



**EWE G/2D**

EUROPEAN WORKSHOP ON EPITAXIAL GRAPHENE AND 2D MATERIALS

20<sup>th</sup> – 24<sup>th</sup> May 2018

Salamanca, Spain

Hotel Alameda Palace \*\*\*\*\*



# Book of Abstracts

## 4<sup>th</sup> European Workshop on Epitaxial Graphene and 2D Materials

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**ASEVA**

It is for us a great pleasure to **welcome you to the *Hotel Alameda Palace* \*\*\*\*\*** where we celebrate the 4<sup>th</sup> edition of the European Workshop on Epitaxial Graphene and 2D Materials conference, called EWEG/2D2018. For this occasion, we have tried to accommodate a widely scoped scientific program paying special attention to combine fundamental science and the latest applicability/technological advances in the field of the graphene and the 2D materials. We tried our best to offer you attractive and exciting scientific talks and posters. We have received around 70 abstracts, around 25% Spanish, 65% from all over the rest of Europe and some contributions from United States.

EWEG/2D conference was foundationally conceived as an international workshop to gather together the wide scientific community with a changeling common interest: the study of the structural, electronic, magnetic and optical properties of graphene and 2D materials epitaxially grown on well-defined substrates. Materials of interest are graphene and its derivatives, its elemental analogues (silicene, germanene, antimonene, among others), hexagonal boron nitride, and transition metal dichalcogenides, but also less common systems as phosphorene or group III monochalcogenides (e.g., GaSe). Also advanced materials in the form of nanostructures and lateral in-plane or vertical van-der-Waals stacked heterostructures fall into the field of the workshop.

In particular, this new edition of the conference, EWEG/2D2018, addresses the experimental determination of structural, electronic, magnetic and optical properties of supported and freestanding 2DMs, as well as theoretical modeling of such properties and prediction of new 2DMs. The workshop includes studies on the interaction of 2DMs with their environment, for example the adsorption of atoms or molecules, or the interaction with light, electric or magnetic fields. Special attention is given to the interaction of 2DMs with their substrates and the way they change their properties.

Besides, maintaining a continuist line characteristic of this conference, most of academic and daily activities (oral and poster sessions, meals, as well as housing) will be carried out at the ***Hotel Alameda Palace* \*\*\*\*\***. This luxurious 5-star hotel located in the center of the World Heritage City of Salamanca is just 10 minutes walk from Salamanca's Main Square and 600 and 1300 meters away from the Railway and Bus Stations, respectively. The conference will take place at the elegant and fancy Pompeya Meeting room.

The choice of Salamanca to celebrate the 4<sup>th</sup> edition of the EWEG/2D conference has been made on the basis a large variety of favorable academic and social factors. On one side, Sciences, Literature and Humanities coexist since the Middle Age at the University of Salamanca, the oldest in Europe, together with Bologna and Oxford. A surprising and exciting microcosm where the foundations of international law were laid, contrasting with its major relevance in today state-of-the-art advances in biochemistry. Proud of the past and looking to the future, the University of Salamanca celebrates and commemorates in 2018 its 800<sup>th</sup> anniversary by remembering Fray Luis de León and waiting for Bob Dylan. On the other hand, the city of Salamanca is known as "La Dorada", or "Golden City", because of the golden glow of its sandstone buildings. This charming town is untouched in its architectural purity. It is one of the five Spanish cities declared by UNESCO as a World Heritage Site. Salamanca boasts a student population of almost 35,000 (approximately 6,000 of whom are foreigners), which provides a lively atmosphere and nightlife. The Roman Bridge used to be the main entrance into Salamanca. It was an essential part of the Roman Silver Route (la "Ruta de la Plata"), which ran from the silver mines in the North, in Astorga, to Mérida. On "El Puente Romano", only the first 15 arches nearest to the city are original, the remainder having been swept away by a flood in 1626. They are made of rustic granite masonry and seated on pillars with cutwaters directed against the river's flow.

The **technological exhibition** and **sponsorship** of this conference is very appealing, with three of the most relevant and representative companies in the field-related technologies: **SPECS** and **TeraTorr**, which will exhibit their products (we strongly recommend you to visit and interact with them), and with **Sigma Surface Science** sponsoring the daily session of the 21<sup>st</sup> of May.

To conclude, we have tried to provide during the conference an attractive offer within the proposed social program, which will start the day 20<sup>th</sup> of May with a “Reception Cocktail” in the famous, stylish and glamorous “Cum Laude” bar, located near the Major Square. To break with the academic routine, the 22<sup>nd</sup> of May the dinner will turn into a typical “Tapas” session around the most emblematic “Tapas” bars near the Salamanca Major Square (“Cervantes”, “Café Real”, among others). We will complete the social program the day 23<sup>rd</sup> of May with a guided excursion across the “old town”, visiting and experiencing the most beautiful and important buildings and monuments of the city, including a visit to the upper part of the Dome of the Cathedral of Salamanca. Afterwards, we will finish the day with the “Gala Banquet”, which will take place in the Hotel Corona Sol \*\*\*\*, where, first, we will visit its penthouse with a welcome drink in the hand to take the traditional conference picture surrounded by beautiful top-views of the city.

Our great hope is that you will enjoy the science and the technology challenges that will be shown in the conference; profit the occasion to establish links between colleagues in your field of research, approaching fundamental basic science and applicability opportunities to technology and vice-versa, and finally that the conference may serve to enhance the friendship between the participant countries represented by a geographically heterogeneous sample of participants.



José Ignacio Martínez

(Chair of the EWEG/2D2018 on behalf the Local Organizing Committee)

## The main organizers:

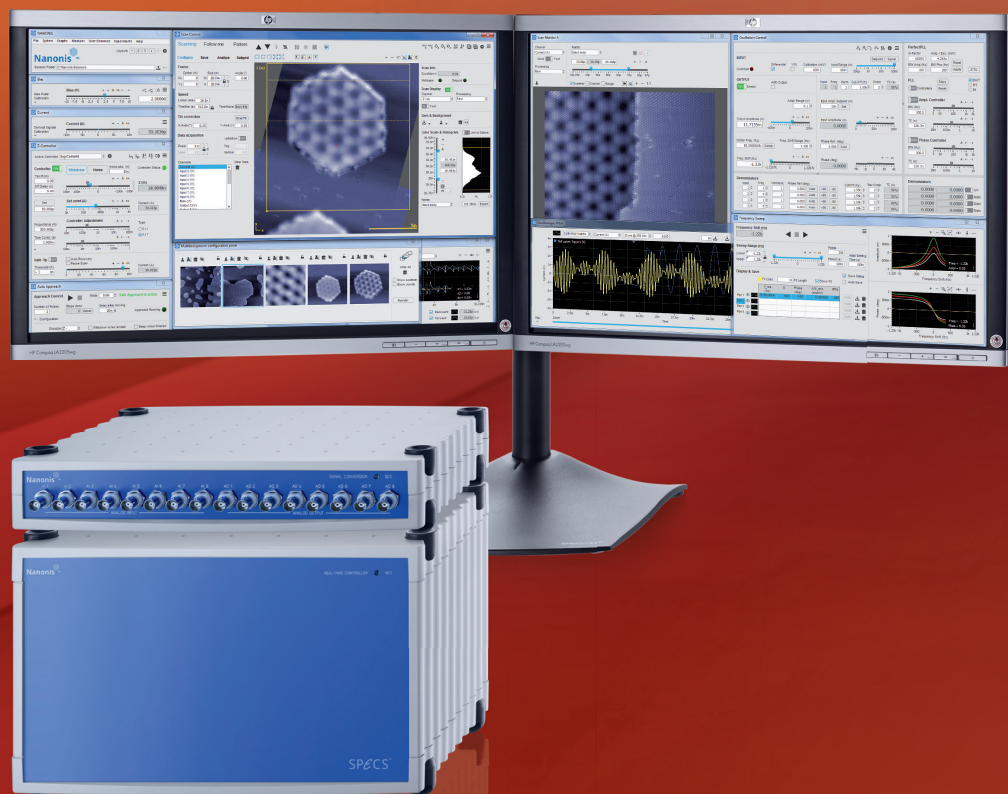
- José Ignacio Martínez (*ICMM-CSIC / Chair of the EWEG2D2018*)
- José A. Martín-Gago (*ICMM-CSIC / President of ASEVA / Scientific Committee*)
- Irene Palacio (*ICMM-CSIC / Technical Secretary of EWEG2D2018*)
- Carlos Sánchez-Sánchez (*ICMM-CSIC*)
- Fabian Calleja (*IMDEA-Nanoscience*)
- M<sup>a</sup> Francisca López (*ICMM-CSIC / Technical Secretary of ASEVA*)
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## Synaptic Schedule/Programme

SUNDAY 20 <sup>TH</sup>	MONDAY 21 <sup>ST</sup>	TUESDAY 22 <sup>ND</sup>	WEDNESDAY 23 <sup>RD</sup>	THURSDAY 24 <sup>TH</sup>
<b>ARRIVAL</b>	09:00-09:50 Dimas G. de Oteyza	09:00-09:50 Eva Y. Andrei	09:00-09:50 Thomas Michely	09:30-10:20 Simone Lisi
	09:50-10:15 A. San Miguel	09:50-10:15 A. Tamtögl	09:50-10:15 M. Batzill	10:20-10:45 M. M. Otrokov
	10:15-10:40 B. Senkovskiy	10:15-10:40 P. Merino	10:15-10:40 T. L. Lee	10:45-11:10 I. Delač-Marion
	10:40-11:05 S. Kraus	10:40-11:05 J. A. Delgado-Notario	10:40-11:05 M. Svec	11:10-11:35 <b>COFFEE</b>
	11:05-11:30 <b>COFFEE</b>	11:05-11:30 <b>COFFEE</b>	11:05-11:30 <b>COFFEE</b>	11:35-12:00 M. Will
	11:30-12:20 José A. Martín-Gago	11:30-12:20 Jaroslav Fabian	11:30-12:20 Philip Hofmann	12:00-12:25 D. Lizzit
	12:20-12:45 J. J. Navarro	12:20-12:45 J. Tesch	12:20-12:45 M. Petrović	12:25-12:35 <b>CLOSURE</b>
	12:45-13:10 B. de la Torre	12:45-13:10 D. Menzel	12:45-13:10 M. Garnica	<b>DEPARTURE</b>
	13:10-14:30 <b>LUNCH</b>	13:10-14:30 <b>LUNCH</b>	13:10-14:30 <b>LUNCH</b>	
16:00-18:50 <b>WELCOME &amp; REGISTRATION</b>	14:30-15:20 Liv Hornekær	14:30-15:20 Sebastian Günther	17:00-20:00 <b>EXCURSION / TOUR &amp; CONFERENCE PICTURE</b>	
	15:20-15:45 J. Knudsen	15:20-15:45 J. I. Cerdá		
	15:45-16:10 S. Simon	15:45-16:10 I. I. Klimovskikh		
	16:10-16:35 C. Romero-Muñiz	16:10-16:35 A. Sala		
18:50-19:00 <b>OPENING</b>	16:35-17:00 <b>COFFEE</b>	16:35-17:00 <b>COFFEE</b>		
Opening Key I 19:00-19:30 Enrique Diez	17:00-17:50 Camilla Coletti	17:00-17:50 Harold Zandvliet		
Opening Key II 19:30-20:00 Rodolfo Miranda	17:50-20:00 <b>POSTERS</b>	17:50-20:00 <b>POSTERS</b>		
20:30 <b>COCKTAIL</b>	20:00 <b>DINNER</b>	20:00 <b>DINNER</b>	21:00 <b>BANQUET</b>	

## Detailed Day-by-day Schedule/Programme

DAY 0 – SUNDAY 20 <sup>TH</sup>
<b>ARRIVAL</b>
16:00-18:50 <b>WELCOME &amp; REGISTRATION</b>
18:50-19:00 <b>OPENING</b>
Opening Key I 19:00-19:30 Enrique Diez (Univ. Salamanca): "Processing and characterization of nanoelectronics devices based on 2D materials"
Opening Key II 19:30-20:00 Rodolfo Miranda (IMDEA Nanosci.): "Magnetism in 2D"
20:30 <b>COCKTAIL</b>

## DAY 1 – MONDAY 21<sup>ST</sup>

09:00-09:50 **Dimas G. de Oteyza (CSIC-UPV/EHU):** "Alternative growth strategies of atomically precise graphene nanoribbons"

09:50-10:15 **A. San Miguel (Univ. Lyon):** "High pressure in 2D science. From adhesion and mechanical properties to nanoribbon elaboration"

10:15-10:40 **B. Senkovskiy (Univ. Cologne):** "Revealing the electronic band structure of atomically precise graphene nanoribbons"

10:40-11:05 **S. Kraus (Univ. Cologne):** "Nanostructures of cyclooctatetraene with rare-earth metals on graphene"

11:05-11:30 **COFFEE**

11:30-12:20 **José A. Martín-Gago (ICMM-CSIC):** "Highly selective covalent organic functionalization of epitaxial graphene"

12:20-12:45 **J. J. Navarro (IMDEA Nanosci.):** "Switching the Kondo effect on TCNQ through a catalytic reaction in CH<sub>3</sub>CN functionalized graphene on Ru(0001)"

12:45-13:10 **B. de la Torre (RCPTM):** "Spin-State control in metal-organic complex by positioning on N-doped graphene"

13:10-14:30 **LUNCH**

14:30-15:20 **Liv Hornekær (Univ. Aarhus):** "Controlling the electronic properties, reactivity and substrate interactions of graphene via intercalation and functionalization"

15:20-15:45 **J. Knudsen (Univ. Lund):** "Understanding how a super-dense water phase below graphene promotes O- and CO- intercalation"

15:45-16:10 **S. Simon (Univ. Konstanz):** "Layer-by-layer decoupling of twisted graphene sheets epitaxially grown on a metal substrate"

16:10-16:35 **C. Romero-Muñiz (UAM):** "Nitrogen doping of graphene on metals: Controlling corrugation and electronic properties with doping and oxygen intercalation"

16:35-17:00 **COFFEE**

17:00-17:50 **Camilla Coletti (IIT):** "Scalable van der Waals epitaxial heterostacks for optoelectronics"

17:50-20:00 **POSTERS**

20:00 **DINNER**

## DAY 2 – TUESDAY 22<sup>ND</sup>

09:00-09:50 **Eva Y. Andrei (Univ. Rutgers):** "Physics of imperfect graphene"

09:50-10:15 **A. Tamtögl (TU Graz):** "Nanoscale mass transport on Dirac materials"

10:15-10:40 **P. Merino (ICMM-CSIC):** "Atomically-resolved edge states on surface-nanotemplated graphene explored at room temperature"

10:40-11:05 **J. A. Delgado-Notario (Univ. Salamanca):** "0.3 THz detection using an asymmetric dual grating gate graphene FET"

11:05-11:30 **COFFEE**

11:30-12:20 **Jaroslav Fabian (Univ. Regensburg):** "Orbital, spin, and magnetic proximity effects in single and bilayer graphene on 2D substrates"

12:20-12:45 **J. Tesch (Univ. Konstanz):** "Landau quantization in graphene/transition metal dichalcogenides probed at the local scale"

12:45-13:10 **D. Menzel (TUM):** "Ultrafast charge transfer from core-excited argon intercalated and compressed under graphene monolayers and in blisters"

13:10-14:30 **LUNCH**

14:30-15:20 **Sebastian Günther (TUM):** "Graphene synthesis by CVD on Cu for the construction of electron transparent membranes"

15:20-15:45 **J. I. Cerdá (ICMM-CSIC):** "Tuning the graphene on Ir(111) adsorption regime by Fe/Ir surface-alloying"

15:45-16:10 **I. I. Klimovskikh (State Univ. Saint Petersburg):** "Graphene on Gd-5d metals surface alloys – superlattice and spin-dependent effects"

16:10-16:35 **A. Sala (Univ. Trieste):** "Growth and electronic structure of graphene on Ni(100)"

16:35-17:00 **COFFEE**

17:00-17:50 **Harold Zandvliet (Univ. Twente):** "Novel elemental 2D materials"

17:50-20:00 **POSTERS**

20:00 **DINNER**

## DAY 3 – WEDNESDAY 23<sup>RD</sup>

09:00-09:50 **Thomas Michely (Univ. Cologne):** "Graphene on Ir(111) as a growth platform for transition metal disulphide layers"

09:50-10:15 **M. Batzill (Univ. South Florida):** "Exploring layer-dependent properties of metallic 2D materials "

10:15-10:40 **T. L. Lee (Diamond Light Source):** "Chemically resolved geometric structures of 2D materials"

10:40-11:05 **M. Svec (Czech Academy of Sciences):** "The Moiré pattern of a 2D iron oxide layer grown on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001)"

11:05-11:30 **COFFEE**

11:30-12:20 **Philip Hofmann (Univ. Aarhus):** "Electronic structure and electron dynamics in novel two-dimensional materials"

12:20-12:45 **M. Petrović (Univ. Duisburg-Essen):** "Lateral heterostructures of hexagonal boron nitride and graphene: alloying and microstructuring"

12:45-13:10 **M. Garnica (TUM):** "h-BN on Cu(111): Geometric corrugation and intercalation of functional molecules"

13:10-14:30 **LUNCH**

17:00-20:00

**EXCURSION / TOUR  
&  
CONFERENCE PICTURE**

21:00 **BANQUET**

## DAY 4 – THURSDAY 24<sup>TH</sup>

09:30-10:20 **Simone Lisi (Inst. Néel):** "Excitons in transition metal dichalcogenides vs. strain, defects and charged impurities"

10:20-10:45 **M. M. Otrokov (CFM-MPC Donosti):** "Evidence of large spin-orbit coupling effects in quasi-free-standing graphene on Pb/Ir(111)"

10:45-11:10 **I. Delač-Marion (CEMS):** "Atomic-scale defects and electronic properties of synthesized molybdenum disulphide monolayer"

11:10-11:35 **COFFEE**

11:35-12:00 **M. Will (Univ. Cologne):** "A monolayer of hexagonal boron nitride on Ir(111) as a template for cluster growth"

12:00-12:25 **D. Lizzit (Elettra – Sincrotrone Trieste):** "Single-orientation high-quality MoS<sub>2</sub> monolayers with complete spin polarization"

12:25-12:35 **CLOSURE**

**DEPARTURE**





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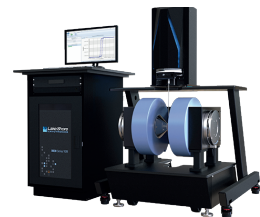
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# PRACTICAL INFORMATION

## - Social program

As commented in the introduction, we have tried to provide during the conference an attractive offer within the proposed social program, which will start the day 20<sup>th</sup> of May with a “Reception Cocktail” in the famous, stylish and glamorous “Cum Laude” bar, located near the Major Square. To break with the academic routine, the 22<sup>nd</sup> of May the dinner will turn into a typical “Tapas” session around the most emblematic “Tapas” bars near the Salamanca Major Square (“Cervantes”, “Café Real”, among others). We will complete the social program the day 23<sup>rd</sup> of May with a guided excursion across the “old town”, visiting and experiencing the most beautiful and important buildings and monuments of the city, including a visit to the upper part of the Dome of the Cathedral of Salamanca. Afterwards, we will finish the day with the “Gala Banquet”, which will take place in the Hotel Corona Sol \*\*\*\*, where, first, we will visit its penthouse with a welcome drink in the hand to take the traditional conference picture surrounded by beautiful top-views of the city.

## - Map with important sites



1. The Hotel: Hotel Alameda Palace (Paseo de la Estación 1)
2. The Gala dinner: Hotel Corona Sol (Av. Villamayor 31)
3. Bus Station (Av. Filiberto Villalobos)
4. Train Station
5. Meeting point Guide Excursion: Cathedral of Salamanca
6. Reception Cocktail: “Cum Laude” Bar (C/ Prior 5-7)



## Alternative growth strategies of atomically precise graphene nanoribbons

D. G. de Oteyza<sup>1,2,3</sup>

<sup>1</sup> Donostia International Physics Center, Paseo Manuel Lardizabal 4, 20018 San Sebastián, Spain

<sup>2</sup> Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain

<sup>3</sup> Centro de Física de Materiales (CSIC-UPV/EHU) - MPC, Paseo Manuel Lardizabal 5, 20018 San Sebastián, Spain

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The challenge of synthesizing graphene nanoribbons (GNRs) with atomic precision is currently being pursued along a one-way road, based on the synthesis of adequate molecular precursors that react in predefined ways through self-assembly processes. The synthetic options for GNR generation would multiply by adding a new direction to this readily successful approach, especially if both of them can be combined. We show how, still based on self-assembly to maintain the atomic precision not yet achievable with top-down methods, selectivity in the GNR synthesis can be guided, instead of by designed reactants, by an adequately nanotemplated substrate. This new strategy's proof-of-concept compares experiments using 4,4'-dibromo-para-terphenyl (DBTP) as molecular precursor on flat Au(111) and stepped Au(322) substrates.

On Au(111), the reactant first polymerizes into poly-para-phenylene (PPP) at moderate temperatures below 200 °C. Annealing to higher temperatures drives the lateral fusion of PPP chains through cyclo-dehydrogenation, ending up with graphene nanoribbons of varying width depending on the number of polymers involved. The resulting samples are thus interesting to study width-dependent properties and phenomena in GNRs. We have used such samples to characterize the width-dependent band gap of GNRs and, most importantly, the associated evolution of the energy level alignment of frontier bands. Doing so, a Fermi level pinning scenario of the valence band has been found for GNRs displaying band gaps below ~1.7 eV.[1] However, from the synthetic point of view, selectivity towards particular GNRs is completely missing.

A completely different scenario is found on Au(322). The polymerization and cyclo-dehydrogenation reactions occur in a similar way. However, the periodic steps of Au(322) limits the number of fusing polymers to two, resulting in the selective synthesis of 6 atom-wide armchair GNRs (6-aGNRs). In addition, all GNRs being uniaxially aligned along the substrate's steps, we have been able to characterize the sample's valence band properties by angle resolved photoemission spectroscopy. Complemented with scanning tunneling spectroscopy measurements and density functional theory calculations, we end up with a fully coherent and complete picture of the electronic properties of 6-aGNRs.[2] Beyond the readily widely accepted band gap predictions for GNRs, this work confirms the reliability of the predictive scaling laws for the effective masses of aGNRs, a similarly important parameter for the ultimate performance of GNR-based devices. Together with the newly demonstrated concept of substrate templating for selective GNR growth, proved with the first report on selective synthesis of 6-aGNRs, these results take a substantial step further in the development of GNR-related research and thus in its track towards real device design and implementation.

### REFERENCES:

[1] N. Merino-Díez, et al., *ACS Nano* **2017**, *11*, 11661-11668

[2] N. Merino-Díez, et al., in preparation.

## Selective covalent organic functionalization of epitaxial graphene: a platform for nano-bio-hybrid composites

J. A. Martín-Gago<sup>1</sup>, R. A. Bueno<sup>1</sup>, I. Palacio<sup>1</sup>, J. I. Martínez<sup>1</sup>, M. Marciello<sup>1</sup>, M. Moreno<sup>2</sup>, M.F. López<sup>1</sup>, F. Mompean<sup>1</sup>, M. García-Hernández<sup>1</sup>, P. Morales<sup>1</sup>, C. Briones<sup>2</sup>, G. Ellis<sup>3</sup>, L. Vazquez<sup>1</sup>.

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Graphene functionalization is an important step for the development of graphene-based materials with tailored electronic properties. However, its high chemical inertness makes difficult a selective covalent functionalization, and most of the works performed up to date report electrostatic molecular adsorption or unruly functionalization. We show a new mechanism for promoting highly specific covalent bonding of any amino-terminated molecule and a description of the operating processes. We show, by different experimental techniques and theoretical methods, that the excess of charge at carbon dangling-bonds formed on single-atomic vacancies at the graphene surface induces enhanced reactivity towards a selective oxidation of the amino group and subsequent integration of the N within the graphene network. Functionalized surfaces retain the electronic properties of pristine graphene as unaltered.

Thus, we use this strategy to link to graphene a molecule with a robust thiol-terminated moiety derived from a *p*-aminothiophenol (p-ATP) molecules. We use this facile strategy to covalently link gold nanoparticles, which remain firmly anchored to the surface after many washing and annealing cycles. In parallel, we also couple *in vitro* a thiol-modified ssDNA aptamer to the p-ATP-functionalized graphene surface, and successfully obtain atomic force microscopy images both in air and in a liquid environment, and demonstrate that the anchored aptamer retains the functionality required to recognize its target protein, PCBP-2. This work opens the door to the integration of high-quality graphene layers in technological platforms for plasmonics, biosensing or advanced field-effect transistor devices.

### REFERENCES:

[1].- Bueno et al. Nat. Comm. 2017; 8: 15306.

## Controlling the electronic properties, reactivity and substrate interactions of graphene via intercalation and functionalization

L Hornekær

Dept. Physics and Astronomy and Interdisciplinary Nanoscience Center (iNANO), Aarhus University

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The extensive control of electronic and chemical properties of graphene/Ir(111) available through chemical functionalization and intercalation will be illustrated via combined STM, XPS and HREELS measurements and DFT calculations. On one hand, functionalization structures can be controlled via intercalation, while conversely, intercalation can be hindered via chemical functionalization. Furthermore, unique oxygen functionalization structures and molecular hydrogen dissociative adsorption pathways are available in this system [1]. Overall this allows for extensive control of electronic properties for band gap engineering [2], as well as control of the graphene-substrate interaction, providing proof-of-principle pathways to e.g. enhance the coating properties of graphene on metal surfaces [3,4].

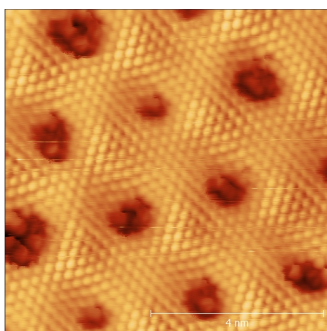


Fig.1 STM image of hydrogen functionalized graphene/Ir(111).

### REFERENCES:

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## Scalable van der Waals epitaxial heterostacks for optoelectronics

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In this talk recent advances on the synthesis and applications of large-scale highly-crystalline 2D van der Waals heterostacks will be presented. The electronic performance of single-crystal graphene arrays obtained via patterned growth [1] will be discussed in terms of homogeneity and repeatability. Particular focus will be put in the heterostack obtained by directly synthesizing via chemical vapor deposition (CVD) tungsten disulfide ( $WS_2$ ) on graphene [2]. It will be shown via microstructural and electronic characterization that  $WS_2$  aligns on top of graphene with a  $0^\circ$  orientation, the interface is atomically sharp and the spin-orbit splitting of monolayer  $WS_2$  on graphene is the largest reported to date [3]. In virtue of its band alignment and remarkable spin-orbit splitting, this system gains strong appeal for optoelectronics and optospintronic applications. Indeed, the fabrication and performance of an entirely scalable hybrid  $WS_2$ /graphene photodetector will be presented.

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## Physics of Imperfect Graphene

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Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries and to the promise of important applications. I will discuss new and surprising phenomena that emerge when the perfect honeycomb lattice of graphene is disrupted by single atom vacancies as revealed by scanning tunneling microscopy and spectroscopy. These include i) the ability to charge the vacancy site into the supercritical regime where atomic collapse leads to the formation of an artificial atom<sup>1,2</sup>; ii) the appearance of a local magnetic moment at the vacancy site and its Kondo screening<sup>3</sup>.

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# Orbital, spin, and magnetic proximity effects in single and bilayer graphene on 2D substrates

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Graphene and novel 2d materials offer new perspectives for spintronics [1]. Graphene can reach spin lifetimes of 1-10 ns, limited currently by spin flips off magnetic moments [2]. However, graphene has no band gap, so its spintronic applications will be limited as a highly efficient spin transfer channel. Heterostructures of graphene and two-dimensional transition-metal dichalcogenides (TMDC) are emerging as systems in which both orbital and spin properties can be controlled by gating, thus offering a materials basis for spintronic applications, such as bipolar spin devices [3]. We have proposed that graphene on TMDCs can be used in optospintronics [4], since the direct gap of TMDCs allows optical spin orientation, with the successive transfer of spin into graphene. But these van der Waals stacks also yield interesting fundamental physics. We have recently shown that graphene on WSe<sub>2</sub> exhibits an inverted band structure, which leads to helical edge states in graphene nanoribbons on WSe<sub>2</sub> [5], with a bulk spin-orbit gap of about 1 meV, which is giant when compared to 24 micro eV in pristine graphene. Even more fascinating is bilayer graphene on TMDCs, as the spin properties of this material can be controlled by gate voltage, creating a platform for spin-orbit valves and spin transistors [6], illustrated in Fig 1.

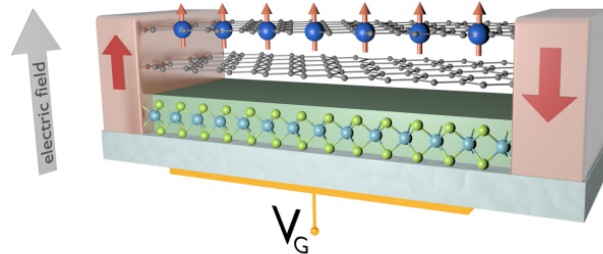


Fig. 1. Spin transistor made of bilayer graphene on a TMDC. Applying electric field we can either increase or decrease spin-orbit coupling and spin relaxation, resulting in ON and OFF states of the transistor [6].

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## Graphene synthesis by CVD on Cu for the construction of electron transparent membranes

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Understanding and controlling the growth kinetics of graphene is a prerequisite to synthesize a membrane material by chemical vapor deposition (CVD) on Cu in a reactive methane/hydrogen atmosphere that fulfills the requirements for the construction of ultra-stable electron transparent windows. We review that Cu foils contain a considerable amount of bulk carbon that significantly exceeds the expected amount of thermally equilibrated dissolved carbon in Cu and that this carbon has to be removed before any high quality graphene may be grown [1,2]. Starting with C-depleted Cu foils, systematic studies of the graphene growth kinetics in a reactive CH<sub>4</sub>/H<sub>2</sub> atmosphere were performed. Considering thermodynamics, we were able to setup a kinetic growth model and predict the equilibrium constant of the graphene formation reaction within a precision of a factor of two. By quantitatively controlling the deviation of the chosen CVD growth parameters from thermodynamic equilibrium, we confirm that the graphene growth proceeds from a C(ad)-phase on Cu which is in thermal equilibrium with the reactive gas phase and extract the respective apparent activation barrier. Finally, we can predict the achievable growth velocity of growing graphene flakes during CVD on Cu. Suitable parameters are identified allowing the synthesis of high quality monolayer graphene with single crystalline domains of 100-1000 μm in diameter within reasonable growth time. Using the synthesized material, we construct free-standing graphene covering large holes [3].

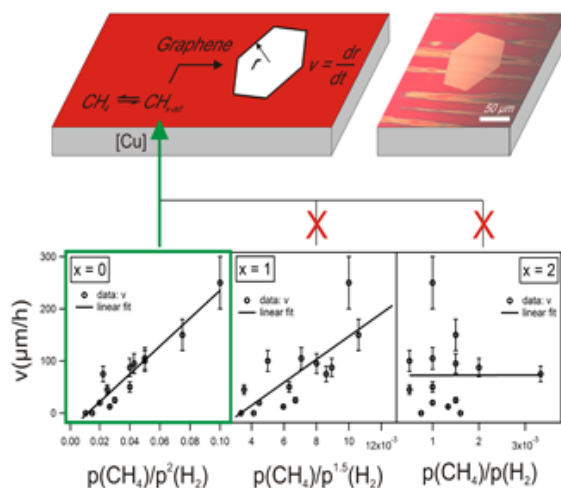


Fig. Correlation analysis proves CVD graphene growth on Cu via a pre-equilibrated C(ad) species. The identified growth kinetics allow to predict the growth velocity of nucleated g-flakes that may exceed 200 μm/h.

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4<sup>th</sup> European Workshop on Epitaxial Graphene and 2D Materials (<http://www.icmm.csic.es/eweg2d-2018/>)

## Novel elemental 2D materials

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Recently, a few research groups have reported the growth of germanene, a new member of the graphene family [1]. Germanene is in many aspects very similar to graphene, but in contrast to the planar graphene lattice, the germanene honeycomb lattice is slightly buckled and composed of two vertically displaced sub-lattices. First principles total energy calculations have revealed that free-standing germanene is a two-dimensional Dirac fermion system, i.e. the electrons behave as massless relativistic particles that are described by the Dirac equation, i.e. the relativistic variant of the Schrödinger equation. We will give a brief update of the growth and electronic properties of germanene on Pt/Ge(110) nanocrystals [2,3]. Subsequently, we will show that large and continuous single germanene layers can be grown on molybdenum disulfide ( $\text{MoS}_2$ ) [4]. The structural and electronic properties of the germanene layer are studied with scanning tunneling microscopy and spectroscopy. The lattice constant of the germanene layer is  $3.8 \pm 0.1 \text{ \AA}$ , i.e. substantially larger than the lattice constant of  $\text{MoS}_2$  ( $3.16 \text{ \AA}$ ), and the interlayer distance between the germanene layer and the  $\text{MoS}_2$  substrate is  $3.2 \pm 0.2 \text{ \AA}$ , suggesting that we are dealing with a low-buckled germanene layer. The density of states of the germanene layer exhibits a V-shape, which is one of the hallmarks of a two-dimensional Dirac system.



**Figure.** Scanning tunneling microscopy image (4.5 nm by 4.5 nm) of buckled honeycomb lattice of germanene. Sample bias -0.5 V, tunnel current 0.2 nA.

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## Graphene on Ir(111) as a growth platform for transition metal disulphide layers

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Graphene and monolayers of hexagonal boron nitride on Ir(111) are excellent templates for the regular arrangement of holes, clusters or molecules and superior substrates for the synthesis of new materials, including organometallic sandwich molecular wires, oxide thin films or transition metal dichalcogenide layers.

In this contribution I will discuss a two-step molecular beam epitaxy synthesis with elemental sulphur enabling the growth of clean, well-oriented, almost defect-free and well decoupled monolayer and multilayer islands and layers of the transition metal disulfides MoS<sub>2</sub>, TaS<sub>2</sub>, WS<sub>2</sub> and VS<sub>2</sub>. Using scanning tunneling microscopy, low energy electron diffraction, and angle resolved photoemission spectroscopy we investigate systematically how to optimize the growth process, provide insight into the growth as well as annealing mechanisms, and characterize the global electronic structure of the layers, using MoS<sub>2</sub> as a paradigm.

With the help of scanning tunneling spectroscopy, ab initio calculations and analytical modeling we investigate one dimensional metallic states hosted by two different types of twin boundaries in MoS<sub>2</sub>. Experimentally, these states are characterized by clear length dependent quantization effects with specific boundary conditions, by a density of states gap of the order of 100 meV around the Fermi level again depending of the wire extension, and by an incommensurate modulation of the measured density of states along the wire and extending deep into the discrete states below and above the Fermi level. We critically discuss the relevance of charge density waves and spin-charge separation to understand the observed complex electronic structure.

Contributions to this work by Joshua Hall, Wouter Jolie, Clifford Murray, Tobias Wekking, Carsten Busse, Fabian Portner, Philipp Weiß, Achim Rosch, Arkady Krasheninnikov, Hannu-Pekka Komsa, Borna Pielić, Marko Kralj, Martin Hell, Nils Ehlen, Boris Senkovskiy, Alex Grüneis, José Márquez-Velasco, Luca Petaccia, and Giovanni di Santo, as well as financial support through CRC1238 within project A01 of DFG are gratefully acknowledged.

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## Electronic structure and electron dynamics in novel two-dimensional materials

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Artificial two-dimensional (2D) materials, such as graphene or single-layer transition metal dichalcogenides, permit the realization of massless and massive Dirac fermions. A special feature of the 2D materials is that their electronic properties, for instance their band gap, can be strongly influenced by either their dielectric environment or by the excited carrier density in the material.

Here we exploit this sensitivity to achieve a static and dynamic change in the electronic properties of 2D materials such as graphene and single layer WS<sub>2</sub>. This control of properties is demonstrated using scanning tunneling microscopy, time- and spin-resolved angle-resolved photoemission spectroscopy, as well as spin-resolved inverse photoemission spectroscopy. We demonstrate the possibility of static and dynamic band gap control, as well as the observation of a substrate-induced semiconductor-to-metal transition in epitaxial single layer WS<sub>2</sub>.

## Excitons in transition metal dichalcogenides Vs. strain, defects and charged impurities

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<sup>5</sup>Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragón, Universidad de Zaragoza, 50018 Zaragoza, Spain

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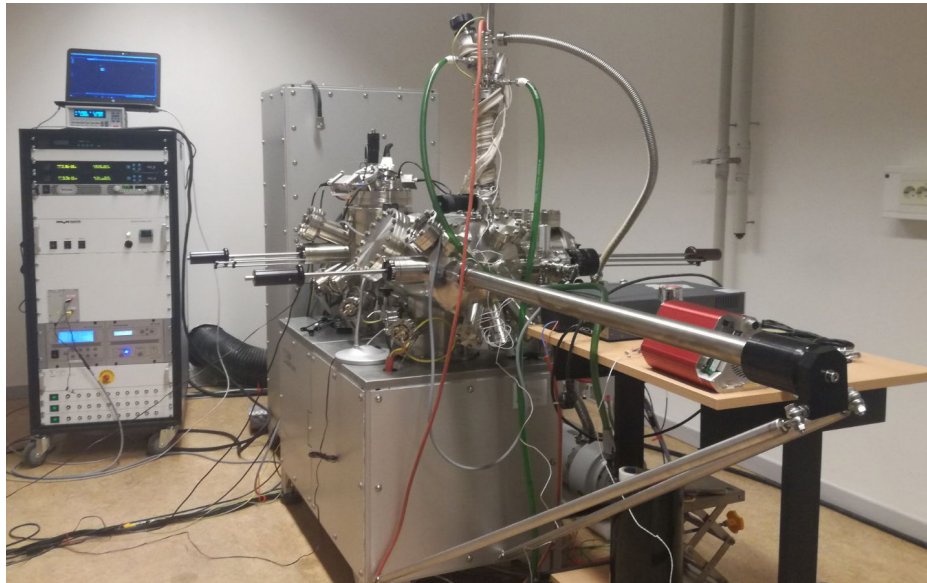
In the last years, the panorama of 2D materials has been rapidly expanding, providing striking illustrations of new, rich Physics related to the reduced dimensionality, precluding possible implementations in actual devices. Strong focus has been given recently to materials complementing the properties of graphene, e.g. atomically thin semiconducting layers. Several such materials have been addressed, which belong to the same class, that of transition metal dichalcogenides (TMDCs) [1]. Similarly to graphite, the bulk crystals can be thinned down to mono-layer 2D flakes thanks to their van der Waals layered nature. Among the others, molybdenum-disulphide ( $\text{MoS}_2$ ) offers some of the strategical properties of graphene, noteworthy abundance and stability. When thinned down to a single layer, quantum confinement effects trigger an indirect-to-direct band gap transition in this semiconductor [2], making it a potential building block for optoelectronic devices [3]. Defects, strains and charge transfers with the environment naturally play a major role in influencing the optical properties of materials, making their understanding, and subsequent control, paramount.

Here I will present our recent study on the role of defects on the optical properties of  $\text{MoS}_2$  [4]. For highlighting their effects on the crystal's optical properties, a novel synthetic  $\text{MoS}_2$  source, hosting specific defects, is compared with a natural one. Supporting the flakes with different substrates (silicon oxide and hexagonal boron nitride) allows for distinguishing intrinsic and extrinsic effects. A cross-characterization, using spatially-resolved Raman spectroscopy and photoluminescence, allows for disentangling concomitant effects with similar spectroscopic signatures, as strain and doping, clarifying the role of defects. Our study suggests the existence of a defect induce exciton localization. A joint density functional theory and scanning tunneling microscopy analysis is carried out to explore the nature of defects in the novel synthetic source.

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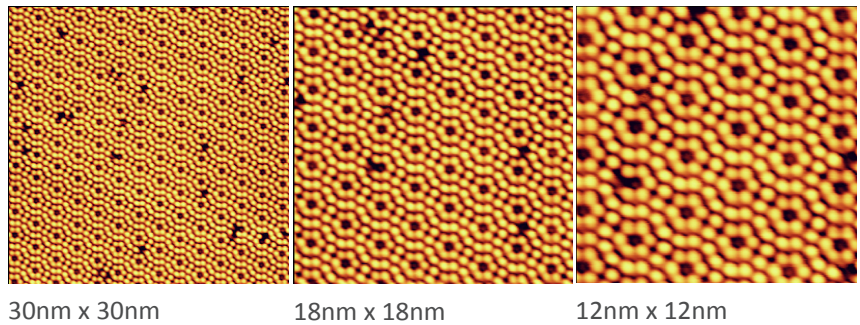
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Low Noise by Design



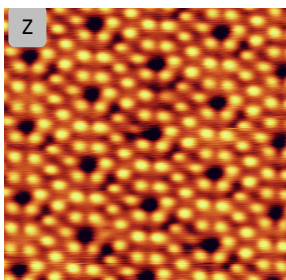
### STM measurement on Si(111) with qPlus® sensor

STM at 10K  
 STM measurements have been carried out with qPlus sensor in STM mode.  
 Vacuum:  $9 \times 10^{-11}$ mbar  
 Sample: Si(111)  $7 \times 7$



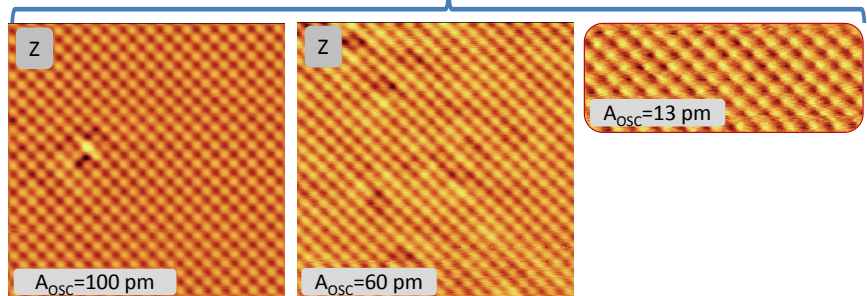
### qPlus AFM on Si(111) and NaCl(001)

qPlus AFM on Si(111) @  $T_{STM}=9.69$ K,  
 10nm x 10nm



Si-measurement parameters:  $f_{RES}=23.161$ ,  
 $df=-4.65$ Hz,  $Q=21.800$ ,  $TC=5$ ms,  $A_{OSC}=190$ pm

qPlus AFM on NaCl(001) @  $T_{STM}=9.69$ K,  
 8nm x 8nm



NaCl measurement parameters:  $f_{RES}=23.157$ ,  
 $df$  ca.  $-3.65$ Hz,  $Q=21.750$ ,  $TC=2$ ms

INFINITY qPlus AFM at  $T < 10$ K  
 Vacuum:  $8.2 \times 10^{-11}$ mbar  
 Temperature: 9.69K  
 Samples: Si(111)  $7 \times 7$  (left), and single crystal NaCl(001) (right)

Results have been obtained with delivered system to University of Lund, Sweden.

Raw data presented with background subtraction only.

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## High pressure in 2D science. From adhesion and mechanical properties to nanoribbon elaboration

D. Machon, C. Bousige, S.D. Silva Santos, R. Alencar, C. Journet, A.C. Torres-Dias, W. Cui, A. Forestier, and **A. San Miguel**

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The high pressure study of 2D-systems brings an additional window for the exploration of the physico-chemical properties of atomic-thick 2D materials as graphene, MoS<sub>2</sub> or h-BN. [1,4]

In particular, we have shown that the pressure response of the Raman signal allows the determination of the strain transfer efficiency between the substrate and the 2D-system, which in turn characterizes the roughness of the substrate, its adhesive character and compressibility [1]. We observe that in the case of a-SiO<sub>2</sub> substrates, graphene displays a homogeneous adhesion pattern [1] whereas MoS<sub>2</sub> interaction with the substrate shows a bimodal nature [2]. The adhesion patterns evolve depending on the substrate nature or the number of considered 2D-layers [1,3].

As an alternative way to synthesize or characterize 2D-systems, we have also explored the high pressure evolution either of carbon or h-BN nanotubes. In particular, we found the high pressure formation of original ribbon-like structures through the unzipping of the tubular structure. In addition, for single-wall carbon nanotubes, the study of the radial collapse pressure as function of the nanotube diameter provides a precise determination of the graphene bending rigidity modulus [4].

In this paper presentation we will review more generally the high pressure contributions to atomic-layer 2D science, including recent propositions of diamondene elaboration.

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## Revealing the electronic band structure of atomically precise graphene nanoribbons

**Boris Senkovskiy**<sup>1</sup>, Dmitry Usachov<sup>2</sup>, Alexander Fedorov<sup>2,3</sup>, Danny Haberer<sup>4</sup>, Niels Ehlen<sup>1</sup>, Vasile Caciuc<sup>5</sup>, Nicolae Atodiresei<sup>5</sup>, Cesare Tresca<sup>6</sup>, Gianni Profeta<sup>6</sup>, Felix Fischer<sup>4</sup>, Alexander Grüneis<sup>1</sup>

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Atomically precise graphene nanoribbons (GNRs) fabricated by the bottom-up approach from the molecular precursors is a promising material for optoelectronic applications. Here we demonstrate the correct way of using the angle-resolved photoemission spectroscopy (ARPES) for unambiguous determination of the electronic band structure of GNRs. The long-standing discrepancy between the ARPES and scanning tunneling spectroscopy data regarding the valence band effective mass of armchair GNRs with a width of  $N=7$  carbon atoms (7-AGNRs) is resolved. We obtain the first true experimental band structure of pristine and boron-doped 7-AGNRs aligned on Au(788) crystals. It is demonstrated that the photoemission intensity of each sub-band of quasi-one dimensional (1D) GNRs is a peaked function of the two-dimensional (2D) momentum. This knowledge allows identifying all 1D sub-bands and visualizing the “hidden” frontier valence sub-band of 7-AGNRs. From the experimental band structure we determine parameters important for the electronic properties of GNRs: effective masses, charge carrier velocities and band offsets. Periodic incorporation of B atoms in GNRs strongly modifies the interaction with the Au substrate. Particularly, hybridization of the B-derived frontier flat valence sub-band with Au states results in energy spreading of the band. From another hand, the second parabolic sub-band with C contribution remains particularly unchanged. Complementary to the ARPES, we investigate the vibrational properties of GNRs by in situ Raman spectroscopy. We find that boron doping strongly affects the Raman active phonon frequencies. In particular, we observe a frequency shift and a doubling of the so-called radial breathing-like mode for boron doped GNRs.

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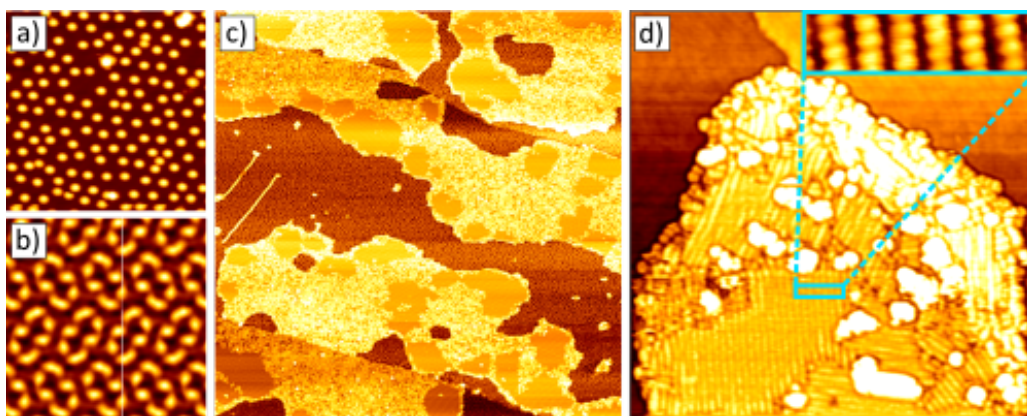
## Nanostructures of Cyclooctatetraene with Rare-Earth Metals on Graphene

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Organometallic compounds containing rare-earth elements are of interest in molecular spintronics owing to the robust magnetic moment of the  $4f$  ion. As a first system, we combine the lanthanide Eu with the organic molecule cyclooctatetraene (Cot) for the growth of organometallic sandwich molecular wires on graphene/Ir(111), which form crystalline islands via self-assembly [1]. Using XMCD techniques we investigate the magnetic properties of the wires at varying temperatures. In order to introduce a magnetocrystalline anisotropy to such a sandwich molecular system, we choose the lanthanide Tm as metal reactant, which has a finite orbital moment as a second system. Rather than only wires, the growth using Tm yields three distinct organometallic phases. Synthesis on the undoped substrate yields a disperse phase of repulsively interacting TmCot monomers [fig. a)], which are stabilized by charge transfer into the substrate leading to a Coulomb repulsion between them. When surpassing a coverage of about 2% ML, an island-forming “coffee-bean” phase emerges [fig. b)] out of the monomer phase and coexists with it as shown in fig. c). The formation of these phases is inhibited by  $n$  doping of graphene via intercalation, as further charge transfer is suppressed. Rather, synthesis on the doped substrate results in the formation of sandwich molecular wires growing in islands as shown in fig. d). Tuning the Tm/Cot ratio during growth controls the achievable wire length, in some islands exceeding 100 Tm ions per wire. XMCD measurements show an anisotropic behavior of the coffee-bean phase and promise exciting magnetic properties of the wire phase.



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## Switching the Kondo effect on TCNQ through a catalytic reaction in CH<sub>2</sub>CN functionalized graphene on Ru(0001)

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The presence of a magnetic impurity in a sea of conduction electrons results in the formation at low temperatures of a many-body ground state in which the electrons from the substrate screen the magnetic impurity. The scattering from a single magnetic impurity by spin flip results in the appearance of a sharp Kondo resonance at the Fermi level that can be detected by STS.

TCNQ molecules acquire magnetic moment when deposited on clean, pristine gr/Ru(0001) under UHV conditions [1] as judged from the appearance of a sharp Kondo resonance at the Fermi level. The gr/Ru(0001) surface can be functionalized by selective adsorption of CH<sub>2</sub>CN<sup>•</sup> radicals at specific positions in the moiré unit cell [2] [3]. Upon deposition of TCNQ molecules on a functionalized gr/Ru(0001) surface, a chemical reaction between TCNQ and CH<sub>2</sub>CN takes place. The new chemical species, product of the reaction, does not show the Kondo resonance. However, the reverse reaction can be induced through STM manipulation techniques, leading to the reappearance of the Kondo signal. This is confirmed by DFT calculations.



Topographic STM image of a TCNQ/TCNQ dimer and a TCNQ/TCNQ-CH<sub>2</sub>CN species on gr/Ru(0001) and corresponding Kondo intensity distribution map. Notice the missing Kondo signal from TCNQ-CH<sub>2</sub>CN.

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## Spin-State Control in Metal-Organic Complex by Positioning on N-Doped Graphene

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Doping of graphene with nitrogen represents a strategic method to control its electronic, magnetic, and transport properties [1-3]. Nitrogen doping can also significantly affect the interaction energies and phenomena on the phase boundary graphene-molecule with a huge impact mainly in sensing and electrocatalysis. Here we demonstrate a novel approach to control spin state of a single molecule of iron (II) phthalocyanine (FePc) by its positioning onto N-doped graphene. The transition is driven by a weak non-covalent interaction based on electron density rearrangement between d-orbitals of iron and the singly occupied  $p_z$  orbital of graphitic nitrogen. High-resolution atomic force microscopy imaging with CO-functionalized tip and theoretical calculations showed that the transition is characterized by sharp differences in the sub-molecular contrast over molecules located on pristine graphene and in the vicinity of N-dopant corresponding to singlet and triplet spin states, respectively. This work demonstrates a unique capability of the imaging technique to discriminate between different spin states of single molecules. Moreover, it shows an emerging possibility to trigger the spin state transition and tune the electronic properties of molecules through weak non-covalent interaction with suitably functionalized graphene.

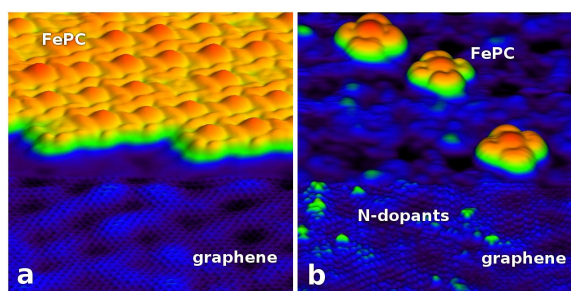


Fig.1: (a) FePc adsorbed on graphene, forming islands. (b) FePc anchored to N-dopants in graphene.

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## Understanding how a super-dense water phase below graphene promotes O- and CO- intercalation

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In this contribution we will present a complete picture of O-, CO- and H-intercalation below pristine graphene supported on Ir(111). Using the interplay of scanning tunnelling microscopy (STM) and x-ray photoelectron spectroscopy (XPS) [1-3] we will give a detailed picture of the adsorption structures formed below graphene. Furthermore, we will discuss how the dosing conditions can be used to control the intercalation: Oxygen intercalates Gr flakes above 400 K while a closed film is stable until 700 K where etching sets in [4]. CO intercalates Gr in the mbar regime [2], while H<sub>2</sub> only intercalates Gr at temperatures close to 100 K [3]. In all three cases we observe digital intercalation of the flakes – i.e. they are either fully intercalated or not at all - indicating that the edges form an initial barrier for intercalation. Once this barrier is surpassed complete intercalation is obtained very fast.

Recently, we found that this picture is changed dramatically if O<sub>2</sub>, H<sub>2</sub>, and CO is dosed sequentially. In contrast to pristine Gr flakes oxygen intercalated Gr flakes are easy to intercalate by subsequent hydrogen dosing at room temperature leading to super dense OH-H<sub>2</sub>O phase trapped below graphene. We find that this OH-H<sub>2</sub>O phase reduce the barrier for sub-sequent oxygen intercalation and room temperature intercalation now becomes possible. The presence of the super-dense OH-H<sub>2</sub>O phase below graphene also has dramatic consequences for CO intercalation. Without the OH-H<sub>2</sub>O phase mbar pressures of CO is needed to overcome the barrier for CO intercalation. In contrast digital CO intercalation is observed when 100 L CO is dosed at UHV conditions when the OH-H<sub>2</sub>O phase is present below graphene. Lowering the dose to 1 L CO leads to insight of the entrance channel for CO intercalation. In this case we observe irregular shaped CO channels growing out from OH-H<sub>2</sub>O islands located at the Ir(111) step edges. This observation suggest a mechanism for the CO intercalation in which CO diffuses along the Ir(111) step edges into dense OH-H<sub>2</sub>O islands and from there spreads out under the graphene flakes.

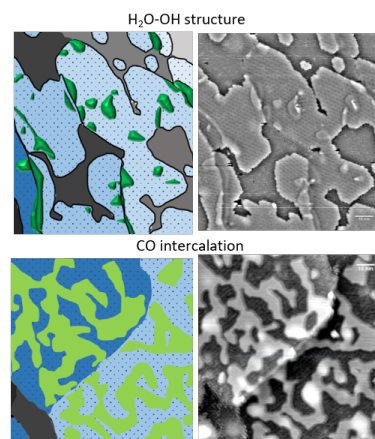


Figure 1: Top right: STM image of graphene flakes after formation of undercover OH-H<sub>2</sub>O islands. Bottom right: STM image of graphene flakes after subsequent exposure to 1 L CO showing the CO channel like structure.

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## Layer-by-layer decoupling of twisted graphene sheets epitaxially grown on a metal substrate

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Epitaxial graphene remains at the center of many theoretical and experimental studies for its potential in the development of new generation technologies, mainly when considering large-scale, high-quality growth [1-3].

In this work, we investigate the electronic properties of graphene multilayers prepared by high-temperature intercalation of atomic carbon underneath epitaxially grown graphene on Ir(111) [4]. We address the controlled growth of multilayers and, by means of Landau-level spectroscopy in high magnetic fields, we study the variation of local electronic properties of the top graphene layer as a function of the twist angle and the number of layers. For the monolayer, as well as for bilayers with small-angle rotations, no Landau levels are observed in magnetic fields up to 6 Tesla. Whereas bilayers with a large twist angle, as well as twisted trilayers, exhibit electronic properties characteristic for a free-standing graphene monolayer, denoting a sufficient decoupling of the upper graphene layer from the metal substrate. Finally, we demonstrate the controlled preparation of epitaxial graphene multilayers with a large degree of decoupling, which represent an ideal platform for future electronic and spintronic applications.

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## Nitrogen doping of graphene on metals: Controlling corrugation and electronic properties with doping and oxygen intercalation

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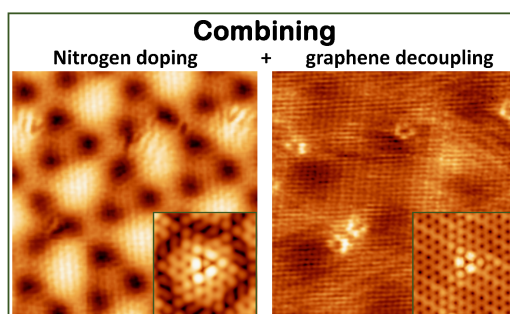
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Nitrogen doping in graphene has attracted a lot of attention due to its catalytic activity in oxygen reduction reactions [1], and as powerful technique to modify the graphene electronic properties [2]. In this work, we study N-doped graphene grown on two different substrates, Pt(111) and Rh(111), which represent weakly and strongly interacting systems respectively. By means of low energy ion bombardment, we demonstrate how it is possible to obtain purely-substitutional N-doped graphene with tunable dopant concentration in both substrates [3,4]. We unveil the STM fingerprints of substitutional defects using first principles simulations, providing additional information about their electronic properties. While in Pt(111), all defects are equivalent due to the flatness of the physisorbed graphene, in the Rh(111) case, the corrugation induced in the graphene structure and the associated change in chemical properties produce a remarkable variation in the electronic properties of nitrogen defects. In a second step, we show how N-doping can be used in combination with oxygen intercalation [4] to tune the position of the Fermi level. The interaction with the substrate (and the associated p-doping) can be controlled by the amount of intercalated species at the interface, while the n-doping level can be adjusted by the concentration of N substitutionals. This combined scheme represents a novel strategy to tailor properties of graphene and other 2D materials.



STM images comparing substitutional nitrogen atoms in the graphene lattice (bright motifs) on Rh(111) (a) and O/Rh(111) (b) substrates. In the insets, the corresponding theoretical STM images according to the Tersoff-Hamann approximation are shown.

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## Nanoscale Mass Transport on Dirac Materials

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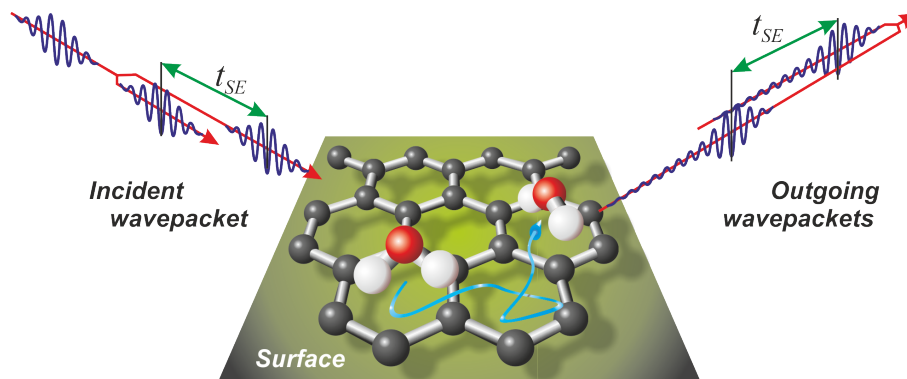
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Recently the reactivity of Dirac materials such as topological insulator surfaces towards adsorbates and the stability of their electronic structure upon adsorption has been widely studied due to being crucial for future devices. However, information about the dynamics and diffusion of adsorbates on these surfaces is scarce and mainly based on theoretical studies.

We have studied the diffusion of water on the surfaces of Dirac materials (graphene and the topological insulator  $\text{Bi}_2\text{Te}_3$ ) using helium-3 spin-echo spectroscopy[1]. Albeit water is ubiquitous in everyday life, the simplest mechanisms controlling its molecular motion at a surface have yet to be revealed by experiment[2-4]. The diffusion of  $\text{H}_2\text{O}$  occurs by an activated hopping motion where in particular in the case of graphene a strong signature for cooperative behaviour due to repulsive forces between the molecules appears. The diffusion of water on  $\text{Bi}_2\text{Te}_3$ , on the other hand, is governed by a large atomic-scale friction between the adsorbate and the substrate.

Our experimental results provide a detailed insight into the diffusion mechanism of  $\text{H}_2\text{O}$  molecules on the surfaces of Dirac materials. Our findings may help to understand the mobility of adsorbates on these surfaces - a key factor for the dynamics of surface chemical reactions.



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## Atomically-resolved edge states on surface-nanotemplated graphene explored at room temperature

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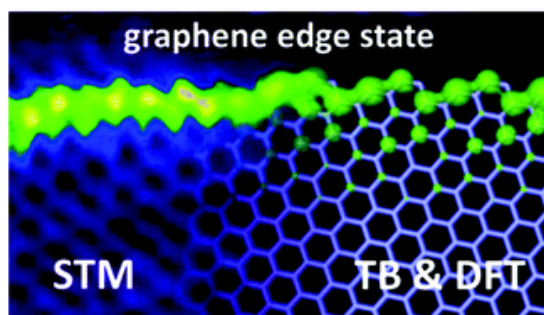
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Graphene epitaxially grown on metal substrates is one of the most promising candidates for obtaining a scalable methodology for high-quality production [1,2]. Graphene edges present localized electronic states strongly depending on their shape, size and border configuration [3]. Chiral- or zigzag-ended graphene nanostructures develop spatially and spectrally localized edge states around the Fermi level; however, atomic scale investigations of such graphene terminations and their related electronic states are very challenging and many of their properties remain unexplored. Here we present a combined experimental and theoretical study on graphene stripes showing strong metallic edge states at room temperature. By means of scanning tunneling microscopy, we demonstrate the use of vicinal Pt(111) as a template for the growth of graphene stripes and characterize their electronic structure. We find the formation of a sublattice localized electronic state confined on the free-standing edges of the graphene ribbons at energies close to the Fermi level. These experimental results are reproduced and understood with tight-binding and ab initio calculations [4,5]. Our results provide a new way of synthesizing wide graphene stripes with zigzag edge termination and open new prospects in the study of valley and spin phenomena at their interfaces [5].



**Figure:** Right hand side, atomically resolved STM image of the edge of a graphene stripe grown on vicinal Pt(111). The region in green corresponds to the graphene edge, where enhanced conductivity is measured. Left-hand side, calculation of the very same edge. The green pockets correspond to the spatial localization of a zero-bias edge state.

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### 0.3 THz detection using an Asymmetric dual grating gate graphene FET

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Graphene based devices shows excellent properties (zero band gap, high mobility, ...) and could be used to reach high frequency operation and specially toward terahertz technology. Exfoliated graphene shows a high value of electronic mobility at room temperature [1] and even higher at low temperatures. Applications of graphene field effect transistors (GFET) operating in the terahertz (THz) range are appealing as it is one of the least explored frequency regions and holds potential to revolutionize different fields like security, medical imaging or high-speed wireless communication. Recent research on vertically stacked heterostructures of graphene with hexagonal-boron nitride (h-BN) and other two-dimensional materials has opened a new realm for intriguing device physics making them ideal candidates for future high-frequency technology [2–3].

Asymmetric grating gate graphene based Field effect transistor (ADGG-GFET) was fabricated and characterize as efficient terahertz detector. The graphene layer was stacked between two layers of h-BN on SiO<sub>2</sub>/Doped-Si (Fig.1-left). The electron density of the channel was controlled by the back gate (substrate doped silicon) and the top gates. The device shows a photocurrent (up to 1.5 nA), when it was excited with terahertz radiations 0.15 and 0.3 THz and at different temperatures from 4K up to room temperature (Fig.1-right).

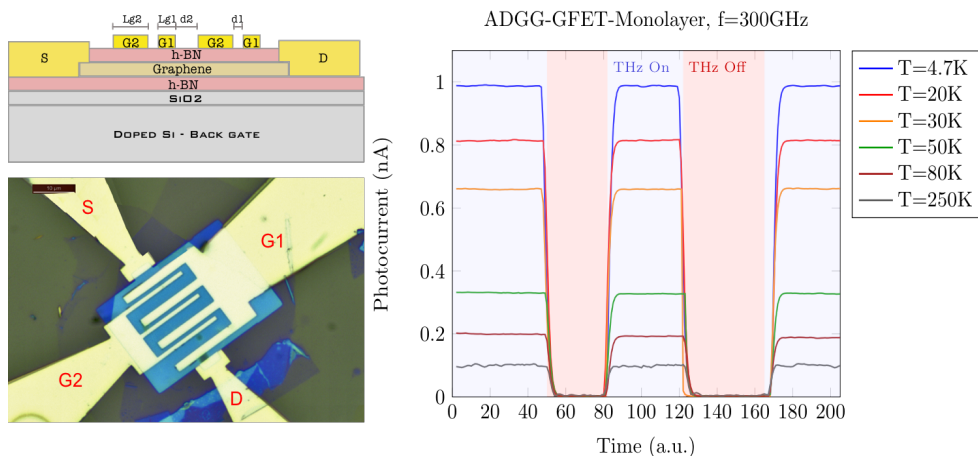


Figure 1: Side description of the GFET structure and top view microscopic image of the GFET (left) and Photocurrent vs time when the THz beam at 300 GHz was switched on and off (right).

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## Landau quantization in graphene/transition metal dichalcogenides probed at the local scale

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The perspective of revolutionizing graphene nanoelectronics by the fabrication of 2D stacked systems from the group of transition metal dichalcogenides (TMDs) has sparked the interest of scientists and engineers alike [1]. The proximity of graphene to the layered van der Waals materials allows for a considerable modification and tuning of the electronic properties of graphene including its spin-orbit interaction (SOI) strength, as has been demonstrated in recent magnetotransport experiments [2,3].

Here, we present the successful preparation of layered systems of a graphene monolayer on tungsten diselenide (WSe<sub>2</sub>), niobium diselenide (NbSe<sub>2</sub>) and molybdenum diselenide (MoSe<sub>2</sub>) accomplished by an adapted wet chemical transfer process and their subsequent investigation with regard to the electronic properties by means of low-temperature scanning tunnelling microscopy and spectroscopy (STM/STS) on the local scale as well as angle-resolved photoemission spectroscopy (ARPES) on a macroscopic scale.

Atomically resolved imaging as well as emerging Moiré patterns due to the lattice mismatch with the underlying substrate indicate a successful transfer procedure. In the presence of high magnetic fields, pronounced Landau level sequences further highlight the effective decoupling from the substrate and confirm the presence of Dirac fermions within the graphene monolayer. A detailed analysis of the Landau level spectrum allows to determine the Fermi velocity as well as the doping level of the layered systems.

The observation of an additional splitting of each Landau level peak into subpeaks is interpreted with regard to a possible TMD substrate induced SOI in graphene. The strength of the splitting as well as the magnetic field behaviour of the peaks is discussed in comparison with a spin-dependent low-energy effective Hamiltonian.

ARPES measurements complement the local investigations of the electronic properties of graphene and confirm the characteristic linear dispersion of graphene as well as the presence of TMD bulk bands.

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## Ultrafast charge transfer from core-excited argon intercalated and compressed under graphene monolayers and in blisters

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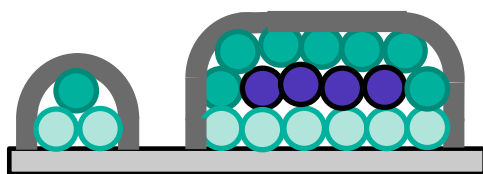
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Argon can be intercalated and compressed into bubbles or blisters under graphene (Gr) monolayers (ML) on metal surfaces, as has recently been shown by several groups (see [1] for references). We have defined these states by XPS, XAS, and STM [1]. On this basis and using XPS as transfer standard, we have now investigated the state of the argon atoms under Gr on Ni(111) by resonant core excitation and decay, using the so-called core hole clock (CHC) method [2]. For intercalated Ar ML we do not detect the Ar  $2p_{3/2} \rightarrow 4s$  resonance at all; the decay signal is weak and consists of Auger electrons only. These findings indicate that in these atoms (state 1) the core excited state is strongly quenched or decays extremely fast. For compressed Ar in blisters containing also Ar in a second layer (state 2) a small resonance is found which decays into Auger states; for blisters containing several Ar layers (at least mono, bi, and tri or more layers as state 3) a stronger, shifted resonance exists leading to spectator decay electrons. We discuss these results in terms of distinguishable contributions from Ar atoms pressed into the Ni substrate (state 1), Ar in contact with the graphene cover only (state 2), and Ar atoms separated (and thus protected) from both interfaces in the interior of blisters (state 3). Besides corroborating our previous interpretations from XPS, XAS, and STM, these new results contribute to the understanding of both the Ar blisters and of the physics of excitation decay in strongly coupled and compressed systems.

Time permitting, further details and extensions to other systems will be reported.



**Fig:** Pictorial representation of the 3 Ar states under Gr ML and in blisters (see text)

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## Tuning the Graphene on Ir(111) adsorption regime by Fe/Ir surface-alloying

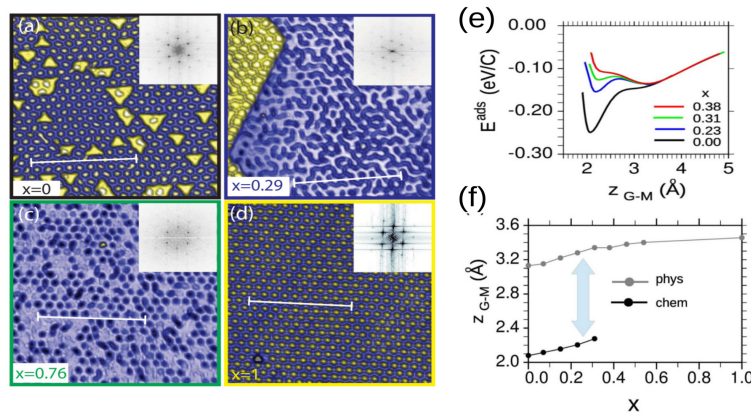
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A combined scanning tunneling microscopy, x-ray photoelectron spectroscopy, angle-resolved photoemission spectroscopy, and density functional theory study of graphene on a Fe-Ir(111) alloy with variable Ir concentration is presented. Starting from an intercalated Fe layer between the graphene and Ir(111) surface we find that graphene-substrate interaction can be fine-tuned by Fe-Ir alloying at the interface. When a critical Ir-concentration close to 0.25 is reached in the Fe layer, the

Dirac cone of graphene is largely restored and can thereafter be tuned across the Fermi level by further increasing the Ir content. Indeed, our study reveals an abrupt transition between a chemisorbed phase at small Ir concentrations and a physisorbed phase above the critical concentration. The latter phase is highly reminiscent of the graphene on the clean Ir(111) surface. Furthermore, the transition is accompanied by an inversion of the graphene's induced magnetization due to the coupling with the Fe atoms from antiferromagnetic when chemisorbed to weakly ferromagnetic in the physisorption regime, with spin polarizations whose magnitude may be tuned with the amount of Fe content.[1]



(a-d) Series of STM images for the Gr/Fe<sub>1-x</sub>Ir<sub>x</sub>/Ir(111) system as a function of the surface Ir concentration x. (e) Evolution of the Gr adsorption energy as a function of its distance to the Metal for various values of x. (f) Gr-Metal distance as a function of x for both the chemisorption and physisorption regimes.

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## Graphene on Gd-5d metals surface alloys – superlattice and spin-dependent effects

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Graphene electronics covers a number of unique effects and most intriguing are based on its interaction with the substrate. Contact of graphene with the lattice-mismatched substrate clones the

Dirac cone and gives rise to Hofstadter spectrum[1], while contact with the heavy/magnetic atoms realizes topological insulator phase.[2]

In this work we study the electronic structure of graphene on Ir(111) and Pt(111) upon rare-earth Gd atoms intercalation by means of angle-resolved photoemission spectroscopy. Gd intercalation results in the formation of the Gd-Ir and Gd-Pt surface alloys with the (2x2) and (9x9) superstructures, relatively. Strong charge transfer from Gd atoms leads to the shifting of the Dirac cone and its replicas towards the higher binding energies while remaining the quasifreestanding character of graphene. The Moire superstructure periodicity of graphene is preserved upon Gd intercalation, but the corrugation strongly increases that is revealed by Scanning Tunneling Microscopy (STM). This peculiar combination of the electron doping and the Moire superlattice leads to the proximity of the Fermi level to the crossing points of the main and replicated Dirac cone bands, that is essential for the superlattice effects application in electronics.

Furthermore, recent works[3] demonstrate the enhanced magnetic properties of the Gd-5d metals surface alloys and thus we analyze the spin texture of the graphene Dirac cone by means of spin-resolved ARPES with the perspective of Quantum Anomalous Hall effect realization.

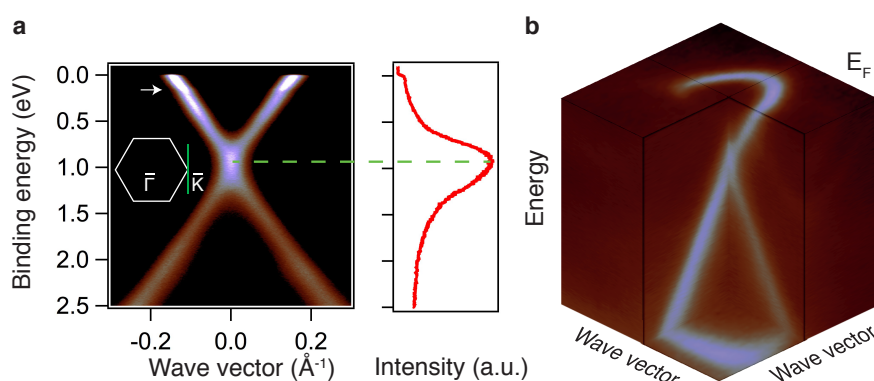


Fig. 1 ARPES dispersion relations of graphene/Gd/Ir(111) system along the direction, perpendicular to GK (a) and in two orthogonal wave vector directions (b)

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## Growth and electronic structure of Graphene on Ni(100)

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Nickel is one of the most technologically relevant substrates for graphene production due to its low cost, large availability and easy removal via chemical etching. The elevated carbon solubility in nickel determines lower growing temperature, appetible for large scale production, but also the tendency to form graphitic multilayers due to surface precipitation. This can be partially overcome in principle by rapid cooling, leaving monolayer graphene sheets heavily interacting with the Ni surface. Our group has already demonstrated how a controlled cooling can lead to the formation of a uniform interfacial layer of nickel carbide between Ni(111) surface and non-epitaxial graphene [1], thus enabling the creation of large non-interacting graphene sheets on this surface. Here we demonstrate how this strategy can be extended to the Ni(100) case, a prototypical example of symmetry-mismatched lattice and the most common surface phase in polycrystalline nickel foils.

Graphene on Ni(100) grows via ethylene dosing (partial pressure  $5E-7$  mbar) at  $\sim 580$  °C and presents a variety of moiré structures with either stripe-like or network morphology [2]. The system was then characterized with complementary surface science techniques. In-situ VT-STM and XPS were used to study the creation of a carbidic phase at the interface via carbon segregation and its relation with the moiré orientation. LEEM/PEEM and  $\mu$ ARPES were employed to demonstrate that the carbidic phase can decouple graphene from the substrate and that this process can be reversed by controlled annealing. The influence of moiré orientation with the electronic state of interacting and non-interacting graphene, as well as a possible route towards the creation of non-interacting graphene on polycrystalline nickel foils will be discussed.

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## Exploring layer-dependent properties of metallic 2D materials

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Metallic transition metal dichalcogenides (TMD) have been extensively studied for their many body physics phenomena in the bulk. In this talk we explore how these properties are modified if these materials are reduced to a single layer and if new functionalities arise in the monolayer regime. Unlike semiconducting TMDs, metallic TMDs are, however, not easily prepared in monolayer-form by simple mechanical exfoliation. Therefore, a bottom-up synthesis of mono- to few-layer (semi)metallic TMDs by van der Waals epitaxy is used to enable studies of properties as a function of number of layers. Specifically, we study the excitonic insulator  $\text{TiSe}_2$  and the novel monolayer-ferromagnet  $\text{VSe}_2$ . Using variable temperature scanning tunneling microscopy/spectroscopy we illustrate strongly enhanced charge density wave (CDW) transition for  $\text{TiSe}_2$  as it is reduced to a single layer. Moreover, we find that the CDW transition is tuned by the substrate material (HOPG or  $\text{MoS}_2$ ), which may indicate dependence on the dielectric environment of the  $\text{TiSe}_2$  monolayer, consistent with an excitonic-origin for the CDW transition in  $\text{TiSe}_2$  [1]. The second material we study is  $\text{VSe}_2$ . Density functional theory has predicted that monolayer  $\text{VSe}_2$  may exhibit intrinsic ferromagnetic ordering, despite being paramagnetic in the bulk. In our studies, mono- to few-layer  $\text{VSe}_2$  on HOPG or  $\text{MoS}_2$  substrates have been protected with a Se capping layer for ex-situ investigation of the magnetic properties by vibrating sample magnetometry, magneto optical Kerr effect and anomalous Hall effect measurements. We find strong room temperature ferromagnetism for the monolayer [2] in all these measurements. This is the first observation of an intrinsically ferromagnetically ordered monolayer TMD, which may have implications for the use of 2D materials in spintronics applications.

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## Chemically resolved geometric structures of 2D materials

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Adsorption on solid surfaces has been a major route for synthesizing 2D materials and is the first step towards device realization. Interaction of a monolayer of a 2D material with the substrate surface can lead to strong deformation and thus alteration of the intrinsic electronic properties of the overlayer. However, characterization of the strength of these interactions at the interfaces as well as the resulting geometric structures of the adsorbed monolayers, either experimentally or theoretically, is far from trivial due to the chemical complexity and often the large sizes of the surface unit cells involved. Here we report combined x-ray standing wave (XSW) and x-ray photoelectron spectroscopy (XPS) studies, which can achieve high spatial resolution and chemical sensitivity, of the geometric structures of borophene on Ag(111) and FeSe monolayer on SrTiO<sub>3</sub>(001).

Earlier theoretical prediction suggests that boron can form small sized clusters with planar structures. Recently, it has been demonstrated by scanning tunnelling microscopy that large-scale 2D sheets of borophene can be synthesized by evaporating pure boron on Ag(111) surface [1]. Unlike graphene or transition metal dichalcogenides, borophene has no corresponding bulk allotrope. Our high-resolution B 1s core-level spectrum reveals distinct multiple components, denoting a unique form of polymorphism consistent with a proposed structure involving vacancy-induced superlattices characterized by the boron coordination number. XSW provides the first experimental evidence that, independent of the specific in-plane structure, borophene exists as a single, atomically flat layer and determines its separation from the underlying Ag(111) substrate to be 2.4 Å, confirming the weak B-Ag interaction predicted by the previous first-principles calculations.

The bulk  $\beta$ -FeSe is a superconductor with a transition temperature ( $T_c$ ) of 8 K. Its tetragonal structure consists of weakly interacting FeSe sheets that are two-dimensional in nature. It has been recently demonstrated that the  $T_c$  can rise to above 60 K when a monolayer of  $\beta$ -FeSe is grown epitaxially on SrTiO<sub>3</sub>(001) [2]. While the origin of this large  $T_c$  enhancement remains debated, progress in theoretical calculations has been hindered by the uncertainty regarding the true structure of the FeSe/STO interface. In this presentation a structural investigation of this interface using XPS, XSW, resonant photoemission and photoelectron diffraction will be also briefly discussed.

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## The Moiré pattern of a 2D iron oxide layer grown on $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001)

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The surface of metal oxides reconstructs in many ways depending on the crystallographic planes and preparation procedures [1]. In the case of iron oxides, the surface reconstruction of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) is still controversial [2]. Under oxidizing conditions, it has been found that a part of the surface accommodates a peculiar phase, called “biphase”, which has been traditionally attributed to a coexistence of tiny alternating islands of FeO and Fe<sub>2</sub>O<sub>3</sub>(0001), based [3].

In this work, we optimize the recipe to grow this particular phase over the entire surface, allowing a reliable analysis with spectroscopic and other techniques with limited resolution. This has allowed us to thoroughly characterize the two main phases of the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) by means of STM, AFM, LEEM,  $\mu$ LEED-IV, XPS, and NEXAFS.

The analysis brings a solid evidence that this surface structure is composed of a single continuous layer of iron oxide with a unique structure, its own lattice parameter and orientation different than that of the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) bulk, giving rise to a distinct Moiré pattern. It may, in fact, be considered as a novel 2D material. Finally, we use the DFT and LEED-IV calculations to single out the atomic model that is best-matching the experimental data.

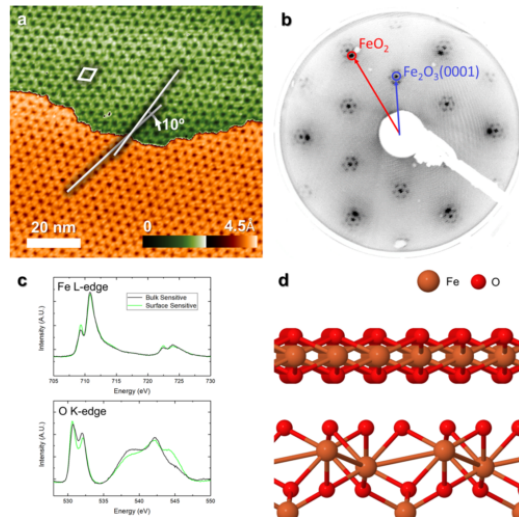


Figure 1 a) STM image showing the characteristic moiré pattern of the oxidized surface b) LEED pattern of the surface. c) NEXAFS spectra of the Fe L-edge and O K-edge. d) A part of the model of the superstructure.

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## Lateral heterostructures of hexagonal boron nitride and graphene: alloying and microstructuring

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A very important step in utilization of 2D materials is their controlled integration into heterostructures, because it enables investigation of new systems of reduced dimensionality and also promises various uses in future technologies. By means of low-energy electron microscopy (LEEM) and selected-area low-energy electron diffraction ( $\mu$ -LEED), here we study lateral heterostructures of hexagonal boron nitride (hBN) and graphene on Ir(111). The method employed for synthesis of the heterostructures is sequential chemical vapor deposition, and this process is tracked *in situ* in ultrahigh vacuum with LEEM. It is found that, besides hBN (insulator) and graphene (conductor), a 2D alloy consisting of hexagonally arranged B, C and N atoms (hBCN, semiconductor) is formed on the iridium surface within the heterostructure (see Figure 1), and its stoichiometry and spatial extension depend on the details of the synthesis.

Additionally, after formation of well-defined heterostructures, a new method is used for *in situ* fabrication of graphene and hBCN microstructures, which relies on decomposition of hBN on Ir(111) at elevated temperatures [1]. In this way, atomically-thin conducting and semiconducting elements of micrometer size, suitable for integration into more complex structures and devices, can be produced.

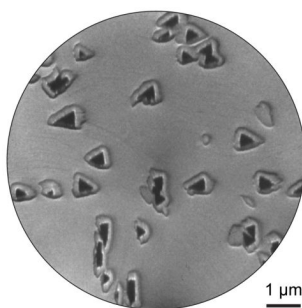


Figure 1. LEEM image of hBN-graphene heterostructures on Ir(111). HBN cores (dark contrast) are surrounded by hBCN and graphene.

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## **h-BN on Cu(111): Geometric corrugation and intercalation of functional molecules**

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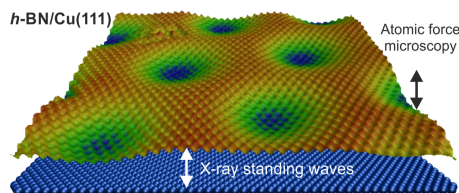
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The synthesis of hybrid materials by combination of different material classes is a promising approach for the fabrication of materials with tailored physical and chemical properties. *h*-BN is one of the prominent building blocks for such architectures due to its insulating behavior, high thermal conductivity, chemical and thermal stability. [1] Here, we present an in-depth structure determination of the *h*-BN/Cu(111) system and discuss the fabrication of a layered architecture through the intercalation of functional molecules between the Cu(111) and the *h*-BN sheet.

The quantification of the geometric corrugation is based on the atomic contrast of *h*-BN resolved by nc-atomic force microscopy. The tip-surface distance dependence of the atomic contrast is used for height calibration. The resulting local corrugation of a few tens of picometers is in good agreement with the spatially averaged X-ray standing waves investigations [2].

Due to the electronic transparency of the insulating *h*-BN layer [3], the intercalated molecules can be characterized and manipulated using scanning tunneling microscopy. While the presence of the capping *h*-BN layer influences the self-assembly, we show that intrinsic molecular functionalities, such as switching between different tautomers or self-metalation, are preserved [4]. Intercalation of functional molecules under *h*-BN provides an opportunity to protect organic materials from atmospheric pressure, and might also be used to control chemical reactions through geometric confinement.



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## Evidence of large spin-orbit coupling effects in quasi-free-standing graphene on Pb/Ir(111)

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A combined scanning tunneling microscopy, angle- and spin-resolved photoemission spectroscopy and density functional theory study of graphene on Ir(111) intercalated with a well-ordered, full Pb monolayer is presented. Lead intercalation between graphene and Ir(111) reduces the coupling to the metallic substrate in such a way that its corrugation becomes negligible and distortions of the linear dispersion largely disappear, while graphene's sublattice symmetry is maintained and it turns out to be *n*-doped. Remarkably, the spin-orbit splittings induced by the proximity of the Ir(111) surface are preserved after Pb intercalation in a wide energy range. We further show that the Pb interlayer induces a complex spin texture with both in-plane and out-of-plane components. Our calculations reveal the origin of the out-of-plane spin components in graphene to trace back to the out-of-plane spin-polarized surface and resonance states of Ir(111), while the Pb interlayer on its own does not induce any vertical spin polarization in the carbon sheet. However, the Brillouin zone folding imposed by the rectangular symmetry of the intercalated Pb layer plays an instrumental role in the spin-orbit coupling (SOC) transfer to graphene, as well as in the linearization of its bands. Finally, since no sizeable gap is observed at the Dirac point, we suggest that an intrinsic (Kane and Mele type) SOC does not exceed the extrinsic (Rashba) SOC for graphene on Pb/Ir(111).

## Atomic-scale defects and electronic properties of synthesized molybdenum disulphide monolayer

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Significant scientific and technological interest in two-dimensional (2D) materials is closely related to the fact that today's microelectronic devices are based on 2D architectures. Along with the most famous and widely researched 2D material, graphene, attention is increasingly turning to other 2D materials, especially those with intrinsic semiconductor properties. One such material is molybdenum disulphide (MoS<sub>2</sub>) monolayer, a prominent member of the transition metal dichalcogenide family.

MoS<sub>2</sub> monolayers researched in this work were synthesized on a SiO<sub>2</sub>/Si wafer and transferred to Ir(111) for nano-scale characterization. The established transfer procedure is applicable to a diversity of substrates, thus opening a way to different applications. Samples were extensively characterized during every step of the transfer process, and MoS<sub>2</sub> on the final substrate examined down to the atomic level by scanning tunneling microscopy (STM). Conducted procedures yielded high quality monolayer MoS<sub>2</sub> of millimeter-scale size with an average defect density in the same range as samples obtained by exfoliation from the natural MoS<sub>2</sub> [1]. By combined use of STM imaging and density functional theory (DFT) calculations we identified the most recurring point-like defects as S vacancies. The electronic band gap measured by scanning tunneling spectroscopy (STS) revealed n-doping of the samples and lateral nano-scale variations of the band gap. From the difference of the electronic band gap measured by STS of 2.1 eV and the optical band gap measured by photoluminescence (PL) of 1.9 eV, an estimated exciton binding energy of ≈0.2 eV is obtained. Comparison of experimental results and simulations considering freestanding and epitaxial MoS<sub>2</sub> on Ir(111) leads to the conclusion that the investigated samples on Ir(111) are quasi-freestanding or weakly coupled to the substrate, based on the observation of the semiconducting band gap, nano-scale rippling of flakes and weak binding of flake edges [2].

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## A monolayer of hexagonal boron nitride on Ir(111) as a template for cluster growth

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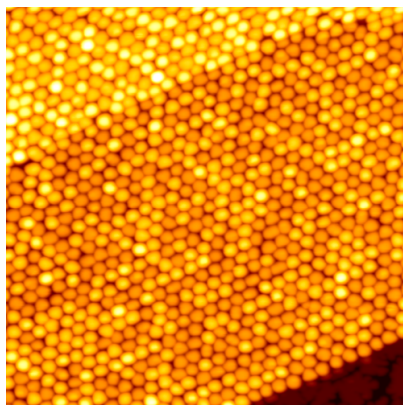
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Chemical vapor deposition of borazine molecules on Ir(111) results in a well aligned monolayer of hexagonal boron nitride (h-BN) which forms an incommensurate (11.7 x 11.7) moiré on (10.7 x 10.7) substrate unit cells. The center of each unit cell provides a chemisorbed valley area, where h-BN is hybridized with the Ir substrate [1]. Through a scanning tunneling microscopy study we provide evidence that the valley regions are reactive and pin deposited atoms. As a result, highly regular cluster arrays with a periodicity of 2.9 nm can be formed. For the case of Ir deposition, the size distribution is narrow. The average cluster size can be tuned from a few to about 200 atoms for room temperature deposition. The thermal stability of the clusters is extraordinary, with a decay of the cluster lattice setting in only above 700 K, through intercalation and Smoluchowski ripening. *Ab initio* calculations explain the remarkably strong Ir cluster binding through selective  $sp^3$  rehybridization of the h-BN sheet, involving a boron-Ir cluster bond and a strengthening of the nitrogen bonds to the Ir substrate in the valley area.

We demonstrate the versatility of the approach and find regular cluster lattice formation also in the case of Au and C deposition at room temperature. Regularly positioned C clusters are even observed after annealing to 1500 K. Compared to cluster lattices using graphene on Ir(111) as a template, the better ordering and the higher thermal stability make the arrays on h-BN/Ir(111) superior for potential applications, *e.g.* in nano-catalysis.



0.57 ML Ir on h-BN/Ir(111) deposited at 250 K, imaged at 300 K

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## Single-Orientation High-Quality MoS<sub>2</sub> Monolayers with Complete Spin Polarization

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The employment of transition metal dichalcogenides, and in particular single layer (SL) MoS<sub>2</sub> for electronic devices, demands for a controllable growth of highly crystalline layers featuring large area with a low concentration of defects to preserve their outstanding electronic properties. Moreover, thanks to the peculiar electronic structure, new degrees of freedom are accessible allowing for spin- and valley-dependent phenomena, that can be retained in devices only through singly-oriented domains. Current chemical vapor deposition methods have not been able to achieve this and have produced mirror twin domains leading to the formation of domain boundaries and dislocations in the layer. We present a comprehensive study of the growth and characterization of SL MoS<sub>2</sub> on Au(111) with a single domain orientation. We demonstrate the structural properties using a combination of surface science techniques, including scanning tunneling microscopy and photoelectron diffraction. Angular resolved photoemission measurements (ARPES) confirmed the single layer character and the high structural quality of MoS<sub>2</sub> while the single domain orientation allowed the measurement, through spin-resolved ARPES, of the complete spin polarization with spin reversal of the states near K and -K points of the Brillouin zone.

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## Helium scattering from 2D Moiré superstructures: A new tool to characterize layered van der Waals heterostructures

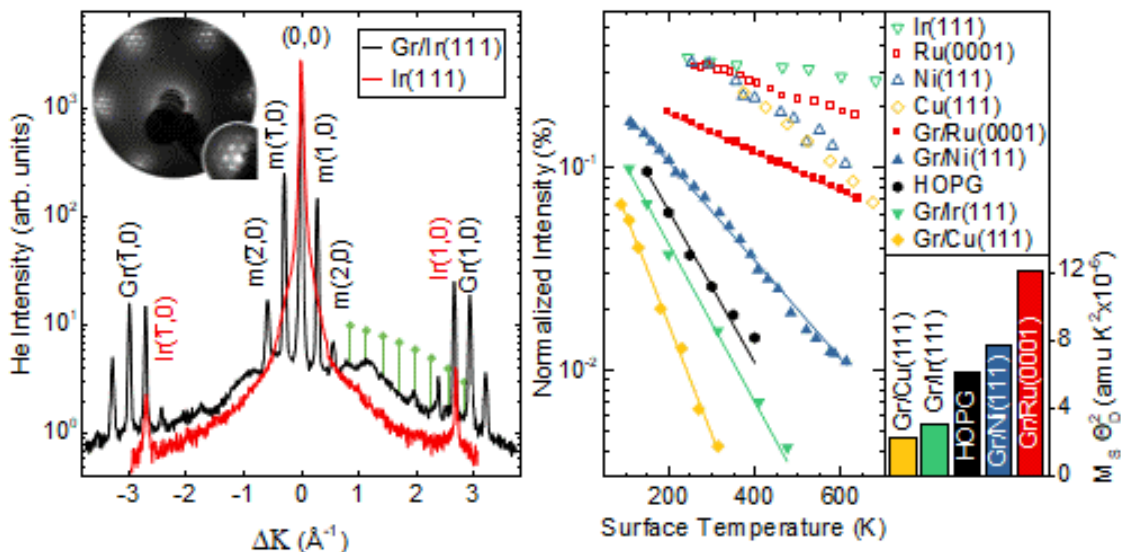
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The rapidly developing field of layered van der Waals heterostructures, in which atomically thin layers of compounds of different nature (graphene, h-BN, black phosphorus, metal dichalcogenides, iron pnictides, etc.) are stacked on top of one another [1], requires an arsenal of experimental techniques that can yield global and local characterization of the fascinating properties of these technologically relevant 2D materials. Specifically, we describe here how properties of the utmost importance, such as crystallographic structure, structural corrugation, interlayer bonding (covalent, ionic, van der Waals, etc), charge transfer or phonon spectrum can be determined by Helium Atom Scattering (HAS) [2] in layered systems (including insulating ones) with examples related mostly to graphene epitaxially grown on a number of single crystal metal surfaces.



1. Diffraction and Debye-Waller measurements of HAS from Gr/Ir(111). The DW factors for graphene grown on different metal surfaces compared with the corresponding metallic substrates yield interlayer bonding.

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## Controllable Switching of the Superconductivity of a Tungsten STM Tip on Epitaxial Graphene

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Epitaxial Graphene on metals has become a playground for a wide range of 2D systems displaying competing interactions that may lead to long range magnetic order, Kondo resonances or superconductivity [1], with STM as a favorite tool to probe their LDOS at the atomic level.

We present a systematic study of a controllable functionalization of tungsten tips on gr/Ir(111) and gr/Pb/Ir(111) that produces superconducting (SC) tips. Starting from Ar<sup>+</sup> sputtered pristine tungsten tips, we reproducibly build a SC nanostructure at the tip apex by means of voltage pulses on several graphene-covered surfaces (see Figure 1(a)). We have further tested these SC tips on a Cu(111) surface, finding that the copper surface state and the tip SC gap can be resolved simultaneously in the STS spectra. The superconductivity of the tip can be switched off by tip manipulation on clean metallic substrates.

We have characterized the resulting SC gap as a function of temperature (see Figure 1(b)) and magnetic field, obtaining a transition temperature close to 3.7 K and a critical field well above 3T in all cases. This suggests the formation of a tungsten-based amorphous nanocarbon compound at the tip, in agreement with the known fact that superconductivity can be present in tungsten carbide alloys [2] and nanostructures [3].

The presented method is currently being used to study the spatial distribution of the Zero Bias Differential Conductance in molecular Kondo lattices of TCNQ on gr/Pb/Ir(111).

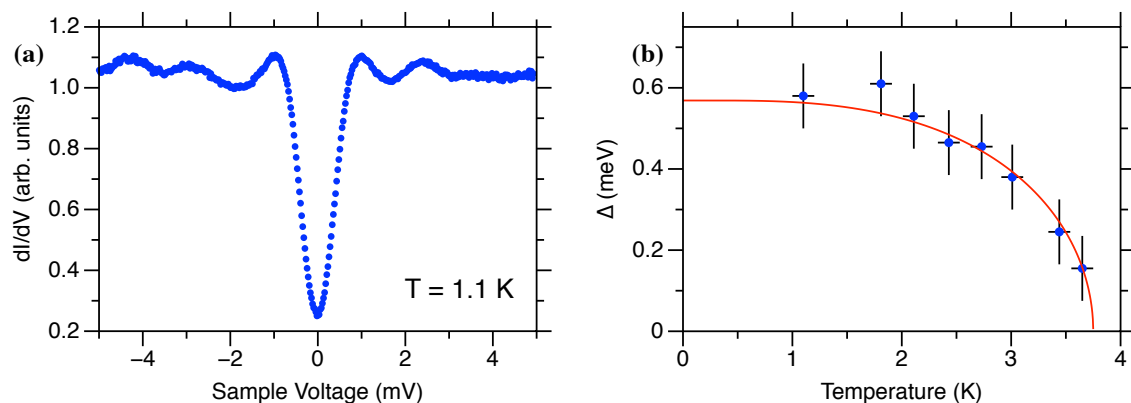


Figure 1: (a) STS spectrum recorded at 1.1 K on gr/Pb/Ir(111) with a functionalized superconducting tungsten carbide tip. (b) Temperature evolution of the superconducting gap.

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## Not all metals are the same: impact of metallic substrates on defected single-layer MoS<sub>2</sub>

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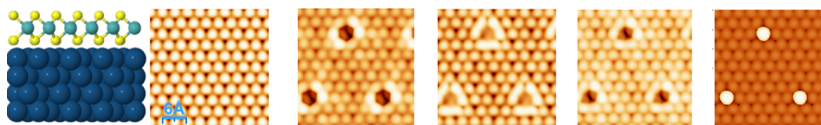
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Defects are present in 2D materials regardless of the growth method, which might imply the presence of metallic substrates. The impact of such substrates on the electronic properties of pristine single-layer MoS<sub>2</sub> has been previously addressed by Density Functional Theory (DFT) calculations [1], showing that the interaction between the metal and the MoS<sub>2</sub> can greatly vary depending on the metal. However, the way a metallic substrate affects the electronic properties of a defected MoS<sub>2</sub> monolayer and its STM characterization has not been systematically analyzed so far.

We analysed the interaction of defects with Ir(111) substrate by means of DFT calculations, revealing the pinning of the defect states to the Fermi level and hence a shift of ~1 eV of the MoS<sub>2</sub> states towards the valence band. STM simulations within the Tersoff-Hamann approximation show the vacancies site as a dark depression with clearly visible S atoms, even at the defect energies, supporting the experimental evidence [2]. The electronic structure of the MoS<sub>2</sub> system is shown to be very sensitive to the hybridization with the metal states, and might induce dramatic changes in the STM contrast depending on the effective coupling between the MoS<sub>2</sub> and the metal. The case of a gold substrate, which presents a much weaker interaction with the MoS<sub>2</sub> monolayer, will be also discussed and contrasted to experimental data [3].



STM images at  $V = +0.1$  V for the epitaxial MoS<sub>2</sub>/Ir(111). From left to right: pristine structure, S vacancy at the top layer, S vacancy at the bottom layer, S divacancy, and S adatom.

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## Determination of graphene-hBN lateral interface structure on Ir(111)

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The same two-dimensional (2d) honeycomb structure with similar lattice constants of graphene and hexagonal boron nitride (hBN) makes it possible to form continuous hybrid atomic-thin membranes. Due to the complementary electronic properties of graphene (semi-metal) and hBN (insulator), this in-plane hetero-structure is a promising prototype for novel 2d electronic circuits. Moreover, emergent electronic behavior (magnetism [1], half-metallicity [2]) is predicted at the interface between graphene and hBN. The absence of a band gap in graphene gives rise to a poor on-off ratio of graphene field-effect transistors. Various methods have been proposed to solve this problem, one of which is lateral hybridization with hBN [3].

The high quality continuous graphene-hBN membranes produced so far are all fabricated with epitaxial growth on metal substrates [4,5]. While this method utilizes the catalytic activity of the metal, it also gives rise to (potentially detrimental) interactions between the 2d membrane and the metal surface. In this presentation, we report our experimental study on the graphene-hBN lateral hybrid system epitaxially grown on transition metal surfaces as Ir(111). Careful determination of the structure with x-ray standing wave measurements show that, although covalent C-B and C-N bonds are present at the interface thus forming a continuous 2d membrane, the interface itself is strongly bonded to the metal substrate (see Fig.).

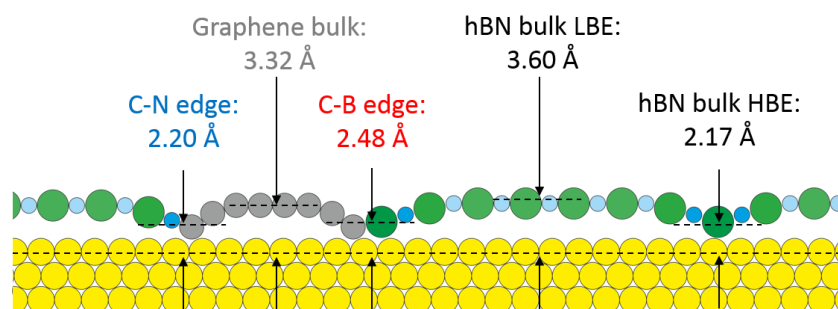


Fig. Side view sketch of the continuous graphene-hBN membrane on Ir(111), displaying the buckling of hBN, and the strongly bonded interface (grey: C; green: B; blue: N; yellow: Ir).

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## Relativistic Dispersion of Massive Electrons in Graphene Nanoribbons

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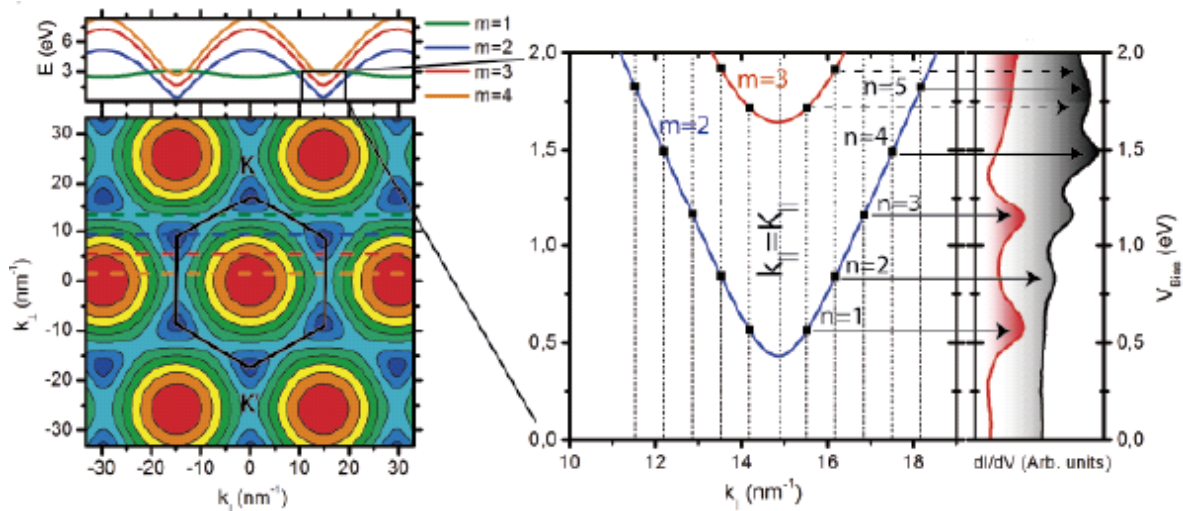
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In recent years Graphene Nanoribbons (GNRs) have raised the interest of the scientific community as they are envisioned to play an important role in futuristic semiconducting all-carbon electronics [1]. As a result of the lateral confinement induced by the finite width, the opening of a gap in the electronic dispersion of graphene is observed, also leading to non-zero values for the effective masses  $m^*$  of the charge carriers. Importantly, determining such  $m^*$  for identical GNRs by means of different techniques such as Scanning Tunneling Spectroscopy (STS) or Angle-Resolved Photoelectron Spectroscopy (ARPES) showed disagreements of almost a factor of 2 [2-3].

Herein, the bottom-up fabrication of 3p-aGNRs via terminal dehydrogenation and the subsequent lateral C-C coupling of linear halogenated precursors is presented. In the specific case of 6-aGNR sections, a quantum box (QB) behaviour is found as a result of the quantization of the Conduction Band (CB). The energy separation of the discrete energy states, inversely proportional to the ribbon length, is investigated by means of STS together with the electronic dispersion relation. By using an analytic model for the electronic structure of GNRs based on the discretization of the full band structure of graphene, the experimental data can be well fitted with a hyperbolic dispersion relation corresponding to relativistic massive particles. This analysis also resolves the contradiction between different values of effective mass previously reported, and reproduces the results from more extensive Density Functional Calculations (DFT) previously published.



**Left:** 2D dispersion relation of graphene and the discrete sub-bands obtained for the confinement in the perpendicular direction. **Right:** Conduction sub-bands with discretized energy levels and their correspondence with the experimental data.

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## Coherent electron transport through graphene nanoconstrictions

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Dirac materials are materials whose low energy electronic properties are a direct consequence of a Dirac spectrum, characterized by the well-known linear energy-momentum relation of relativistic massless particles [1]. Among Dirac materials, graphene possesses unique electronic, thermal and mechanical properties [2, 3] and it represents a promising candidate for replacing silicon in future nanoelectronics. For this aim it is very important to understand electron transport properties in nanostructures based on graphene.

We fabricate GNCs (Graphene Nano Constrictions) on HMDS (hexamethyldisilazane) deposited on a substrate of silicon and silicon oxide. The achieved mobility in a bar geometry is over  $10000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  [4]. Our purpose is to investigate the effects of the fabrication conditions on electron transport through with one or two nanoconstrictions. The electrical transport measurements we carried out allow us to perform a comparison between theory and experiment.

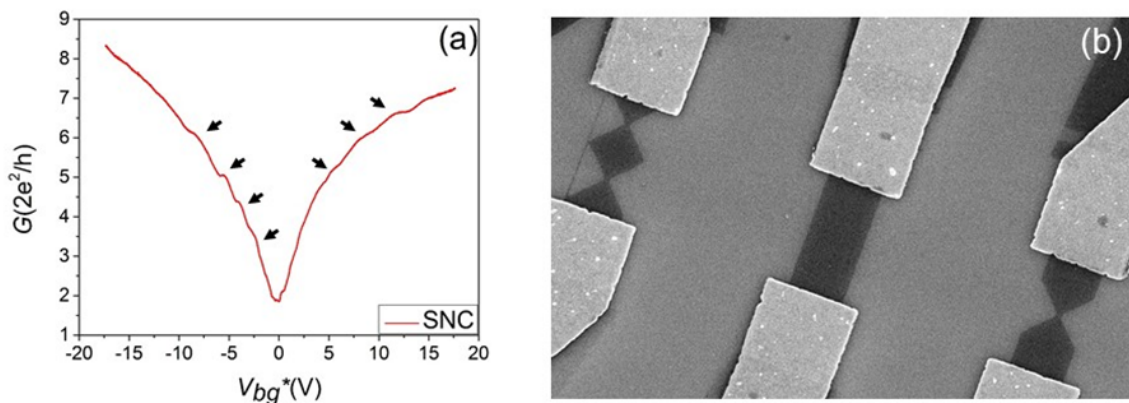


Figure: (a) Quantized conductance in a single nanoconstriction (b) Sem image of the device, the scale bar is given by the width of the Bar (1  $\mu\text{m}$ )

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## Post-synthesis metal incorporation into MoSe<sub>2</sub> or MoTe<sub>2</sub> leads to crystal modifications into metallic line-network

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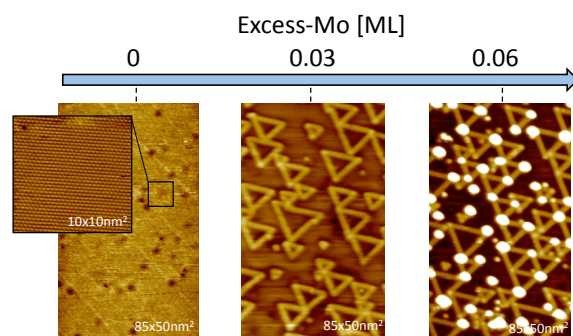
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Modifications of MoSe<sub>2</sub> or MoTe<sub>2</sub> with mirror twin grain boundary (MTB) networks in films grown by molecular beam epitaxy have been previously reported [1,2]. These MTBs are metallic and exhibit 1D quantum liquid behavior [1]. The goal of the study reported here is to understand the formation of MTB networks and use this gained knowledge for controlled modifications of these 2D materials. In a combined scanning tunneling microscopy and density functional theory approach we demonstrate that excess Mo can easily diffuse into the pristine MoSe<sub>2</sub> or MoTe<sub>2</sub> (but not into MoS<sub>2</sub>) layer and cause the crystal modifications into Mo-rich twin grain boundaries. Figure 1 shows STM images for sequential deposition of Mo at 350°C on MoSe<sub>2</sub> single crystal. Initially excess Mo is incorporated in the crystal structure to form triangular inversion grains with Mo-rich grain boundaries. Only after a critical density of MTBs is reached Mo-clusters are formed at the surface. The energetics and barriers for Mo-incorporation is calculated by DFT and shows that the formation of twin grain boundaries in the presence of excess Mo is favorable for MoTe<sub>2</sub> and MoSe<sub>2</sub>, but not for MoS<sub>2</sub> - in agreement with the experiment. These findings show that MoSe<sub>2</sub> and MoTe<sub>2</sub> can be readily modified by post-synthesis incorporation of excess Mo. The achievable dense networks of MTBs constitute a new Mo-rich metallic phase that may be used for controlled electric contacts or creation of active sites in electro-catalysis and thus adding new functionalities into transition metal dichalcogenide-based materials and devices.



**Figure 1.** STM images for sequential deposition of Mo at 350°C on MoSe<sub>2</sub> single crystal surface.

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<sup>4</sup> European Workshop on Epitaxial Graphene and 2D Materials (<http://www.icmm.csic.es/eweg2d-2018/>)

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## **Spectroscopic investigation of graphene nanoribbons showing room temperature ballistic electron transport**

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Graphene nanoribbons (GNRs) have been shown to exhibit ballistic transport properties and buckling effects [1], depending on the edge chirality. Multiple possible effects could lead to this extraordinary transport, for example the local modification of the band structure by anomalous quantum Hall-like strain effects [2]. Scanning tunneling microscopy is used to investigate the local density of states in order to clarify on the origin of this exceptional conductance of GNRs. Furthermore, DF(P)T calculations are used to investigate what effects strain have on the lattice- and electronic dynamics of graphene nanoribbons.

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## Two Phases of Single Layer Tantalum Disulfide on Gold

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We investigate single layer tantalum disulfide ( $\text{TaS}_2$ ) grown on the Au(111)-surface by a combination of physical and chemical vapor deposition [1]. With scanning tunneling microscopy (STM) we observe two different contrasts (see figure 1), referred to as  $\beta$  (bright) and  $\delta$  (dark) phase of  $\text{TaS}_2$ . Both phases have a similar lattice structure and exhibit a moiré pattern due to the lattice mismatch with the underlying gold substrate. However, the  $\beta$ -phase has a larger apparent height and a stronger corrugation of the moiré pattern than the  $\delta$ -phase.

We probe the unoccupied states with scanning tunneling spectroscopy and find a shift of the resonance peak associated with the local band maximum at  $\Gamma$ . Angle resolved photoemission spectra of the occupied states reveal an even more drastic difference: the  $\delta$ -phase exhibits the characteristic bands of 1H- $\text{TaS}_2$  with a spin-split hole pocket along the  $\Gamma\text{K}$  direction, whereas the bands of the  $\beta$ -phase cross the Fermi level only once and become extremely flat near K. We also observe replica bands for the  $\beta$ - but not for the  $\delta$ -phase.

By varying the growth parameters we can ascribe the two phases to differently sulfurized  $\text{TaS}_2$ .

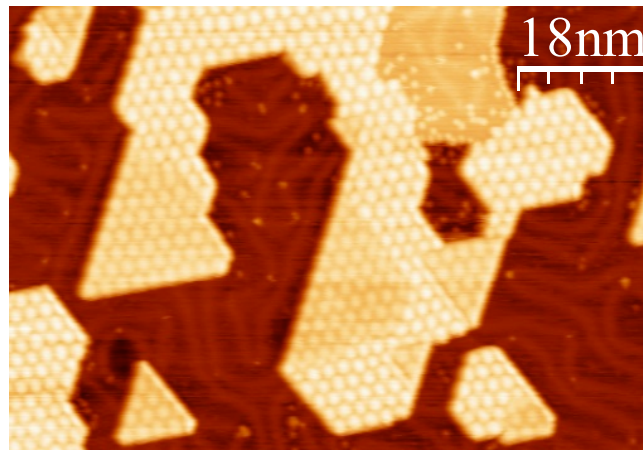


Figure 1. STM image of  $\text{TaS}_2$  grown on Au(111)-surface. Visible are  $\delta$ -phase triangles and a network of  $\beta$ -phase  $\text{TaS}_2$ .

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## Spin textures of graphene/Pb systems on various substrates

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To facilitate the implementation of the graphene-based devices, an essential change of its electronic and spin structure should controllably be done. Spin splitting and Dirac-point (DP) gap can be induced via spin-orbit coupling (SOC) enhancement in graphene by contact with heavy metals, e.g. Pb. Indeed, recent works demonstrate the giant SOC-related effects in graphene intercalated with Pb on Ir(111) [1] and Pt(111) [2]. Depending on the substrate and Pb atoms arrangements the topological phase or Rashba splitting of the Dirac cone can be realized. Therefore, the systematic study of the Dirac cone spin texture of graphene/Pb system on various substrates is required for applications purposes of the SOC-related effects in novel electronics.

In the present work we continue our studying of graphene based systems grown on top of transition metal substrates Ir(111) and Re(0001) with subsequent Pb atoms intercalation. Studies were performed by means of spin- and angle resolved photoemission spectroscopy with the application of synchrotron radiation. The impact of Pb atoms intercalation on electronic structure is close for both substrates [3] and also for Pt(111) [2]. Intercalated layer reduces the coupling between graphene and the substrates in such a way that the linear dispersion of the Dirac cone recovers, graphene's corrugation becomes insignificant and DP places below the Fermi level. Noteworthy, graphene's sublattice symmetry is maintained. Nevertheless, the spin structure of the Dirac cone dramatically depends on the substrate. We observed an absence of spin splitting for gr/Pb/Re(0001) and sizable splitting of both in-plane and out-of-plane spin components for gr/Pb/Ir(111). These results show that induced SOC in graphene cannot be described only by Pb impact but as joint influence of intercalated layer and substrate. Different substrates and Pb atoms arrangements allow to vary the spin texture of the graphene  $\pi$ -state with preserving its linear dispersion that is essential for application in spintronics.

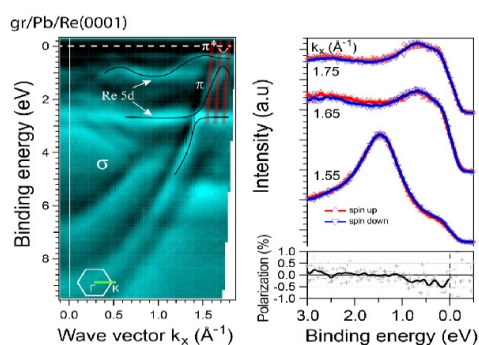


Fig.1 Electronic dispersion and spin resolved spectra of gr/Pb/Re(0001)

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## Investigation of hexagonal boron-nitride (hBN) and graphene Gr-R0° on SiC(0001)

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Graphene and hexagonal boron-nitride (hBN) are frequently studied 2D materials. While graphene is a semimetal, hBN is a wide band gap ( $> 5$  eV) insulator with a similar lattice parameter, but very different optical and electronic properties. Hence, the investigation of the mixing of both materials within one 2D layer, the so-called hBNC layer, is very promising for new device applications like, e.g., resonant tunneling field-effect transistors [1].

Here, we report on the formation of single layer hBN on the wide band gap semiconductor silicon carbide SiC(0001). After the preparation of hBN on SiC, the hBN layer can be gradually (or completely) replaced by graphene by annealing the sample. The orientation of the first graphene layer (Gr-R0°) is determined by the lattice orientation of hBN [2]. This orientation (R0°) is untypical for epitaxial monolayer graphene grown on SiC(0001), which usually is rotated by 30° with respect to the SiC substrate (Gr-R30°). Further annealing leads to the growth of Gr-R30° (i.e., the “normal” orientation) beneath the Gr-R0° layer, so that a twisted bilayer of graphene (TBLG) is formed. In contrast to TBLG grown, e.g., on Cu, the tilt angle between the two layers of TBLG on SiC is exactly 30° on the entire sample.

We used the x-ray standing wave (XSW) technique to accurately determine the vertical structures of hBN, hBNC, and Gr-R0°, and performed angular resolved photoelectron spectroscopy (ARPES) of the valence levels to determine the orientation and doping of the twisted bilayer system (see Fig. 1).

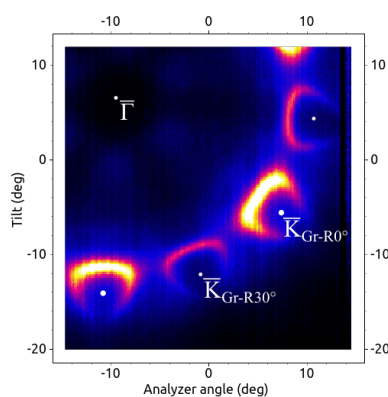


Fig. 1: Constant binding energy ARPES ( $E_B=2.0$  eV) of TBLG on SiC

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## “Two-dimensional molecular crystals with non-trivial electronic properties”

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Condensed matter research has been focused in the generation of novel classical and quantum phases in the past years. The emergence of topological insulators (TIs)[1,2], materials characterized by the presence of conducting states in their edges and an insulating behaviour in their bulk, brings new candidates for the fields of spintronics, micro-electronics and thermoelectricity.

The long-term goal of this work is to demonstrate the concept of a TI in the form of a crystalline organic material, obtained through the synthesis of a two dimensional molecular crystal. Polymerization of molecular units can yield low-cost crystalline materials with the additional advantage of properties engineering thanks to molecular unit design. Covalently-bond polymers are in fact expected to host electronic states having long spatial extension, possibly conducting or semiconducting throughout the whole material or its edges. In fact, the addition of metallic centers in such networks is besides predicted to bring significant spin-orbit coupling to the material, producing under the right circumstances a splitting, at Fermi level, of electronic bands that otherwise would be degenerate — this is the essence of bulk semiconducting properties evolving to dissipationless conductive states at the edges of the material.

A novel 2D polymerization method in solution has indeed recently been discovered at Institute FEMTO-ST (with which keep a close collaboration), which yields soluble organometallic 2D polymers that were successfully dispersed in the form of a single molecular layer onto high-oriented pyrolytic graphite (HOPG) [3]. In this contribution we will present the (still under progress) physical-chemistry and physics characterization of these polymers onto different substrates.

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## Growth and structure of mono- to few-layer vanadium disulphide on graphene on Ir(111)

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Using scanning tunnelling microscopy and low-energy electron diffraction we study the growth and structure of vanadium disulphide  $VS_2$ . The mono- to few-layer samples of  $VS_2$  on graphene on Ir(111) are grown by in situ molecular beam epitaxy. Depending on the specific growth parameters, a variety of growth scenarios evolves. Monolayer  $VS_2$  displays smoothly joined domains of a  $(3 \times 1)$  superstructure that appears to result from an uniaxial distortion and buckling of the hexagonal  $VS_2$  lattice. In X-ray circular magnetic dichroism experiments, the ferromagnetism proposed in monolayer  $VS_2$  [1] is not found. In few-layer  $VS_2$ , the hexagonal lattice is restored, still exhibiting multiple superstructures.

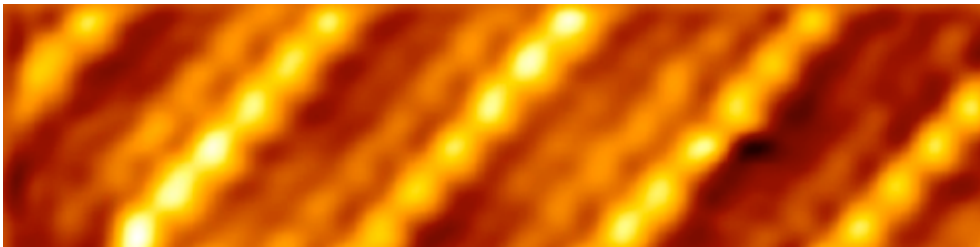


Figure 1: Scanning tunneling microscopy topograph of  $VS_2$  on graphene on Ir(111) showing a  $(3 \times 1)$  superstructure. Image size:  $6.0 \times 1.5 \text{ nm}^2$ .

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## Inelastic Excitations in Bilayer Graphene on Ru(0001)

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Bilayer graphene on Ru(0001) was prepared via decomposition of ethylene and subsequent carbon segregation [1]. Scanning tunneling microscopy unravels a bilayer moiré lattice that matches the moiré pattern of the monolayer. Inelastic electron tunneling spectroscopy (IETS) was used to explore vibrational excitations of bilayer graphene. The IET spectra reveal spectroscopic signatures of graphene phonons [2,3] and a feature that is compatible with a graphene plasmon [4]. Spatially resolved IETS unveils that the signal strength of these features depends on the moiré lattice site. Possible mechanisms are discussed that appropriately describe the influence of the different atomic stacking in the moiré lattice sites on inelastic excitations.

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## Optical response of doped epitaxial graphene and chemically grown MoS<sub>2</sub>

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Specific potential applications of two-dimensional (2D) materials relate to their versatile electronic properties and related photonic, optoelectronic or photovoltaic functionality. The leading member of the 2D family, graphene has a semimetallic character which is a drawback in context of electronics application but enables continuous tuning of optical properties and in particular plasmon resonance frequency, which can be achieved e.g. by electrostatic gating and is nevertheless by now limited to near-infrared energies. However, chemical doping in epitaxial graphene reveals possibility to launch plasmons in graphene on Ir(111) highly doped with alkali-atom intercalation, where a periodic spatial modulation originating from interaction between graphene and substrate compensates momentum mismatches between visible light and graphene plasmons [1].

While linear bands in semimetallic graphene lead to record charge carrier mobility, mono- and few-layer transition metal dichalcogenides (TMDs) attract increasing attention due to their intrinsic semiconducting and optoelectronic properties and corresponding advantages over graphene. MoS<sub>2</sub> monolayers researched in our work were synthesized on a SiO<sub>2</sub>/Si wafer and transferred to Ir(111) for nano-scale characterization. The established transfer procedure is also applicable to a diversity of substrates, thus opening a way to different applications. The electronic band gap measured by scanning tunneling spectroscopy (STS) revealed n-doping of the samples and lateral nano-scale variations of the band gap. From the difference of the electronic band gap measured by STS of 2.1 eV and the optical band gap measured by photoluminescence (PL) of 1.9 eV, an estimated exciton binding energy of  $\approx 0.2$  eV is obtained. Optical characterization indicates a quasi-freestanding character and versatile advantage for optical sensing, such as specific molecular adsorption [2].

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## Universal Trends in the Covalent Functionalization of Epitaxial Graphene by Amino-terminated Organic Molecules

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With the aim of designing and developing novel and emerging graphene-based materials with tailored electronic properties, an important step forward in the graphene functionalization with organics has been recently given by our group.[1, 2] We have proved, by a combination of different experimental techniques and theoretical methods, that we covalently link p-aminophenol molecules into single atomic monovacancies created in graphene via a selective oxidation of the amino group and subsequent integration of the nitrogen within the graphene network in a  $sp^3$ -like configuration. Interestingly, functionalized surfaces retain the electronic properties of pristine graphene, as unaltered Shubnikov-de-Haas oscillations and Dirac cone.[3]

Motivated by this recent work, herein we present a combined experimental and first-principles based exhaustive study on the incorporation within the graphene lattice of a large variety of amino-terminated organic molecules. Results demonstrate how the incorporation into the graphene lattice of the different molecules is produced in a similar way that the previously reported case of p-aminophenol, independently of their size, chemical nature and electronic character. In all cases, graphene locally n-dopes in the graphene molecular vicinity accommodating around 0.4–0.5  $e^-$  per molecule, where an important molecular charge rearrangement is produced after the incorporation into the graphene lattice. DFT-based calculations of the N1s core-level-shifts (CLSs) for all the functionalizing molecules reveal that the charge accumulation in the incorporated N atom produces similar CLSs towards lower binding energies w.r.t. a purely graphitic N atom. Although all these computed values are similar, it is possible to find interesting trends between these values and the molecular incorporation free energy for all the molecules, as well as with the out-of-plane buckling displacement of the N atom w.r.t. the graphene plane and the local graphene n-doping level. All these findings can be integrated within a sort of highly predictive universal behavior that fully rationalizes the incorporation process of amino-terminated molecules within the graphene lattice.

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## Formation of a AuIr 2D alloy by intercalation of Au in graphene/Ir(111)

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Atom intercalation in metal supported graphene is an effective way to decouple graphene from the underlying metal, giving a certain control over its doping and allowing the observation of inter- or intra-valley scattering processes. In addition, if the intercalants are heavy-metal atoms, the intrinsic spin-orbit coupling of graphene could be enhanced to the point of turning it into a 2D topological insulator [1]. So far, by intercalation of gold and lead atoms it has been possible to enhance graphene's spin-orbit coupling to the order of 100 meV (including Rashba type), in particular in gr/Au/Ni(111) [2], gr/Pb/Ir(111) [3] and gr/Au/Pt(111) [4].

In this work we study the intercalation of Au in gr/Ir(111) by means of LEED and STM. We show that, under certain growth conditions, a 2D Au-Ir surface alloy is formed underneath graphene, preserving the original moiré periodicity of gr/Ir(111). In addition, we observe inter-valley scattering processes, a hallmark of the effective decoupling of graphene from the substrate, which we use to estimate the Dirac point.

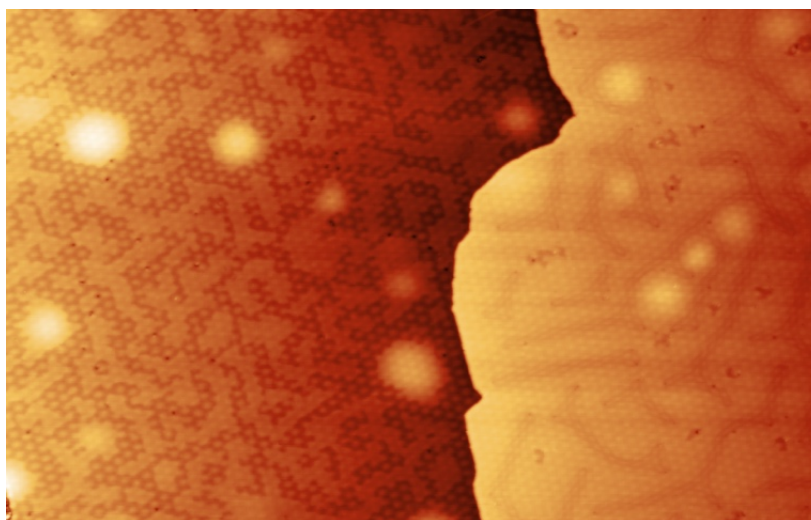


Figure 1: 150nm-wide STM topographic image of Au-intercalated gr/Ir(111) exhibiting two terraces with different degree of intercalation. The extended lighter-colored areas are the Au-intercalated regions.

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## Studies on Point Defects and Heterostructures of Transition Metal Dichalcogenides

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The transition-metal dichalcogenides (TMDCs) family has been rapidly growing and now encompasses various kinds of materials with different electronic properties (metals, semiconductors, insulators, superconductors...). The exciting aspect of these materials is their ability to be isolated, transferred and stacked on top of each other to create new heterostructures. Within this family, semiconducting TMDCs have triggered a great interest, especially in next-generation optoelectronic nanodevices. In this poster, we present DFT calculations for electronic properties of point defects in MoS<sub>2</sub> monolayer and for in-plane heterojunctions between two monolayers of MoSe<sub>2</sub> and WSe<sub>2</sub>. In the study of defects, various types of point defects are considered: sulfur vacancies, the substitution of Mo atom by Fe atom and the replacement of S atom by B, C or N atom. It was found that, the point defects do not lead to a significant strain in MoS<sub>2</sub> films. Our calculations for the TMD heterojunction reveal a type-II alignment between MoSe<sub>2</sub> and WSe<sub>2</sub> parts of the junctions. This finding is supported by scanning tunneling microscopic/spectroscopic measurements in ultra high vacuum at 8.5K. The sample was made by depositing MoSe<sub>2</sub> and WSe<sub>2</sub> monolayers one after another onto a graphitized SiC substrate. Our STM/STS measurements provide values of 0.3 eV and 0.1 eV for the valence band offset and conduction band offset, respectively.

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## Decoupling Graphene From Metals By Electrochemical Oxidation

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While high-quality defect-free epitaxial graphene can be efficiently grown on metal substrates, strong interaction with the supporting metal quenches its outstanding properties. Thus, protocols to transfer graphene to insulating substrates are mandatory, and these often severely impair graphene properties by the introduction of structural or chemical defects. Here we describe a simple, fast and easily scalable general methodology to structurally and electronically decouple epitaxial graphene from metal surfaces. A multi-technique characterization of the different steps involved in the process, combined with ab-initio calculations, shows that after a controlled electrochemical oxidation process a single-atom thick metal-hydroxide layer intercalates below graphene decoupling it from the metal substrate. The decoupling process takes place without disrupting the morphology and electronic properties of graphene. The electrochemical protocol has been proved to work on Gr/Pt(111) and Gr/Ir(111) substrates. Epitaxial graphene was grown in UHV conditions by thermal decomposition of fullerenes and the samples were characterized in-situ by STM and LEED. Subsequent ex-situ characterization with AFM, XPS and Raman before and after the electrochemical treatment demonstrates the efficiency of the decoupling process. This work suggests that suitably optimized electrochemical treatments may provide viable alternatives to transfer protocols for graphene and other 2D materials on diverse metal surfaces.

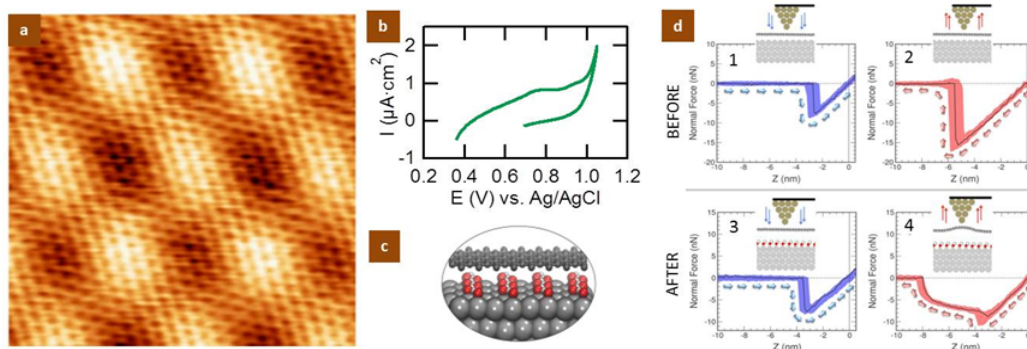


Fig.1. a) STM image of Gr/Pt(111) showing a characteristic Moiré ( $(4 \times 4) \text{nm}^2$ ,  $I=4 \text{nA}$ ,  $V=10 \text{mV}$ ). b) Cyclic voltammetry of a Gr/Pt(111) sample in 0.1M aqueous  $\text{HClO}_4$ . c) A  $\text{Pt}_2\text{OH}$  submonolayer is formed beneath the graphene surface. d) FZ curves of a Gr/Pt(111) sample before (1,2) and after (3,4) the electrochemical treatment. Black lines correspond to a typical curve while the colored areas represent  $> 100$  repeated curves. 1- FZ plot in forward direction showing the characteristic jump-to-contact from zero-force and the sloped straight-line of contact. 2- Corresponding retracting curve where a higher force is achieved due to the adhesion force. 3- FZ plot in forward direction showing a similar jump-to-contact. 4- Corresponding retracting curve direction showing a different behavior: the adhesion force is reduced and a bump in the force is perceived.

## Tuning the chemical reactivity of graphene grown on metals:

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Graphene is commonly regarded as an inert material. Using first principles calculations, we explore different ways to enhance its chemical reactivity and to tune its electronic properties, what can be useful in the design of molecular electronics devices. For instance, we can use nitrogen defects to increase the reactivity of the layer, creating preferential adsorption sites for oxygen trapping. We find interesting electronic properties in these oxygen-decorated nanopatterns, especially when more than one oxygen atom is absorbed and collective effects are displayed [1]. As a result, a gap of  $\sim 1$  eV is opened in the electronic structure (see figure). In addition, we show that it is also possible to induce a remarkable increment in the chemical activity of a graphene layer by simply growing it on an appropriate substrate [2]. In strongly-interacting substrates like Rh(111), graphene adopts highly rippled structures that exhibit clearly different areas with distinctive chemical behaviors. According to the local coupling with the substrate, we find areas whose properties resemble free-standing graphene, but also, more reactive regions leading to different pathways of adsorption and diffusion for both atomic and molecular oxygen.

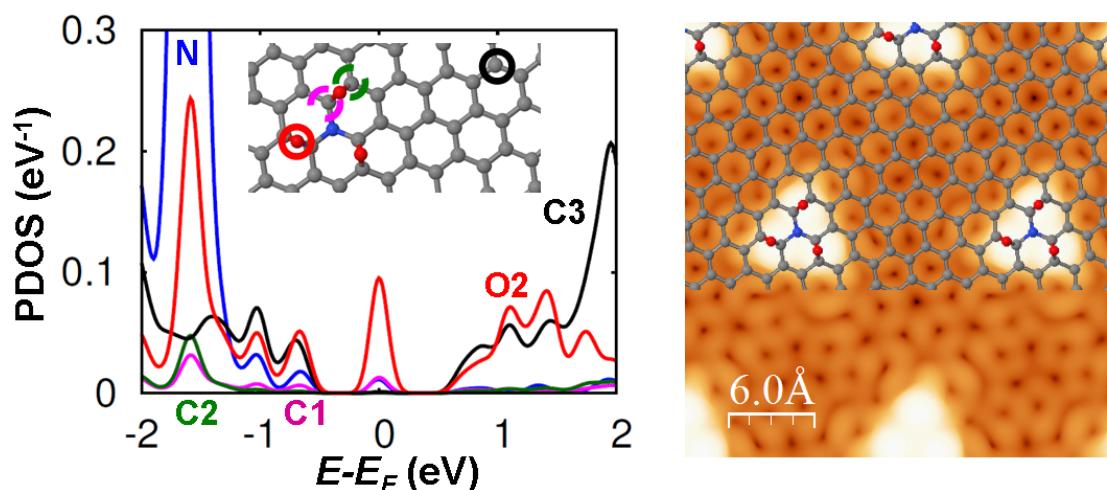


Fig. 1: Electronic properties of an oxygen-decorated nanopattern N-doped graphene showing the opening of 1 eV band gap in the projected DOS (left). Theoretical STM image of the pattern (right).

### REFERENCES:

[1] C. Romero-Muñiz, et al.: (submitted)

[2] C. Romero-Muñiz, et al.: (submitted)

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## Morphology and electronic properties of ultrathin molybdenum disulphide and tungsten disulphide grown on various substrates

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Two-dimensional (2D) materials beyond graphene give rise to a number of new possible applications. While graphene has many extraordinary properties, its lack of a bandgap is a limiting factor for (opto-)electronics. Transition metal dichalcogenides (TMDCs) overcome this problem. Depending on e.g. the chemical composition, the thickness, doping and strain, electron-hole pairs may be created with light in the visible regime, and the band gap may be either indirect or direct. Especially excitonic effects are even more pronounced than in common three-dimensional materials, because the excitonic binding energy are orders of magnitudes larger [1]. Furthermore, the unavoidable presence of defects (edges, grain boundaries, point-like defects etc.) lead to additional changes such as e.g. catalytic activity [2].

Here, we present results obtained from samples prepared in our custom-made system for chemical vapor deposition (CVD) of molybdenum disulfide (MoS<sub>2</sub>) and tungsten disulfide (WS<sub>2</sub>), two representatives of the TMDCs. These materials are grown on various substrates and are characterized by scanning probe microscopy (SPM) complemented by other techniques. Applying various modes of SPM several properties of those samples as well as the influence of intrinsic and artificial defects could be studied on a microscopic level. In particular, scanning tunneling microscopy (STM) and kelvin probe force microscopy (KPFM) exhibit information about the electronic properties of 2D materials, thus information about their semiconducting and catalytic nature.

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## Graphene synthesis via segregation of carbon atoms through a thin metal film: features of growth and electronic structure

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<sup>1</sup> St.Petersburg State University, 198504, ul. Ulyanovskaya 1, Saint-Petersburg, Peterhof, Russia

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The work is devoted to a study of graphene monolayer growth on a thin metal film deposited on graphite under a certain heat treatment due to segregation of carbon atoms from metal-graphite interface to the surface. We have studied different metal (Ni, Co) layers deposited on two types of graphite substrates: singlecrystalline graphite and highly-oriented pyrolytic graphite (HOPG). Photoemission data indicate the graphene is easily formed on Ni film deposited on HOPG: growth process starts after annealing at 180°C and a monolayer thickness of graphene is obtained at annealing temperature 310°C. However it consists of a lot of rather small variously oriented domains following the surface structure of HOPG. Usage of cobalt film allowed to obtain better-ordered graphene, the diffraction pattern indicated the presence of a large area domain. But the temperature is a bit higher: annealing Co/HOPG system at 350°C is a bit not enough to form full monolayer graphene coverage. Usage of single-crystal graphite with a Co layer atop allows form a well-ordered graphene of monolayer thickness, but it requires higher temperatures – ~450°C. Nevertheless, the study of intermediate synthesis stages showed that annealing the metal/graphite or metal/HOPG system always leads to formation of the surface carbide phase, which at higher temperatures transforms to graphene [1-3].

Experiments were conducted in the Resource Center "Physical methods of surface investigation" of St.Petersburg State University and at Russian-German beamline at BESSY-II synchrotron facility (Helmholtz-Zentrum, Berlin).

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## An efficient device for growth of graphene samples on 6H-SiC(0001)

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Thermal decomposition of SiC wafers in Ar atmosphere was proven to be a suitable method to obtain epitaxial graphene samples [1-4]. However, the state-of-the-art setups that reach the needed conditions for sublimation of Si from SiC substrates are complex and require precise tuning of the growth parameters [1]. Therefore, we devise a compact furnace in which high-quality graphene samples can be prepared efficiently with minimum requirements on the equipment.

The design of the furnace is based on a directly heated element with an extremely high heat localization, which can reach temperatures over 1600 °C with a modest power dissipation. We study quality of the produced samples by a number of methods - the terrace widths and number of graphene layers by STM, presence of graphitic carbon is proven by X-ray photoelectron core level spectroscopy and near-edge X-ray absorption fine structure. Finally, the low amount of defects is detected by Raman spectroscopy.

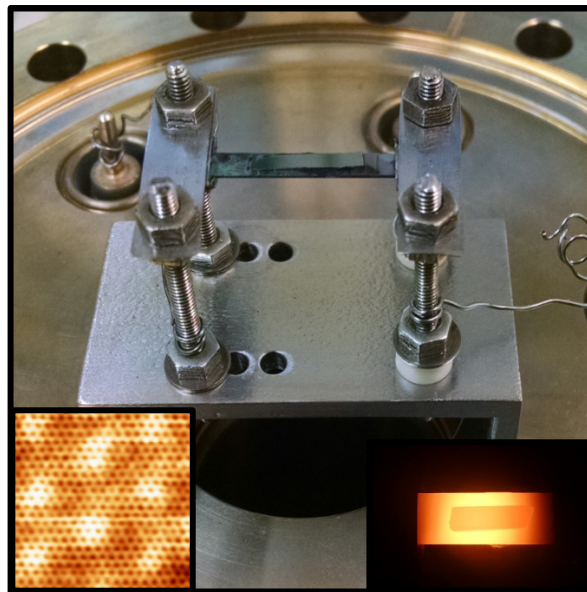


Figure 1 Device for graphene growth on SiC(0001). Left inset STM image of graphene/6H-SiC(0001). Right inset sample uniform annealing

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## Spin-orbit and exchange coupling induced in graphene under contact with heavy and magnetic metals and possibility of topological phase formation

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Graphene is one of most perspective material in modern nanoelectronics due to linear dispersion of electronic states near the Fermi level at the K-point. At the same time, recently a series of works appear in literature demonstrating an enhanced induced spin-orbit (SO) coupling in graphene under contact with heavy metals [1]. It allows assuming a practical realization of topological phase formation predicted in graphene [2] with the energy gap at the Dirac point induced by SO coupling. It allows realization of the Quantum Spin and Anomalous Hall effects in graphene which are manifested in creation of the 1D-edge states in the open SO gap. In the present talk a possibility of an enhanced induced spin-orbit coupling in graphene and formation of corresponding topological phase in graphene under contact with heavy metals (Au, Pt, Pb) will be analyzed. In relation to it, the induced contributions of the intrinsic (internal) and extrinsic (Rashba-like) SO coupling realized in the studied systems and also the influence spin-dependent hybridization will be analyzed and estimated. The experimental investigation of spin and electronic structure was carried out by photoemission with angle and spin resolution and crystalline structure - by STM and LEED. Comparison with theoretical calculations is carried out. As a result, we estimate a relation between the intrinsic and extrinsic contributions in the induced SO coupling in dependence on the mutual arrangement of graphene and metal atoms. It is shown that for graphene on Au/Ni(111) and Au/Co(0001) the Rashba-like contribution prevails in the induced SO coupling that is followed by the induced spin splitting up to 100-150 meV without the Dirac gap formation [1]. For graphene on Pt(111) [3] and on Pt(111) with intercalated Pt monolayer [4] a contributions of intrinsic SO coupling increases leading to opening SO gap at the Dirac point. For graphene on Pt(111) with intercalated Pb monolayer the spin structure in the upper and lower Dirac cone was studied [4], which was predicted for topological phase. Additionally, a possibility of interplay between SO and exchange coupling and manipulation of the induced SO splitting in graphene by the induced magnetic moment is demonstrated in the system included both heavy (Au) and magnetic (Co) atoms.

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## Dependence of the adsorption height of graphene-like adsorbates on their dimensionality

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Graphene nanoribbons (GNRs) attract attention because unlike pristine graphene they have a bandgap, making them applicable in semiconductor technology. Because their electronic, magnetic and transport properties depend on their width and edge shape, efforts are made to control their geometry. An open question remains, however, how the shape and precise atomic configuration of the edges influence the interaction with the substrate. An important aspect by which the substrate interaction may be affected is the dimensionality of the adsorbate. GNRs are confined in one direction and extended in the other, hence they are quasi one-dimensional (1D)  $\pi$ -conjugated objects. This is in contrast to graphene-like platelet molecules (quasi-0D graphene flakes) and graphene (2D).

Here we address the question whether and, if yes, how local bonds via the edges on the one hand and the dimensionality on the other influence the interaction between graphene-like adsorbates and the surface. To this end, by means of x-ray standing wave technique we directly measured adsorption heights of several GNRs on Au(111) and Cu(111) and graphene on Cu(111) and compared these to the adsorption heights of organic molecules. We find that, regardless of their edge shape and their chemical edge structure (armchair or chiral vs. chevron geometry, nitrogen-doped vs. undoped edges), GNRs have a backbone height that is similar to that of graphene-like platelet molecules, but very different from graphene. We assign this to a consequence of the adsorbate dimensionality and to the related spill-out charge redistribution at the adsorbate/metal interface.

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## Supported 2D materials under low energy He ion irradiation

P. Valerius<sup>1</sup>, A. Herman<sup>1</sup>, C. Speckmann<sup>1</sup> and T. Michely<sup>1</sup>

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He ion irradiation is used to tailor the 2D materials graphene (Gr) and a monolayer hexagonal boron nitride (h-BN), both resting on Ir(111), in a useful way.

First we induce single vacancies in the h-BN monolayer on Ir(111) by low fluence 500 eV He<sup>+</sup> ion irradiation at elevated temperatures in order to form vacancy clusters that are located in the initial valley regions of the h-BN/Ir(111) moiré. Consequently, a 2D antidot lattice of small holes with diameters of 0.5-1 nm is formed. The vacancy cluster formation is traced back to single vacancy mobility and preferential bonding of vacancy cluster edges to Ir(111) in the valley regions. Moreover, similar irradiation experiments for an h-BN monolayer on Pt(111) show that our observations represent a general principle of irradiation induced antidot lattice formation, rather than a unique case. Compared to irradiation induced vacancy cluster arrangements in Gr/Ir(111) [1] the order of the vacancy cluster in the h-BN/Ir(111) moirés is superior due to a single preferred agglomeration site. Possible uses of such nanomesh membranes based on low energy irradiation are outlined.

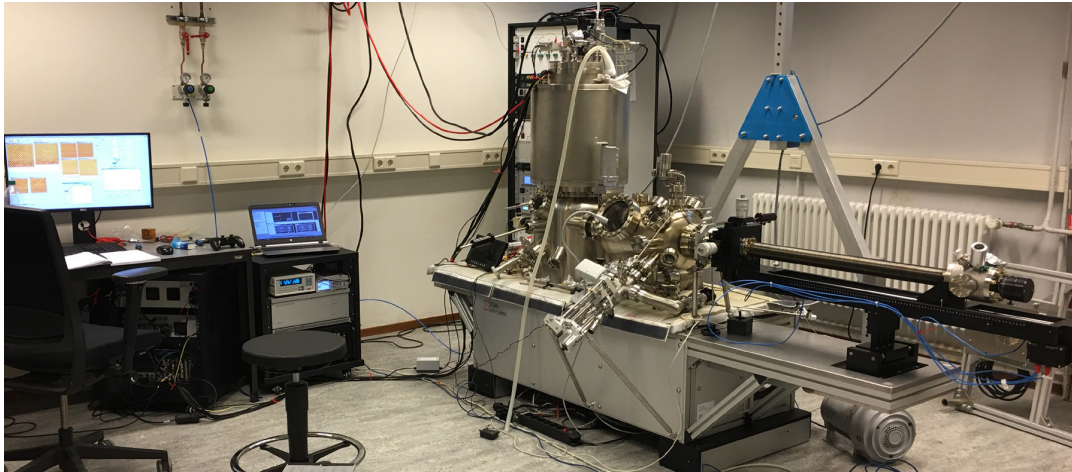
Further, we use He ion irradiation in order to remove wrinkles in Gr resting on Ir(111), which form during the growth process due to the thermal mismatch of substrate and Gr. With low fluence, low energy noble gas ion irradiation at temperatures around the CVD growth temperature the height and length of the resulting wrinkles can be reduced until they are eventually completely eliminated. However, as side effects of the He ion irradiation small vacancy clusters are pinned to the moiré of Gr on Ir(111).

### REFERENCES:

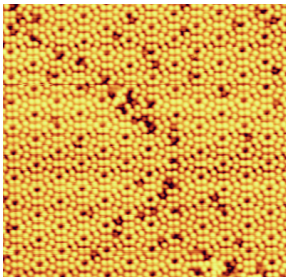
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# POLAR

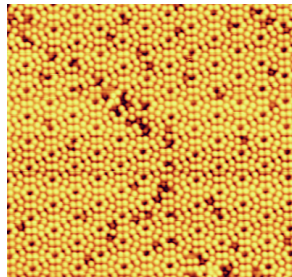
## LT-SPM with Variable Magnetic Field



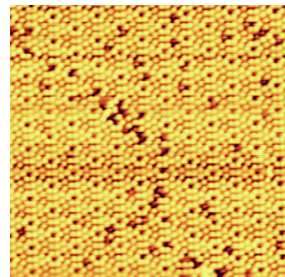
### Low Temperature STM in variable magnetic fields



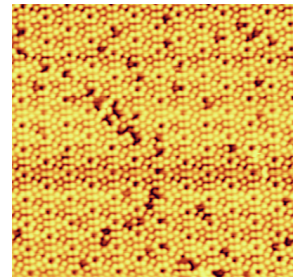
$B_z = 2T$



$B_z = 3T$



$B_z = 4T$

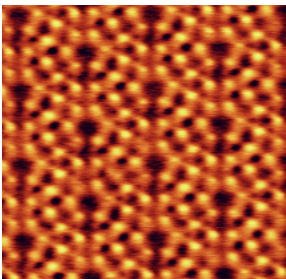


$B_z = 4.5T$

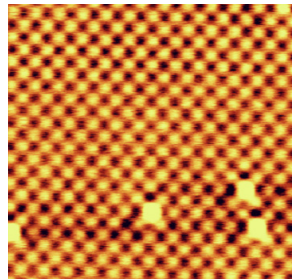
Si(111)7x7  
20nm x 20nm  
T=4.4K

Series of STM images at the same spot on the sample at different magnetic fields.

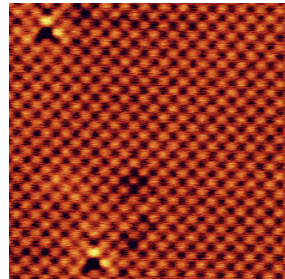
### Low Temperature qPlus® AFM



Si(111)7x7  
7.8nm x 7.8nm  
A=550pm<sub>pp</sub>, f=20.005,5Hz,  
df= -13.534Hz, Q=35.123,  
U<sub>gap</sub>=0V, T=4.4K

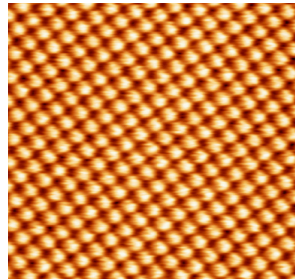


Single crystal NaCl(001)  
7.2nm x 7.2nm  
A= ~100pm, f= ~23.000Hz  
U<sub>gap</sub>=0V, T=4.4K



$B_z = 4.5T$

7.8nm x 7.8nm  
A=300pm<sub>pp</sub>, f=23.999,7Hz  
df=-8.54Hz, Q=53.221  
U<sub>gap</sub>=0V, T=4.35K



$B_z = 5T$

5nm x 5nm  
A=300pm<sub>pp</sub>, f=24.006,1Hz  
df=-6.432Hz, Q=31.700  
U<sub>gap</sub>=0V, T=4.35K

First qPlus results in magnetic field with POLAR SPM at T=4.35K  
Sample: single crystal NaCl(001)

Results have been obtained during the test and installation of a POLAR system to University of Utrecht, Netherlands.

## List of Posters (*referenced as "P\*" to be located in the exhibitor panels*)

- P1. Al Taleb A.** "Helium scattering from 2D Moiré superstructures: a new tool to characterize layered van der Waals heterostructures"
- P2. Ayani C. G.** "Controllable switching of the superconductivity of a tungsten STM tip on epitaxial graphene"
- P3. Biel B.** "Not all metals are the same: impact of metallic substrates on defected single-layer MoS<sub>2</sub>"
- P4. Cai J.** "Determination of graphene-hBN lateral interface structure on Ir(111)"
- P5. Cirera B.** "Relativistic dispersion of massive electrons in graphene nanoribbons"
- P6. Clericò V.** "Coherent electron transport through graphene nanoconstrictions"
- P7. Coelho P. M.** "Post-synthesis metal incorporation into MoSe<sub>2</sub> or MoTe<sub>2</sub> leads to crystal modifications into metallic line-network"
- P8. De Vries N.** "Spectroscopic investigation of graphene nanoribbons showing room temperature ballistic electron transport"
- P9. Dombrowski D.** "Two phases of single layer tantalum disulfide on gold"
- P10. Estyunin D. A.** "Spin textures of graphene/Pb systems on various substrates"
- P11. Franke M.** "Investigation of hexagonal boron-nitride (hBN) and graphene Gr-R0° on SiC(0001)"
- P12. Gómez-Herrero A. C.** "Two-dimensional molecular crystals with non-trivial electronic properties"
- P13. Hall I. J.** "Growth and structure of mono- to few-layer vanadium disulphide on graphene on Ir(111)"
- P14. Halle J.** "Inelastic excitations in bilayer graphene on Ru(0001)"
- P15. Kralj M.** "Optical response of doped epitaxial graphene and chemically grown MoS<sub>2</sub>"
- P16. Martínez J. I.** "Universal trends in the covalent functionalization of epitaxial graphene by amino-terminated organic molecules"
- P17. Navarro J. J.** "Formation of a AuIr 2D alloy by intercalation of Au in graphene/Ir(111)"
- P18. Nguyen V. D.** "Studies on point defects and heterostructures of transition metal dichalcogenides"
- P19. Palacio I.** "Decoupling graphene from metals by electrochemical oxidation"
- P20. Pérez R.** "Tuning the chemical reactivity of graphene grown on metals"
- P21. Pollmann E.** "Morphology and electronic properties of ultrathin molybdenum disulphide and tungsten disulphide grown on various substrates"
- P22. Pudikov D. A.** "Graphene synthesis via segregation of carbon atoms through a thin metal film: features of growth and electronic structure"
- P23. Redondo J.** "An efficient device for growth of graphene samples on 6H-SiC(0001)"
- P24. Shikin A.** "Spin-orbit and exchange coupling induced in graphene under contact with heavy and magnetic metals and possibility of topological phase formation"
- P25. Soubatch S.** "Dependence of the adsorption height of graphene-like adsorbates on their dimensionality"
- P26. Valerius P.** "Supported 2D materials under low energy He ion irradiation"

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