of ~10 eV (larger than both pure graphane CH and pure fluorographane CF [4]) and embodies a huge excitonic effect (~3 eV). Fluorographane C₂FH is therefore a material with the widest electronic gap and a largest binding energy of exciton in the class of currently known 2D materials.



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Charge and energy transfer in two-dimensional heterostructures

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Research into two-dimensional materials is one of the hottest topics in physics and material science. These thin, flexible structures exhibit many unique material, optical, and electrical properties that make them well suited to applications as diverse as photodetectors, solar cells, light-emitting screens, and biosensors. Taking this a step further, innovative devices could be built by tightly stacking atomically thin layers to create designer materials. These structures, known as van der Waals heterostructures (vdWHs), can exchange charge carriers and energy across the interfaces between layers on short timescales following optical excitation. These competing processes govern the optoelectronic response of vdWHs but remain poorly understood. Here, we experimentally study a model vdWH to better understand these interlayer charge and energy transfers [1].

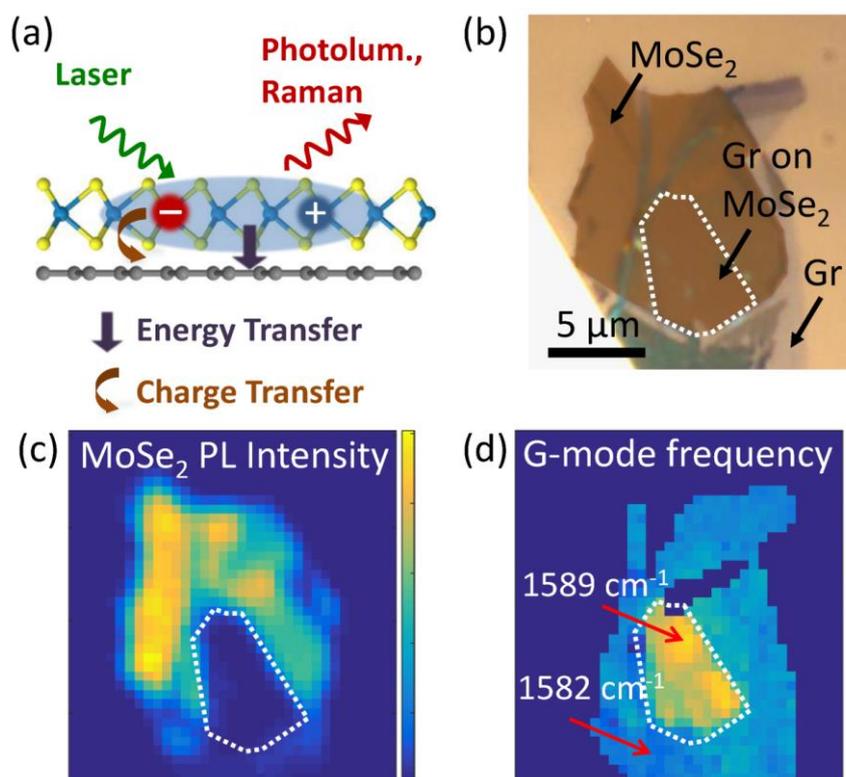


Figure 1: Illustration of photoinduced charge and energy transfer from a monolayer of transition metal dichalcogenide (here MoSe₂) to graphene (Gr) (b) Optical image of a MoSe₂/graphene (Gr) heterostructure. The map of the Gr Raman G-mode frequency (c) and of the MoSe₂ photoluminescence intensity (d) reveals clear signatures of interlayer coupling on the heterostructure (dashed contour in b-d).

Specifically, we investigate a metal-semiconductor junction made of a graphene monolayer transferred onto a transition metal dichalcogenide (TMD, here molybdenum diselenide) monolayer. By measuring light emission from the TMD, we demonstrate that interlayer coupling to graphene drastically reduces the photoluminescence yield and exciton lifetime. Additionally, using Raman spectroscopy, we finely probe the frequency and linewidth of the optical phonon modes in the monolayers. These parameters are highly sensitive to the charge carrier density and show a net photo-induced electron transfer from TMD to graphene. Remarkably, exciton dynamics in a TMD-graphene vdWH is largely independent of the existence of a net charge transfer.

This key result strongly suggests that picosecond interlayer energy transfer from TMD to graphene dominates the photoresponse of these heterostructures. Highly efficient energy transfer now has to be carefully considered when designing devices based on 2D materials. As an outlook, implications of our results for opto-valleytronic applications will be discussed in light of our recent studies of valley polarization and coherence in TMD-graphene vdWH [2].

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Acknowledgement:

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Plasmon Induced Magneto-Optical Enhancement in Metallic Ag/FeCo Core/Shell Nanoparticles Synthesized by Colloidal Chemistry

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Photonic materials for the control of the polarization of light have been demonstrated a powerful tool to develop information carriers in optical communication, sensing and imaging.^[1,2] A special case is the so-called magneto-plasmonic metamaterials where ferromagnetic and plasmonic structures are combined in a unique entity. While ferromagnetic structures are characterized by large magneto-optical Faraday and Kerr effects (namely, dependence of optical polarization of light transmitted and reflected on magnetization); plasmonic materials enable the electromagnetic energy confinement at the nanoscale and enhanced interactions with external magnetic fields due to the electromagnetic excitation of collective oscillations of the free-like electrons. The interplay between magneto-optical and plasmonic functionalities in a nanostructure can be then used to build 2D metasurfaces for the active control of light polarization, where the magnetic field is used as a polarization control knob for light reflected and/or transmitted by nm-thick surfaces,^[3] as well as to ultrasensitive bio-detection schemes.^[4]

Up to now, the physical growth methods have shown the only exploitable approach to prepare these types of nanostructures. Here, we demonstrate the chemical synthesis of magneto-plasmonic core/shell nanocrystals with enhanced magnetic control of optical properties comparable to the best results reported for nanostructures growth by physical method. Ag/FeCo core/shell nanocrystals were synthesized in a combination of hot injection and polyol approaches, demonstrating that the well-defined structures of both components, their interface and the optimized morphology, where the plasmonic and magnetic components are placed in the core and the shell regions, are the responsible of the observed large enhancement of magnetic control of light polarization. Therefore, it is confirmed the possibility to develop tunable magneto-optical materials by hybrid magneto-plasmonic structures synthesized by chemical methods.

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Electrochemically Controlled Winding and Unwinding of HOPG Supported Carbon Nanoscroll

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The carbon nanoscroll (CNS) is carbon nanostructure formed by rolling of graphene sheets. However, in contrast to carbon nanotube (CNT), the CNS open-coil structure is more radially flexible, because to overcome van der Waals interlayer interactions requires less amount of energy than the deformation of sp² carbon bond in close tubular CNT structure. Thus DFT calculations[1] predict electroactuation effects order of magnitude higher for CNS than for CNT.

CNSs were first reported in 1960 as byproducts of arc discharge experiments using graphite electrode [2]. Later, several different methods[3] producing CNSs at high yield, low cost and offering better control of final product were developed.

In our study[4], we have utilized CNSs spontaneously formed after peeling off basal plane HOPG surface by adhesive tape. Scrolled nanostructures with length range of 10²-10³ nm and diameter within the range of tens nanometers were considered. Freshly cleaved basal plane HOPG serving as a working electrode with supported CNS was immersed in an aqueous 0.1 M H₂SO₄ solution and successive potential steps from 0 V up to -0.9 V were applied. The CNS potential-driven actuation was monitored by in-situ AFM imaging during electrochemical experiment. Reversible changes of radial dimension exceeding 10 nm in axial and 50 nm in lateral direction were observed selectively on scrolled nanostructures, while other parts of HOPG surface including planar areas, lifted and simple bended steps remain intact. The mechanism explaining observed phenomenon is discussed.

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2D materials: preparation, functionalization and application in sensing

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Achieving the full control over the production, and processability of high-quality 2d sheets from bulk crystals represents a major challenge with potential interest for numerous applications in opto-electronics, energy, sensing and composites. The outstanding effort dedicated to tackle this challenge in the last decade revealed that certain organic molecules are capable of leveraging the exfoliation of graphite and related materials in liquid media. The use of small organic molecules such as dispersion-stabilizing agents is expected to promote the exfoliation of graphite when the chosen molecules have a strong affinity for the basal graphitic planes, being stronger than that of the solvent molecules interacting with graphene. In this framework, we have demonstrated that by mastering a supramolecular approach it is possible to improve the yield of graphene in liquid-phase exfoliation (LPE) process and produce high-quality 2d nanosheets flakes from bulk crystals [1-6].

The functionalization of 2d nanosheets allows creating foams and coatings integrating novel functions, which comes from the intrinsic design of the molecular units. We will demonstrate that the use of hygroscopic molecules allows the generation of humidity sensor whereas the use of molecules with different rigidity allows creating pressure sensors with high sensitivities. Graphene based humidity sensors are promising for their low cost and low temperature operation, however they presents critical drawbacks, such as low sensitivity, long response and recovery times and poor stability. With the aim of improving the sensing performances, we have developed a novel humidity sensor based on a layered film of functionalized graphene oxide (f-GO), which exhibits an improved sensing performance compared to the neat GO. In particular our f-GO sensor is characterized by ultrafast response and recovery in the sub-second range, a high response, especially towards low humidity levels, low hysteresis, and excellent repeatability and stability. Moreover, we will demonstrate a series of pressure sensors based on GO functionalized with organic molecules having different rigidity. The rigidity of the molecular linkers was found to affect the sensitivity of the GO-based sensors. In general, the as prepared pressure sensors display high sensitivity (ca. 0.8 kPa⁻¹) at low-pressure region (0-0.6 kPa) has been achieved within a short response time (≈ 24 ms) and detection limit as low as 7 Pa. Finally, we will demonstrate that the GO-based pressure sensors can be used to monitor heart pulses and easily transformed into a matrix able to provide a 3D mapping of the pressure exerted by different objects.

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Chemistry on and with graphene: Introducing Selectivity, Functionality and Motion

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Reaching the ultimate potential of graphene in multitude of fields requires means of on-demand tuning of its properties. Covalent chemical functionalization of the graphene monolayer provides merely unlimited space for targeted attachment of various moieties and thus manipulation of intrinsic parameters of the material. The approach, however, is facing three crucial challenges on the way towards its goal: achieving the chemical reaction, properly characterizing its product, and application of the chemical functional group in extending functionality of the material.

The covalent modification of graphene can now be realized by three mechanistically different approaches, by i) radical grafting,[1] ii) nucleophilic[2] or iii) electrophilic substitution.[3] This is crucial to overcome incompatibilities of functional groups with the grafting protocol. The characterization of 2D materials is traditionally dominated by Raman and X-ray photoelectron spectroscopies, however they provide only limited insight into the actual chemical transformation taking place at the surface. Successful application of several other methods, including mass spectrometry,[4] SERS[2] or IR spectroscopy[5] has been demonstrated, thus completing the information about structure and integrity of the grafted species to the monolayer material regardless the functionalization protocol employed.

The introduced moieties indeed modulate the electronic structure of graphene, e.g. Fermi level, which consequently for instance tune the efficiency of graphene-enhanced Raman scattering.[6] However, the grafted groups also bring new functionalities inherent to their chemical properties, such as sulfonyl groups on graphene serving as the catalyst and stabilizing layer for selective polymerization of PEDOT.[7] Prior patterning of graphene provides selective formation of such heterostructures with superb spatial resolution.[8] Finally, covalently dynamic bonds can be envisaged, allowing for thermodynamically controlled connectivity and out-of-equilibrium manipulation with species on the nanoscale.

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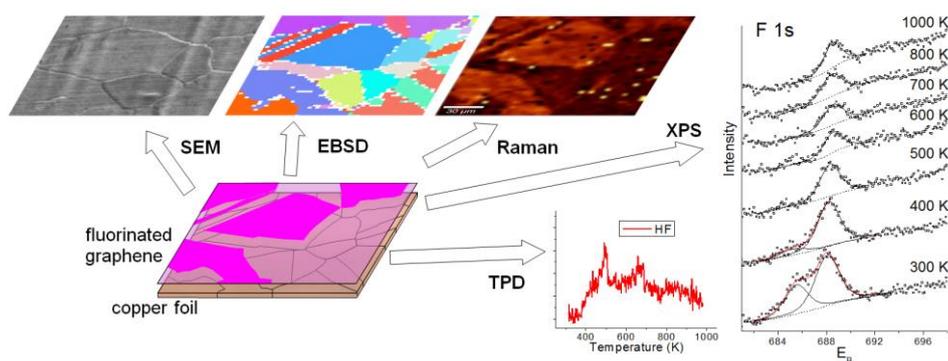
Fluorinated Graphene on Copper – Reactivity Driven by Support Phase Orientation and Decomposition under Heat Treatment

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Exploring the local tailoring of reactivity is very attractive because it may allow the achievement of patterned chemical functionalization of graphene, which may lead to local changes in mechanical, chemical and optical properties. Fluorine functionalization is preferred because of stronger bonding than e.g. hydrogen to carbon. Fluorine can be replaced by other molecules in the gas phase and is thus an attractive starting material for further functionalization reactions. Additionally, fluorinated graphene is one of the most interesting two-dimensional ‘graphene-based’ materials because it exhibits attractive electronic and optical properties, etc.

In spite of the relatively weak Cu-graphene interaction, the growth of graphene depends on the underlying Cu crystal structure. However influence of underlying Cu structure on interaction of graphene with fluorine and the reaction mechanism of the decomposition of fluorinated graphene is still not well understood.



Graphene prepared by CVD on copper foil was exposed to XeF_2 , and the results of the fluorination were analyzed using Raman spectroscopy, EBSD, XPS, and TPD. It was found that the graphene above Cu grains with orientations close to (111) is the most reactive. Variations in reactivity were observed for graphene on (100), whereas graphene on grains with orientations close to (110) is the least reactive. Long term tests showed that the most stable fluorinated graphene is on copper grains with orientation close to (111). Graphene, both coupled and decoupled from the copper substrate, was identified in the XPS C 1s spectrum after fluorination, whereas heating above 800 K resulted in completely coupled graphene to the substrate. The coupling process was associated with desorption of intercalated water and OH species. Gradual loss of fluorine and carbon was observed by XPS during annealing up to 700 K. The loss of fluorine was associated with broad desorption of HF species monitored by TPD. The desorption of CF species at 670 K was rationalized by a defect formation process in the fluorinated graphene layer. A significant number of vacancy-like defects in the graphene layer after annealing was confirmed by Raman spectroscopy.

Effect of hydrogenation on the particular layer in isotopically labelled Turbostratic- and Bernal stacked bilayer graphene

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One of the most efficient methods allowing manipulation and modification of the graphene properties is its chemical functionalization [1]. Many applications have been already found for the hydrogenated graphene (graphane): opening the bandgap, enhancement of the spin-orbit coupling and appearance of the magnetic moment make it a great candidate for the purposes in spintronics, sensors or thermoelectric devices. Moreover, the prior hydrogenation of graphene may create the possibility for its further functionalization with the compounds that do not react with the pristine graphene [2].

Functionalization of graphene bilayers (BLGs) is currently used for the modification and control of their bandgaps, since in contrast to the linear bands of monolayer their electronic structure consists of the parabolic energy bands. On the other hand, BLGs are known for lower efficiency of functionalization [3]. Here, we have investigated the effect of hydrogenation on BLGs, both Turbostratic- and Bernal stacked. Thanks to the isotopically labelled layers we could distinguish the effect of hydrogenation on the particular layers. We have found that reactivity of BLGs is lower than in case in SLG in general, for both types of stacking. However, hydrogenation of the Turbostratic stacked BLG resulted with the appearance of the D mode of the top layer, whereas in case of Bernal stacked BLG the D modes were not observed for neither top nor bottom layer.

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Tuesday, May 29th

Atomic-Scale Defect-Engineering of 2D Materials with Electron and Ion Beams

Title of Contribution

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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 manipulate 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 provide an overview of our latest results in using ion irradiation at a large energy scale to modify graphene and to implant foreign atoms into it [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. I will also describe our new experimental setup (to be finished soon) combining low-energy ion irradiation line in the same vacuum as a state-of-the-art aberration-corrected scanning transmission electron microscope fitted for in situ manipulation during imaging.

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Defects and interlayer coupling in in van der Waals heterostructures

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Van der Waals heterostructures give access to a wide variety of new phenomena that emerge due to the combination of layered materials with different properties.

One of the key engineers the properties of 2D materials could be in the ability to alter their structure in a controllable way. Different methods are possible: functionalization, intercalation, inducing defects etc. Whatever the chosen method the consequences is a strong modification of their structure and thus on their electronic and vibrational properties. All these effects can be probed efficiently by optical phonons. Up to now various methods have been used as argon bombardment, electron beam irradiation, graphene oxidation, ..ect.

In this work we will try to unravel the structural modification induced by defects in the case of graphene and MoS₂. In the case of few- and single-layer MoS₂ hosting substantial defects densities, these defects are thought to influence the doping level, the crystal structure, and the binding of electron–hole pairs. We disentangle the concomitant spectroscopic expression of all three effects and identify to what extent they are intrinsic to the material or extrinsic to it, i.e., related to its local. We discover a defect-bound state having a low binding energy of 20 meV that does not appear sensitive to strain and doping, unlike charged excitons. Conversely, the defect does not significantly dope or strain MoS₂ [1].

We also show here that due to an enhanced interaction cross section in such structure, made of molybdenum disulphide and boron nitride, electron-hole pairs can be generated by incident electrons and give rise to cathodoluminescence. Using Raman spectroscopy and photoluminescence, we show that low energy electron beam irradiation can nevertheless cause irreversible structural damages in molybdenum disulphide. A correlation between molybdenum disulphide/boron nitride coupling and the defect creation is established. Our work demonstrates that cathodoluminescence is powerful tool images the electronic properties in van der Waals heterostructures at the nanometer scale.

In the case of graphene, we report the observation of an intense anomalous peak in the Raman spectrum in specific growth conditions that cannot be attribute to structural defects. In fact, bombardment with an electron beam demonstrates that this new peak is clearly distinct from the well-studied D' peak appearing as defects are created in graphene [3].

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X-ray Scattering on Highly Perturbed Carbon Nanomaterials

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Carbon based materials are extensively used in different industrial applications for decades. Besides the well-known crystalline allotropes diamond and graphite, industrially important are the carbonaceous materials in the forms of carbon black, coal tar pitches and resins, hydrogen containing carbons, hard/soft non-graphitizing carbons etc. Because of their specific physical properties, they are increasingly important in high added value products as carbon bonded refractory materials, in the surface chemistry as catalyzers, as different types of filters, as fuel storages for natural and hydrogen gas, and as well as in the microelectronics as electrode materials for Li storage in Li-ion batteries.

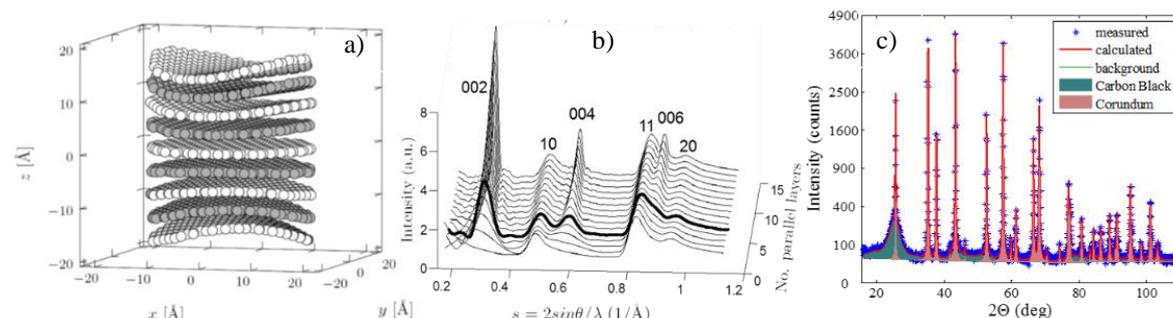


Fig. 1 Turbostratic carbon cluster of cylindrical shape (a). Calculated scattering pattern from cylindrical turbostratic carbon cluster with diameter $L_a = 10 \text{ \AA}$; number of parallel layers varied between 1 and 15 (b). Measured and refined x-ray scattering patterns from mixture of crystalline material (corundum) and turbostratic carbon (25 wt. %) sample (c).

Such nanocrystalline, highly defect forms of carbon materials are called turbostratic carbons. Structurally they are built from graphene layers where the carbon atoms, bounded with strong covalent bonds, form hexagonal honey-comb structure. Weak van der Waals bonds between individual graphene layers allow random fluctuations in the parallel layer spacings, random lateral translations of graphitic layers, the curvatures of layers and mutual disorientations of individual parallel layers around the layers normal direction. The structural disorder – loss of the 3D periodicity together with very small cluster sizes leads to the formation of pronounced $00l$ peaks coming from the scattering on mutually disoriented parallel layer groups and asymmetrical hk bands originating from the scattering on individual layers, in the scattering pattern. Additionally the scattering pattern of turbostratic carbon is highly diffuse and cannot be described with well established powder diffraction procedures (Fig. 1).

Simulations of scattered intensity distributions from two and three dimensional carbon structures of different shapes and sizes were done using the general Debye scattering equation [1]. The influence of the lattice defects typical for the turbostratic structure, i.e. random fluctuations in the parallel layer spacings, random lateral translations of graphitic layers, the curvatures of layers and mutual disorientations of individual parallel layers around the layers normal direction, on

the resulting simulated scattered intensities were studied and discussed [2]. The microstructure-induced changes in the line broadening, in the shape parameter in the Scherrer formula and in the lattice parameters determined from the positions of the X-ray diffraction lines are discussed in particular. The set of presented Scherrer parameters allows the calculation of the cluster sizes along and normal to the basal planes from the measured X-ray scattering. The applicability of the Warren-Bodenstein's approach [3] and paracrystalline model [4, 5] for description of scattering on turbostratic carbon structures was proven. Intensity distributions simulated using both approaches were compared to those obtained using the general Debye scattering equation.

A computer program adopting Warren-Bodenstein's approach and paracrystalline model allowing fitting of whole measured scattering powder patterns was written. The program enables refinement of physical parameters of turbostratic carbon materials, i.e. the mean lattice parameters a_0 , c_0 , the mean cluster sizes parallel and perpendicular to the graphitic planes L_a and L_c , their distributions as well as the mean square atomic displacements $\langle u_a^2 \rangle$ and $\langle u_c^2 \rangle$. A series of high melting coal-tar synthetic pitch specimens, annealed at different temperatures, was prepared and investigated [6]. In studied samples we observed the increase of the clusters sizes, changes in the mean lattice parameters a_0 , c_0 , and decay of disorder with increasing annealing temperature.

The generalized Warren-Bodenstein's method describing the scattering on turbostratic carbon was implemented into the Rietveld program MStruct [7] allowing fitting of measured scattered intensity distribution from mixtures of crystalline materials with turbostratic carbon, refinement of essential microstructural parameters and quantitative phase analysis.

Acknowledgement

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Electron Irradiation-Induced Defects and Phase Transformations in Two-Dimensional Transition Metal Dichalcogenides

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Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN, transition metal dichalcogenides (TMDs) and silica bilayers were manufactured. All these systems contain defects and impurities, which may govern the electronic and optical properties of these materials. Moreover, defects can appear during the characterization of the materials in transmission electron microscope. All of these calls upon the studies on defect properties and mechanisms of their formation under electron beam. In my talk, I will present the results [1-4] of our recent first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in close collaboration with several experimental TEM groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of inorganic 2D materials. I will also present the results of our theoretical studies of electron-beam induced phase transformations in 2D TMDs 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.

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In-situ spectroelectrochemistry of catalytically active sites in molybdenum dicalcogenide mono- and fewlayers for HER

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Optically active, atomically thin semiconductors are an emergent class of two-dimensional materials. Particularly, monolayers of semiconducting transition metal dichalcogenides (SC-TMDs), such as MoS₂, excel in their large optical response. The light-matter interaction in such monolayers is dominated by exciton phenomena, resulting in a layer- and energy-dependent extraordinarily high absorbance of more than 15% for a less than 1nm thick crystal. Its high optical in the visible range for monolayers together with catalytic activity and photocatalytic stability makes single-layer MoS₂ a very promising material for sunlight driven photocatalytic applications such as photocatalytic hydrogen evolution (HER) [1,2,3].

We recently developed a photo-electrochemical microcell enabling photo-catalytic measurements on individual micron-sized two-dimensional materials and other nanostructures. The microcell provides full optical access with a lateral resolution in the electrolyte better than 500nm for *in-situ* and *in-operando* photoluminescence, Raman and reflectance measurements [3,4]. In this way, we studied the photocatalytic stability of MoS₂ edges and basal planes under light irradiation in different electrolytes [3]. Furthermore, the photocatalytic activity regarding HER of exfoliated single- and few-layer MoS₂ immersed in an acid electrolyte by cyclic voltammetry is investigated [4]. We observe an increased catalytic activity of MoS₂ with decreasing number of layers. In particular, monolayers exhibit high current densities, low onset potentials and high turnover frequencies. Edge sites and defects show higher activities than the basal plane. Much higher turnover frequencies and photon-to-current conversion efficiencies are observed at the edges. A statistical analysis points towards a non-negligible contribution of catalytically active defect sites on the basal plane to the overall catalytic activity. We furthermore demonstrate that HER activity is increased by illumination in the visible range.

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Magnetoplasmonic Heterostructures for Theranostic Applications

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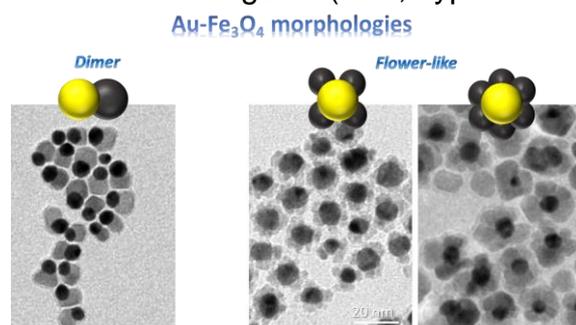
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The continuous development and evolution of nanotechnology requires the design and optimization of high-engineered materials for widespread applications.¹ In this sense, one of the most versatile strategies is the growth of hybrid heterostructures with at least two different properties (optical, magnetic, catalytic,...) into a single entity.² Interestingly, the functionality of such nanostructures can be tailored by the synergic combination of the diverse properties of each counterpart. One example is the gold-magnetite system, where magnetite nanoparticles are used as T2 contrast agents in magnetic resonance imaging and nano-heaters in magnetic hyperthermia.² On the other hand, gold particles can be imaged by optical means or by X-ray computed tomography due to its large Z number. Moreover, gold nanoparticles are able to generate heat by the absorption of light due to their unique surface plasmon resonances (photothermia).

In this work we will show different strategies to tune the size and morphology of Au-Fe₃O₄ nanostructures based on thermal decomposition approaches, ensuring an intimate contact between both phases.³ In fact, exploring the reaction parameters allows us to understand the reaction mechanism and thus to control the final morphology of the nanostructures (Fig. 1). The magnetic and optical properties of the nanoparticles are rather dependent on the size and morphology of the nanostructures. Finally, the nanostructures were transferred to aqueous media in order to be tested as theranostic agents (MRI, hyperthermia).



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Single 3d transition metal atoms on multi-layer graphene systems: electronic configurations, bonding mechanisms and role of the substrate

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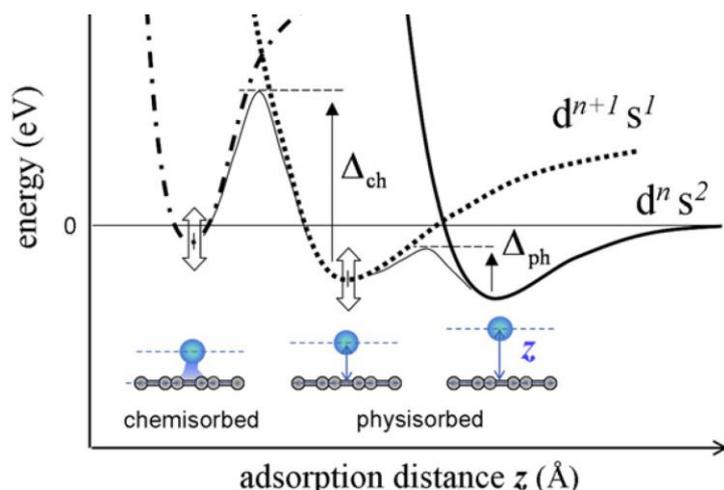
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Two-dimensional (2D) materials are of large interest for spintronics, in particular if transport can be influenced by accessory magnetic degrees of freedom.

We are interested in minimum invasive methods where magnetic atoms are implemented via surface adsorption, leaving the structure of 2D systems intact.

Here we present a study on electronic configurations of Fe, Co, Ni and Cu adatoms on graphene and graphite by x-ray magnetic circular dichroism and charge transfer multiplet theory [1]. A delicate interplay between long-range interactions and local chemical bonding is found to influence the adatom equilibrium distance and magnetic moment (see image below).

The results for Fe and Co are consistent with purely physisorbed species having, however, different 3d-shell occupations on graphene and graphite (d^{n+1} and d^n , respectively). On the other hand, for the late 3d metals Ni and Cu a trend towards chemisorption is found, which strongly quenches the magnetic moment on both substrates.



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Electronic detection of DNA on graphene

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Fast, cheap and reliable identification of the exact order of nucleobases within a DNA/RNA molecule is an important goal of next-generation genome sequencing. Graphene has recently attracted enormous attention for next-generation DNA/RNA sequencing and sensing thanks to its unique electronic and structural properties. Here we present a combined experimental and theoretical study of the electronic detection of DNA and RNA on graphene field-effect transistors (GFETs). We compare the device sensitivity for direct detection of DNA on GFETs in vacuum and liquids, providing an estimate of the GFET sensitivity limit. Furthermore, we analyze the ability of GFETs to directly discriminate individual DNA nucleobases in electronic transport measurements. We demonstrate that GFETs are able to measure distinct, coverage dependent, conductance signatures upon adsorption of DNA nucleobases in vacuum [1]. To get a deeper insight into the origin of the sensing mechanism and molecular recognition in GFET measurements we performed *ab initio* electronic structure calculations using density functional theory (DFT) [2]. We identify that the in-plane dipole moments of the nucleobases play the dominant role in the modification of the electronic structure of graphene, demonstrating both p- and n-type of doping depending on the direction of the dipole moments. We demonstrate that intermolecular interactions have a strong influence on the adsorption geometry, resulting in a tilt of the molecules on graphene. The predicted tilt of nucleobases causes significant changes to the electronic structure and molecular fingerprints of nucleobases in graphene, supporting our recent experimental observations [1]. Our findings have important implications for identification and understanding of molecular fingerprints of DNA/RNA nucleobases in graphene-based sensing and sequencing methods.

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Multi-responsive nanocomposites based on liquid crystals

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Today's information age is from a big part possible thanks to devices, which are based on thermotropic liquid crystals (LCs). These materials are used not only in different types of displays, but also in tunable lenses and optical filters, organic photovoltaic cells, switchable windows, memory-storage systems, artificial muscles prototypes. LCs based systems for the primary diagnostics of cancer as well as temperature sensitive spots that indicate the correct storage conditions of drugs, foodstuffs etc. are also being investigated¹.

LCs are used so widely due to their unique ability to form achiral and chiral mesophases between crystalline and liquid states at heating or cooling². These well defined self-organized structures are responsive to external stimuli, such as electric field. Commonly, mixtures of LCs exhibiting achiral mesophases with additives causing helical twisting of molecules are used for applications³. Supramolecular structures of mesophases can be easily modulated by electric field, but they are rather resistant towards magnetic field. To induce some structural changes very strong magnetic fields of strengths ~ 1 T must be applied to the sample⁴. This drawback can be circumvented by the addition of magnetic nano-objects to LC hosts. In this case another problem arises - stability of the mixture, since magnetic nano-objects tend to aggregate being doped into a LC. Aggregation can be avoided, when the surface of nano-objects is modified with suitable ligands. So far only few publications described stable mixtures of LCs with magnetic nano-objects,^{5,6} and in all of them ligands carried only one function - stabilisation.

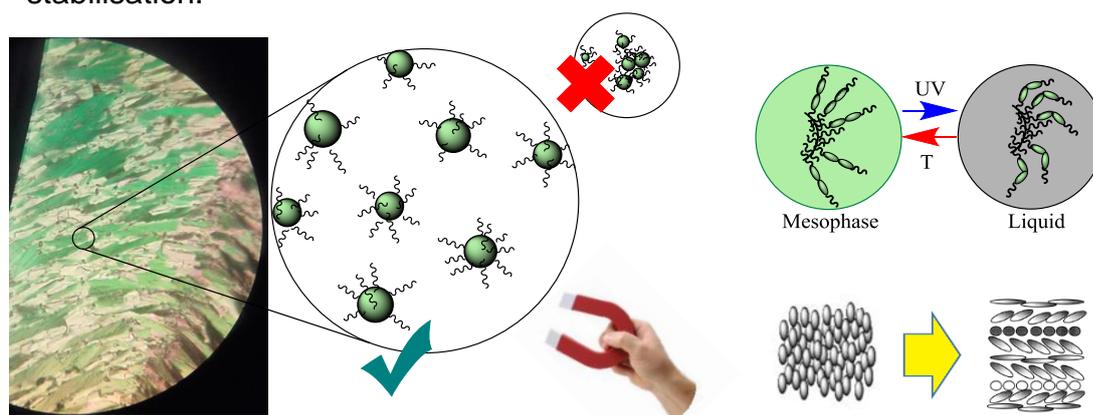


Fig.1: Combined functions of the prepared ligands.

In this study, we have focused on the development of ligands, which will at the same time stabilize magnetic nanoparticles (NPs), twist the achiral mesophase structure and enable mesomorphic properties photomodulation (Fig. 1). Our approach leads to the creation of complex multi-responsive materials, where UV-light, electric and magnetic fields can be used as external stimuli to influence the state of the prepared materials.

To reach our aim, ligands of several structures were developed. All of them have a structure similar to the LC hosts, which includes anchor group (phosphonic acid), chiral unit (lactic acid or BINOL) and photosensitive unit (N=N group). Structure, purity and mesomorphic properties of prepared ligands were characterised using common techniques. Stability of Z-isomers formed after ligands UV-light irradiation was determined in solutions using ¹H NMR spectroscopy. Obtained ligands were used for cobalt ferrite NPs modification using the methodology based on the “ligand exchange” principle. After subsequent characterisation, NPs with the modified surface were used as dopants for different LC hosts. The effect of the NPs addition on host properties (Fig. 2) will be also discussed during the presentation.

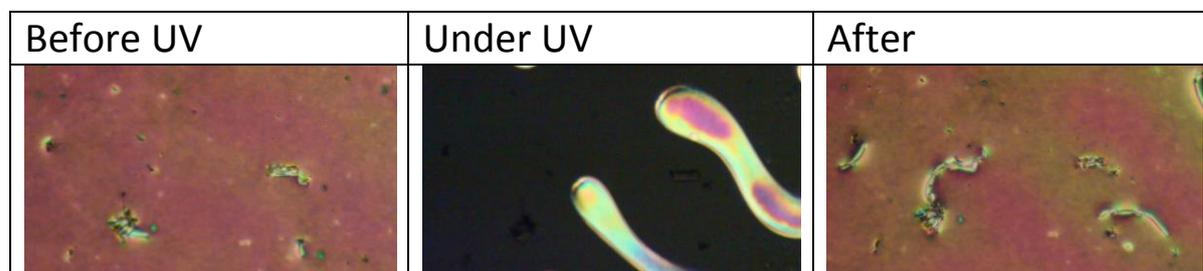


Fig. 2: Photomodulation of mesophases exhibited by a LC host doped with NPs.

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Wednesday, May 30th

Resonance Raman spectrum of epitaxial graphene doped towards the Lifshitz transition

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We employ in situ Raman spectroscopy in tandem with angle-resolved photoemission (ARPES) to investigate the doping-dependent Raman spectrum of epitaxial graphene on Ir(111). The evolution of Raman spectra from pristine to heavily Cs doped graphene up to a carrier concentration of 4×10^{14} electrons per cm^2 is investigated. ARPES proves that the Fermi surface at such extreme doping levels undergoes a Lifshitz transition resulting in a single hexagonal contour around the zone center. Ultraviolet (UV) light excitation is then needed to achieve resonance Raman conditions. The position of the Raman G band of graphene doped close to the Lifshitz transition is characterized by a 60 wavenumber downshift due to the combined effects of phonon renormalization and lattice expansion. Its line shape assumes a strong Fano asymmetry with increasing doping. Our work establishes ultra high vacuum UV Raman spectroscopy at variable temperatures as a versatile surface science tool.

Quasi-2D Liquid Nanofoam on Water-Immersed Solid Surface

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Gaseous nanobubbles residing on water-immersed solid surfaces extend concept of binary solid-liquid interface to 3-phase solid-gas-liquid system. They represent relatively stable gaseous nanostructures, which existence on the interface is often not anticipated. As the appearance density of nanobubbles on solid-liquid interface can vary widely (Fig. 1), it may bring uncertainty pattern to efficiency and kinetics of heterogeneous interfacial processes.

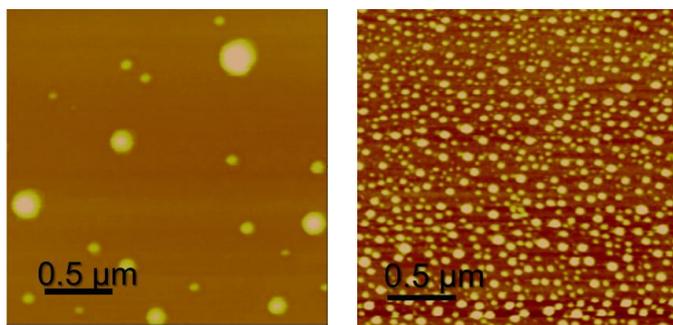


Figure 1: Ambient gaseous nanobubbles on water immersed solid surface imaged by AFM *in situ*. Nanobubble appearance density corresponding to surface coverage by gaseous nanodomains ~ 10% (left) and ~60% (right).

The nanobubble research thus becomes significant for various fields including heterogeneous (electro)catalysis, electrodeposition, charge storage, photochemical energy conversion, immersion lithography etc.

Quasi-2D liquid nanofoam represents a special form of gaseous nanostructure, which, unlike regular liquid foams appearing at gas-liquid interface, exists at solid-liquid interface. It consists of gaseous nanobubbles pinned to immersed solid surface and organized into close-packed assembly covering up to 90% of solid-liquid interface.

Research performed at the J. Heyrovský Institute of Physical Chemistry is focused on nanobubble interactions with solid surfaces leading to nanobubble-assisted nanostructuring¹ and nanoporation² of polymer films and on nanobubble shielding effect in electrochemical deposition and adsorption.

Special attention is paid to nanobubble imaging by AFM *in situ* and to application of novel imaging technique utilizing nanobubble imprint in polymeric matrix to evaluate nanobubble distribution *ex post*, by *ex-situ* AFM, avoiding interaction of nanobubble with AFM tip. The last technique³ is particularly useful for imaging dense nanobubble assemblies - nanofoams (Fig. 2), where AFM resolution is limited by the elasticity of nanofoam surface.

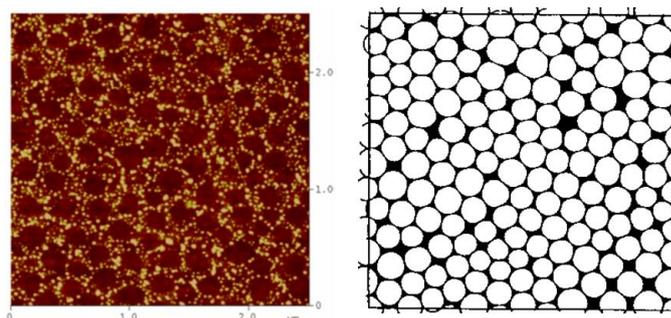


Figure 2: Imprint of quasi-2D gaseous nanofoam (“wet” type) formed in polystyrene film during its immersion in water (left) and corresponding “wet” foam model⁴ (right). Quasi 2D nanofoam is composed from single layer of gaseous nanobubbles in close-packed arrangement - circular voids (left) represent imprints of positions of individual gaseous nanobubbles in nanofoam imaged by AFM *ex situ*.

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Physical properties of metal-organic frameworks doped with TCNQ

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Metal-organic frameworks (MOFs) represent a new class of compounds that consist of metal nodes and organic ligands to form 1D, 2D and 3D nanostructures exhibiting advanced optical, electronic and magnetic properties. Their interior spaces allow foreign atoms and molecules to be assembled in low dimension as well as to functionalize the host frameworks. Optimally functionalized MOFs with defined properties can potentially be implemented in electronic devices such as solar cells, batteries and sensors. Magnetic transition metal arrays in MOFs are ideal systems in which we study anisotropic magnetic coupling. Metal ions exposed to the interior voids react with infiltrating molecules, leading to MOF's sensing abilities. Our experiments using Raman, photoemission, SQUID, electron microscopy, and magnetotransport measurements aim to probe electronic and magnetic interactions at molecular interfaces that are responsible for their unique physical properties. We demonstrate that the MOF's electrical conduction can be tuned by doping with TCNQ.

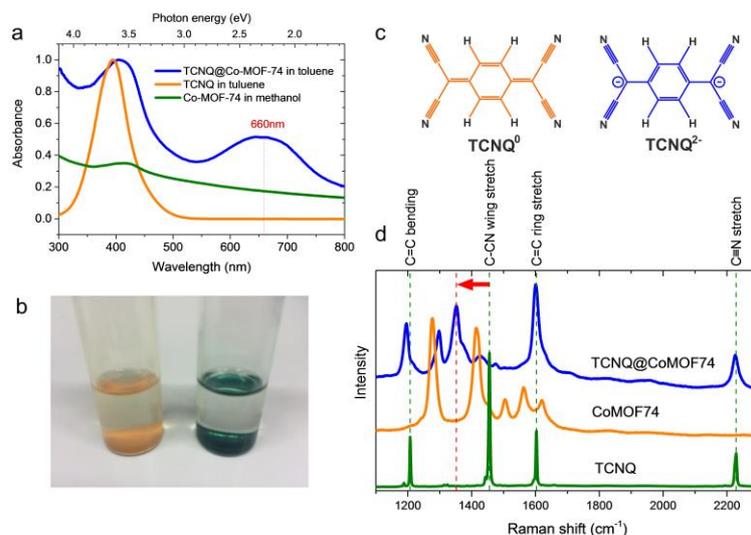


Figure: **a.** Absorption spectra for TCNQ, Co-MOF-74 and TCNQ@Co-MOF-74 nanocrystals. **b.** A photograph of the glass vials containing Co-MOF-74 (left) and TCNQ@Co-MOF-74 (right), both in methanol. **c.** Diagrams for neutral TCNQ⁰ (bottom) and divalent TCNQ²⁻ (top). **d.** Raman spectra for TCNQ, Co-MOF-74 and TCNQ@Co-MOF-74 collected at 633 nm laser wavelength.

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Thermoelectric properties of thin films

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Optimisation of thermoelectric materials requires a process of structural tuning on the nano/meso-scale to reduce thermal conductivity with minimal effect on electrical properties. Here we use in-plane thermal conductivity measurements which are particularly sensitive to thin film morphology, and use these measurements to study several materials including conductive polymers and halide perovskites.

Methyl ammonium lead iodide films of various thicknesses and morphologies were formed by co-evaporation of methyl ammonium iodide with PbCl₂, or by aerosol-assisted chemical vapour deposition. Despite an intrinsically low thermal conductivity, we measure a sizeable Kapitza resistance (thermal boundary resistance) and find a further reduction in thermal conductivity when grain sizes are in the range 10-100nm. The Kapitza resistance shows an unexpected increase with temperature, which can be interpreted through first principals calculations of the rotational and translational modes methyl ammonium ions at the grain boundaries.

Our studies on thermal transport in highly aligned thermoelectric polymer films will also be presented. Remarkably, we find the thermal conductivity of the polymer to be tuneable over an order of magnitude. An asymmetry in thermal conductivity of ~2.5 is observed between the directions parallel and perpendicular to the chain alignment for doped films and an asymmetry of ~5 in undoped films. Surprisingly, we observe that doping these polymers induces a large increase in thermal conductivity to >1 W/mK. The magnitude of this increase in thermal conductivity far exceeds predictions of the Wiedemann-Franz law and we explain it through a doping-induced structural changes. This has implications for using highly oriented polymer films for thermoelectric applications.

Back-gated epitaxial graphene on SiC

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Epitaxial graphene on SiC provides one of the most promising routes towards application of graphene in novel electronic and optoelectronic devices. The new concept is to exploit semi-metallicity of graphene. This feature allows using graphene as a conductive electrode with tunable Fermi energy. Although graphene can be grown on Si-face of SiC in high quality, it is difficult to back-gate epitaxial graphene due to the presence of so called buffer layer. This layer exhibits large density of localized states which pin Fermi level [1]. Such pinning is prohibitive for successful gating. For this reason, hydrogen intercalation is necessary to decouple buffer layer from SiC substrate [2]. Decoupling eliminates localized states formed by buffer layer and allows Fermi level to be tuned. It is also convenient for optoelectronic devices to have direct optical access to the conducting graphene channel [3]. Therefore we have fabricated a back gate by growing thin layer of semi insulating SiC on top of conducting SiC wafer. The modified physical vapor transport method has been used to grow thin layers of SiC. The semi-insulating behavior is reached by vanadium doping. Vanadium is incorporated by mixing SiC powder with VC powder. We polish chemically-mechanically these layers to recover atomically smooth SiC surface. The epitaxial graphene is grown on top of such conducting-semi insulating SiC layers. The method of buffer growth and hydrogen intercalation is used to eliminate buffer layer [4]. We present Raman depth scans as a tool to probe thickness of grown layers and two-dimensional mapping is used to determine epitaxial graphene quality. We show quasi-free standing graphene on back gated SiC $n/n++$ junction.

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Graphitization of diamond through different routes

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The electronic properties of diamond and graphene, though both built of carbon, differ in extremities. While the energy bandgap of about 6 eV in the diamond electronic structure leads to the electrical resistivity as high as 10^{18} $\Omega\cdot\text{m}$, graphene, a semimetal, exhibits excellent electrical transport properties with charge carrier mobility of 10^5 cm^2/Vs .

Our aim is to form a diamond/graphite system and to investigate the properties at the interface when these two extremities meet in a tight vicinity.

We have synthesized graphitic layers through structural transformations of various diamond substrates: monocrystals (111), (001) and nanocrystalline layers (200 nm thick). Three different methods have been employed for syntheses: direct graphitization of the diamond surface, catalytic transformation and transfer of externally-grown graphene for comparison.

Here, we study the mechanism of surface transformation of single-crystal diamonds (SCD) and CVD-grown nanocrystalline diamond (NCD) when covered with thin Ni films and annealed at 800 °C for a certain time period. The structure of the diamond/graphite interface formed during the catalytic reaction of Ni with diamond is studied by high-resolution transmission electron microscopy (HR TEM) in atomic-scale using specimens in cross-sectional geometry.

Upon heating, highly mobile Ni nanoparticles catalytically dissolve C atoms of diamond which then diffuse under the surface of Ni particles and, after saturation, carbon precipitates on the surface in a form of graphite. In the case of SCDs, the Ni particles stay on the diamond surface and lead to a progressive transformation of surface layers to horizontally aligned graphite. By contrast, in the NCDs Ni particles penetrate along the grain boundaries deep inside the NCD film and yield graphite grown vertically to the diamond surface.

Besides methods of electron microscopy (SEM, TEM and STEM in atomic resolution) we also study electrical transport through the graphitized layers. The temperature dependent conductance reflexes graphene morphology and crystalline quality on a macroscopic scale.

XPS measurements demonstrate that the direct graphitization of diamond surfaces performed under high vacuum and temperatures above 1000°C leads to a thin graphitic layer covering diamond.

Thursday, May 31st

Controllable synthesis of highly crystalline single and few layer MoS₂ and the role of growth-induced strain

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Molybdenum disulphide (MoS₂) is a layered Van der Waals solid enabling, as in the case of graphene, the isolation of a single MoS₂ layer which is essentially a 2D-crystal. Being an indirect-gap (1.3 eV) semiconductor in its bulk form, MoS₂ attracted significant attention in the past years when it was found that its 2D counterpart is a direct-gap (~1.9 eV) material [1, 2]. Before this material can be properly incorporated into commercial devices, efficient large area growth methods are required.

In this work, a two-step atmospheric pressure CVD method is presented, exhibiting controlled and large area growth of single and few-layered 2D-MoS₂ crystals through the reaction between sulphur vapours and pre-deposited sodium molybdate (Na₂MoO₄) on a Si/SiO₂ substrate. Depending on the precursor concentration the lateral size of the crystals can be controlled. Moreover, a monotonic increase of the substrate coverage with the precursor concentration is established, which enables the preparation of either isolated monolayers homogeneously distributed on the substrate or continuous MoS₂ films with single and few-layer domains. X-ray photoelectron spectroscopy was used to verify the stoichiometry of the produced crystals, while Transmission Electron Microscopy confirmed the high quality of the crystals.

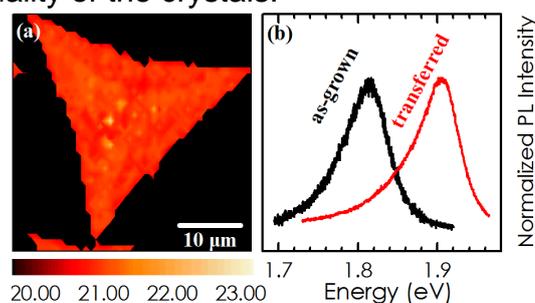


Figure 1 : (a) Raman image of the $\Delta\omega = \omega(A_1') - \omega(A_1'')$ of an a CVD-grown MoS₂ monolayer with average of 20.7 cm⁻¹. (b) PL spectra of a CVD-grown (black) and transferred (red) monolayer. PL peak shifts by 100 meV

Raman and Photoluminescence (PL) spectroscopies are employed to study the fabricated crystals before and after transferring them onto a polymer substrate. Significant spectral variations between the as-grown and transferred crystals were found. An optical analysis [3] was conducted, identifying mechanical strain as the main source of the spectral variations. It was found that strain relaxation takes place due to the transferring of the 2D-crystal. The magnitude of the residual strain imparted on the as-grown crystals -which can be

as large as 0.5%- is adequate to shift the direct transition of MoS₂ by almost 80 meV. The large residual strain experienced by the as-grown crystals enabled an estimation of the deformation potential of the direct optical transition of MoS₂.

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Graphene as substrate for selective self-assembly of 2-D materials for optoelectronic applications

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Graphene is well known as archetype of the 2-D materials, it is a multifaceted species widely recognized for a broad range of applications, including (opto)-electronics due to its outstanding ambipolar charge carrier mobilities and high transparency.

These factors together with the highly ordered 2-D structure, makes graphene an ideal substrate for the growth of layered structures, enabling the assembly of heterostructures with graphene as the key step for the realization of complex hybrid device architectures. In optoelectronic applications, a proper electrical contact is critical for the optimal functioning of the device and graphene has been identified as a very efficient ambipolar charge carrier thus it is possible to use it as electrode. Recently, we achieved highly selective growth of PEDOT on patterned graphene, providing unique hole-conducting/electron-blocking heterostructures. This achievement tempted us to investigate the formation of other graphene heterostructures in a selective fashion and to explore their potential for (opto)-electronic applications. Here, we describe a highly efficient process of selective and oriented growth of various 2-D crystalline materials (optically active) on monolayer graphene. To achieve this we have chosen different organic precursors for the active material which is composed of alternated organic and inorganic layers. Varying the length of the aliphatic chain or size of the aromatic moiety (present in the organic part) affects the selectivity of film formation on graphene due to the hydrophobic interactions and/or π - π stacking, respectively. Thank to this, high spatial resolution down to 5 μm was achieved, as well as uniform coverage of up to centimeter scale graphene sheets.

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Transport and incommensurate quantum-size oscillations in oligoacene molecular wires

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In conventional electronics, the conductance of a wire decreases with length according to Ohm's law. In molecular electronics, quantum effects lead to a richer phenomenology. Oligoacenes are organic molecules which consist of (linearly) fused benzene rings. Recently, Yelin and coworkers studied conductance of oligoacenes directly coupled to Ag leads and found increase of conductance with molecular length [1]. I will show that electronic transport through oligoacenes is governed by a quantum size effect which controls the alignment and width of the lowest unoccupied molecular orbital. These ideas will be supported by first-principles transport calculations using density-functional theory.

Linear oligoacenes are one of the simplest realizations of zig-zag terminated graphene nano-ribbons. In the long-wire limit, I will demonstrate that the optical gap as a function of the molecular length shows surprising oscillations with period of approx. 11 rings [2]. These incommensurate oscillations (IO) arise from a band-structure crossing. I will discuss the effect of electronic correlations on the IO [3].

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2D-3D Interfaces from the Topography Standpoint

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Graphene is almost never perfectly flat. When suspended, Angstrom-sized stabilizing ripples are present, or, if strained, nano- or even micrometer-sized wrinkles appear due to the low bending rigidity of this monoatomically thin material. When supported by a substrate, various corrugations in graphene appear due to homogeneous or heterogeneous stress fields at the interface with the bulk material. In this contribution, two different methods, which allow to exert a reasonable level of control of the graphene's topography, are discussed.

In the first setting, graphene is supported only locally by nanopillar arrays made of a stiff material. Various kinds of wrinkles are formed in the graphene, from short random to long oriented ones. The origin of the long oriented wrinkles is driven by the presence of linear defects acting as edges, where stress instabilities occur. The instabilities give rise to parallel wrinkles spreading at an angle as close to normal from the "edge" as allowed by the symmetry axis of the pillar array. The wavelength of the wrinkles is determined solely by the interpillar pitch.

The second scene features graphene and a soft, compliant polymer. When treated properly, usually by heating, biaxial compressive stress field is and results in the creation of hierarchically wrinkled graphene flakes. The wrinkling characteristics (amplitude, wavelength) are linearly related to the thickness of the graphene. The orientation of the wrinkles is controlled by the geometry of the flakes, such as that long and narrow flakes exhibit perfectly parallel wrinkles perpendicular to the longer edge, while more equilateral specimens are wrinkled without any preferred orientation in the flake interior. Wrinkles were also observed at the edges of the graphenes flakes and their resulting morphology was examined by an analytical approach. A continuum model was developed showing both qualitative and quantitative agreement was found between theory and experiments. Finally, the wrinkles in graphene are imprinted perfectly into the underlying polymer, (i) making the interface homogeneous from the interaction point of view, and (ii) demonstrating a simple patterning method of the polymer.

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Mastering the topography of graphene.

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The transfer of either exfoliated or chemical vapour deposition (CVD) grown graphene to another substrate is one of the key steps during the fabrication of graphene based devices. The creation of rugae, a single state of a corrugated material configuration which in graphene can be mostly observed as either wrinkles, ripples, folds, wrinkles and crumples, during the transfer is generally seen as unwanted, as these topographic features deteriorate the properties of graphene.

In recent years, graphene research has partly shifted their focus from the investigation of as 'perfect as possible' graphene to explore these 'imperfections'. Those topographic features can be very suitable to further explore graphene's potential. One of the more significant changes due to these rugae is a change in the pyramidalization angle, which describes the angle between the σ - and π - orbitals of graphene, and which is a measure for the chemical reactivity of graphene [1]. The chemical reactivity can be further controlled at a rugae via the doping level, as graphene is locally delaminated at the rugae. Furthermore, rugae can act as a generator for pseudo magnetic fields [2] or induce anisotropic transport properties.

In this presentation, I will discuss how we can modify the topographical landscape of graphene using either temperature [3, 4], the used transfer method, (plasmonic) nanoparticles [5, 6] or nanopillars [6]. Using temperature dependent Raman spectroscopy microscopy and atomic force microscopy, the created topographic states in graphene are studied. Using a careful analysis of the measured data of these different graphene based systems, a correlation between the topography of graphene and the temperature, induced strain, doping and defects in graphene can be found. Using this knowledge, we will be able in the future to control spatially the functionalization of graphene.

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Posters

Micromagnetics overview and its application on nanoparticle magnetic studies.

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Micromagnetics is a very useful field of study that helps bridge the gap between purely theoretical and experimental physics. This by allowing us to see the dynamics between different magnetic domains inside a magnetic material, through the use of computer simulations [1]. Within this field of research the magnetization dynamics is attained by numerically solving the Landau-Lifshitz-Gilbert (LLG) equation. This takes into account the contributions of fields due to Exchange, Demagnetization, Oersted, Zeeman, (and others if needed) to resolve the dynamics of a certain material under different conditions. Micromagnetics has been successfully used throughout the years to describe the magnetization dynamics of different devices and structures, such as spin-valves, magnetic tunnel junctions, domain wall motion, vortex oscillations, etc.

Magnetic nanoparticles have been gaining increasing interest in both industry and research due to its possible applications in different areas like in engineering and biomedical fields. Typical sizes of such particles are around the 10 nm scale, and thus very much on the limit of the mesoscopic scale used in micromagnetics. Nonetheless, micromagnetic simulations should be able to give us some insight into the magnetic responses of nanoparticles without the need of an atomic model. The goal is to try and apply it to structures like bi-magnetic core/shell nanoparticles [2], so has to better understand its properties and experimental results.

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Control of diindenoperylene molecular layer orientation by means of crystallographic orientation of underlying few-layer MoS₂ thin film

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Using ion beam sputtering of Mo on Al₂O₃ (0001) substrate and subsequent sulfurization in vapors at high temperatures, it is possible to prepare thin films of MoS₂ with a high degree of crystallinity¹. In our contribution, we show that it is possible to control the orientation of MoS₂ crystallographic *c* axis via the thickness of Mo layer deposited during the sputtering. In particular, we found *c* axis normal and parallel to the substrate for 1 nm and 3 nm thick Mo layers, respectively, by employing grazing-incidence wide-angle X-ray scattering (GIWAXS). Furthermore, we show that when a layer of small organic molecules, such as diindenoperylene (DIP), is thermally evaporated on these MoS₂ thin films, DIP phase exhibits lying-down and standing-up configurations for MoS₂ *c* axis normal and parallel to the substrate, respectively (Fig. 1). This result has direct implications for a tailored preparation of small-molecule organic films for diverse applications.

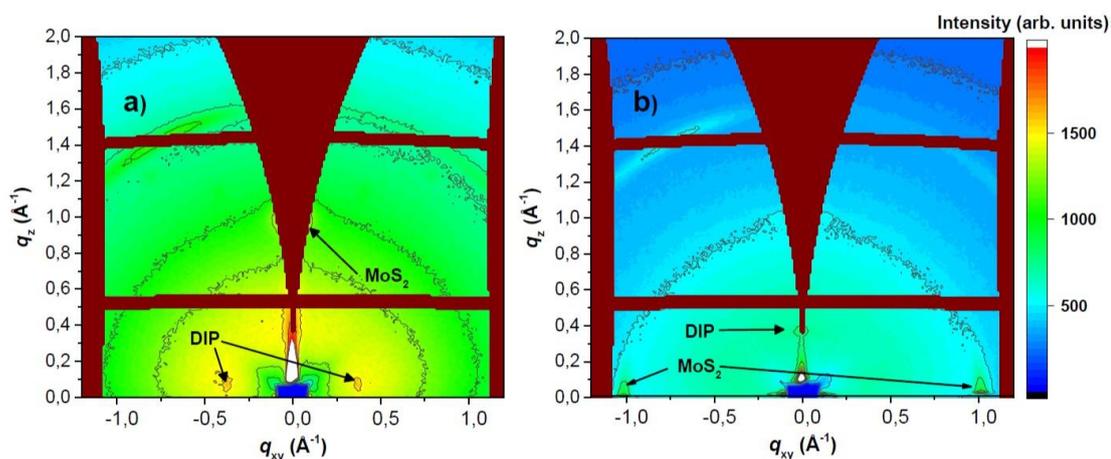


Fig. 1: GIWAXS reciprocal space maps show 002 MoS₂ and deposited 001 DIP diffraction spots for the samples deposited on sulfurized a) 1 nm b) 3 nm thick Mo layers.

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SERS of isotopically labelled $^{12}\text{C}/^{13}\text{C}$ graphene bilayer: graphene layer as spacer and probe

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Graphene is envisaged to improve significantly the substrates for surface-enhanced Raman scattering of planar aromatic molecules as it can ensure a more even enhancement at different places of the substrate. For this purpose, the role of graphene as a spacer in such SERS platforms has to be addressed. Here, we prepared and probed by Raman spectroscopy hybrid systems constituted by $^{13}\text{C}/^{12}\text{C}$ bilayer graphene covered by nanostructured gold. Hybrids with both the ^{13}C over ^{12}C layers and in the flipped geometry, and with both the turbostratic and the A-B stacked order have been investigated, and qualitative as well as quantitative information about the enhancement experienced by phonons of the individual graphene layers by the electromagnetic mechanism of SERS were addressed. Here, the top layer of the isotopically labeled bilayer

graphene represents the graphene spacer, while the bottom layer mimics a monolayer of target planar aromatic molecules. Both the calculation and the experiment based chiefly on comparison of the relative intensity ratio of the clearly distinguished ^{13}C layer and ^{12}C layer G mode bands jointly indicate that the enhancement of Raman scattering of the molecular monolayer on graphene spacer by the electromagnetic mechanism of SERS will be only 0.7 times lower than that of a monolayer located directly on the nanostructured Au surface.

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Thermodynamically driven self-organization of dynamic covalent polymers on graphene

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Heterostructures on graphene are particularly interesting for a broad range of (opto)electronic applications.^[1,2] Epitaxial growth of such systems represents a unique approach to let the device assemble by itself. To demonstrate the potential of this method, we studied spatially resolved self-assembly of van der Waals epitaxial heterostructures based on graphene and six different dynamic conjugated polyimines. Such polyimines were prepared by the copolymerization of three types of bifunctional aromatic aldehydes with different diamines. Dynamic character of imine bonds was studied using ¹H NMR and extended conjugation of the prepared polymers was characterized by UV/Vis and fluorescence spectroscopy. The heterostructures on graphene were prepared by two methods: (i) spin-coating of corresponding polyimines and (ii) on-surface growth. The analysis of the prepared systems using Raman, XPS spectroscopy and AFM microscopy, showed that both methods led in most of the cases to selectively assembled polymer films on graphene. In addition, STM analysis revealed that while spin-coating produced short randomly distributed polymer chains, on-surface dynamic polymerization provided highly organized structures with much longer polymer chains.

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Nanoscale electrical properties of thin films after laser irradiation

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The continuous appearance of emerging applications for organic nanostructured materials makes the generation of micro and nanostructured functional surfaces to be a demanding challenge. Different advanced lithographic processes are being investigated in order to produce surface nanostructures. In particular, laser induced patterning of organic surfaces is a versatile strategy to produce functional materials [1]. The formation of Laser Induced Periodic Surface Structures (LIPSS) is a method which may occur by irradiation of solid surfaces by intense either nanosecond or femtosecond laser pulses. In these cases spontaneous formation of periodic structures on the surface takes place. The structures typically consist of ripples although also more complex structures have been described whose periodicities are closely related to the wavelength of the irradiating laser [1,2].

Here we will discuss the nanostructure and electrical properties of LIPSS formed on spin-coated thin films of poly 3-hexylthiophene (P3HT) and fullerene [6,6]-phenyl C71-butyric acid methyl ester (PC₇₁BM). A heterogeneous electrical pattern consisting in conducting valleys and less conducting hills is observed by C-AFM. On the basis of both X-ray scattering and AFM experiments we propose that laser irradiated films suffer a fast heating/cooling process tending to reduce the overall crystallinity of the LIPSS and therefore decreasing the electrical conductivity of the hills. We will present a method to obtain resist-free PC₇₁BM imprinted regions decorated with nanoscale conducting patterns.

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Local Photocurrent Characterization of Graphene-Silicon Schottky Junction

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Graphene and numerous other 2D materials (e.g. TMDCs like MoS₂) exhibit interesting electrical properties which are, however, significantly influenced by surrounding environment. Thus, interfacing of materials with different dimensionalities becomes increasingly relevant for many applications which can utilize the exceptional properties of low-dimensional materials on one hand, and build-up on the existing production know-how for bulk (3D) materials on the other. Numerous appealing possibilities are offered by such combinations. This work is focused on 2D-3D heterostructures composed of mechanically exfoliated single- and few-layer graphene in combination with n-doped crystalline silicon. Photovoltaic characteristics (PV) of this heterojunction were studied at nanoscale under different light conditions.

Flakes of the studied 2D materials of various thickness were prepared by exfoliation on polydimethylsiloxane (PDMS) substrate, followed by oriented transfer onto the final bulk, freshly etched Si substrate (3D material). Electrical properties of the thus formed 2D/3D heterostructures were studied mainly by methods based on the principles of Atomic Force Microscopy: local photocurrents were studied by conductive AFM (CAFM), as well as using I-V sweeps, and changes in surface potential (i.e., work function) were acquired using Kelvin Probe Force Microscopy.

From CAFM, the fill factor (FF) and open-circuit potential (VOC) can be safely determined, however, the short-circuit current (JSC) values can be compared only for a particular tip, otherwise JSC needs to be normalized. The PV characteristics of p-Gr/n-Si Schottky junction shows strong dependence on light conditions as well as on the overall quality of 2D/3D contact within individual graphene flakes. The parameters of solar cell efficiency further also differ according to the number of graphene layers and level of graphene doping. Connection between aging of heterostructure and changes in photovoltaic properties is briefly discussed.

Even though the quantitative information provided by the local PV characterization methods has its limits, we have shown such methods to be very useful for revealing details invisible to macroscopic measurement.

This work was supported by the Czech Science Foundation (GACR 17-18702S) and Charles University Grant Agency (GAUK- 1484218).

Nanoscale Photovoltaic Characterization of WSe₂-MoS₂ Monolayer Diodes

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P-N diodes are the basic active components in all type of modern electronics and opto-electronics. Due to selective doping, making of thin layer P-N diode is challenging. As a solution, naturally available semiconducting 2D transition metal dichalcogenides are promising candidates to serve as active components of the diodes. Due to layer number-dependent on/off ratio and unique electro-optical properties, the naturally available n-doped MoS₂ and p-doped WSe₂ are attractive for constituting a vertically stacked type-II P-N diode in our work. We focused on n-MoS₂/p-WSe₂ composed of monolayer compounds due to their direct band gap and lower dielectric screening effect [1, 2]. Dry transfer technique using PDMS was used to prepare vertically stacked 2D layer heterojunction directly on gold/chromium electrode finger on SiO₂ substrates. Keithley semiconducting characterization system was used to assess the general electronic characteristics to confirm the operation of the stack as a photosensitive diode. Local electrical and photovoltaic properties were examined by Atomic Force Microscopy (AFM) techniques, mainly conductive AFM (C-AFM) and Kelvin Probe Force Microscopy (KPFM) with and without illumination. The illumination was provided either by white light or red AFM diode (Bruker Dimension Icon) [3] or by a laser (532 and 633 nm) focused to a selected spot (HR Evo Nano, Horiba – AIST-NT). I-V curves obtained locally with the AFM tip show quantitative evolution of the photocurrents across the diode and at a small distance away from its edge on the respective monolayer. On top of that, hysteresis in the I-V curves point to specific capacitive processes taking place in the circuit. Surface potential evolution measured under different laser illumination without the AFM diode interfering (the diode's wavelength is 1300 nm) show the dependence of the charge carrier accumulation and separation on the laser wavelength. The charge depletion region is confined to the edges of the diode, similarly to observations in [4]. We note that the utilization of 1300 nm diode in such an experiment provides more precise data, where the information is not obscured by the effects caused by the common red diode falling into the band gap of the studied material.

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Spin Seebeck effect in ϵ -Fe₂O₃ thin films

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The Spin Seebeck effect, discovered in 2008 by Uchida et al. [1], is a combination of two phenomena: the generation of a spin current by a temperature gradient applied across a magnetically ordered material, and a conversion of the spin current to electrical current by means of the inverse spin Hall effect [2] in the attached metallic thin layer.

We present the experimental observation of the longitudinal spin Seebeck effect in Pt/ ϵ -Fe_{2-x}Al_xO₃ (x = 0 and 0.3) bilayers. The ϵ -Fe_{2-x}Al_xO₃ thin films with 40 – 70 nm thickness were prepared by chemical solution deposition method on (h00)-oriented single crystal yttrium-stabilized zirconia substrates. The prepared films are highly oriented with the crystallographic c-axis perpendicular and the easy magnetic a-axis parallel to the film surface. The magnetic hysteresis loops measured at room temperature on samples with x = 0 with magnetic field parallel to the film surface exhibit coercive fields up to 11.6 kOe, which is the highest value observed so far for ϵ -Fe₂O₃ thin layers. It was observed that the spin Seebeck signal increases proportionally to film thickness. Al substitution led to increase of spin Seebeck effect and decrease of coercive field values. The shape and coercivity of the spin Seebeck hysteresis loops closely resemble shape and coercivity observed in magnetization loops. A difference was encountered in the case of films with a small amount (1–2 volume%) of secondary soft ferrimagnetic phase, which manifested itself in a constricted shape of magnetization loops. In contrast to spin Seebeck loops, where no constriction is observed.

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Spin hybrids – a new concept of magnetic matter

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The concept of spin hybrids introduced within the TSuNAMI project (ERC-Stg-2016) will be presented. The aim of the research is to build prototypes of trans-spin nano-architectures composed of at least two divergent spin entities, the TSuNAMIs. The spin entities of interest correspond to single atomic spin embedded in spin crossover complexes (SCO), molecular spin of molecular magnets (SMM), superspins of single-domain magnetic nanoparticles (SuperS) and pseudospins in two-dimensional transition metal dichalcogenides (PseudoS). Ultimate goal of the project is to identify a profit from trans-spin cooperation between the different spin entities coexisting in a single 'TSuNAMI'. Within the proposed high-risk/high-gain trans-spin strategy, we thus expect: 1. Enhancement of magnetic anisotropy in SMM-SuperS with enormous impact on cancer therapy using magnetic fluid hyperthermia, 2. Control over SCO via coupling to giant classical spin giving rise to miniature 'on-particle' sensors, 3. Mutual visualization of electronic states in SCO-PseudoS pushing frontiers of nowadays pseudospintronics, and 4. Control over electronic states with nanometer resolution in SuperS-PseudoS giving rise to novel functionalization strategies of graphene successor. Finally, first results of the research gained during the first year will be disseminated.

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Prof. Jaroslav Heyrovský (20. 12. 1890 – 27. 3. 1967)

Academician Jaroslav Heyrovský is considered to be the founder (1922) of a method (polarography) that enables the fast and extremely exact determination of metals and their concentrations in solutions.

In 1924 Heyrovský, together with his Japanese disciple Masuzo Shikata, designed and built an automatic device which he named a polarograph. After World War II, the method of polarography, which was employed in science, medicine and a range of industries, achieved a massive expansion.

In 1950, J. Heyrovský founded the Institute of Polarography that was attached to the Academy of Sciences in Prague.

Heyrovský is the only Czech scientist to be awarded the Nobel Prize for chemistry (10.12.1959) in recognition of his invention of polarography, pioneering achievement and the development of polarography.

The tradition of Heyrovský Discussion was started in 1967. The Heyrovský Discussion took place always in one of the conference centers of the Czech Academy. Originally, the Discussions were held at the Liblice castle, later in castle Bechyně and recently it has taken place at the renaissance castle Třešť in southeastern Bohemia, in an attractive, peaceful locality rich in historical monuments and of beautiful natural scenery.



NOTES

