September 28th – 29th, 2021

STiBNite

1st Summer School: Surface-Confined Synthesis and Advanced Surface Characterization Tools

Project Coordinator: *Prof. Davide Bonifazi*, University of Vienna, Austria
School Organizers: *Prof. Willi Auwärter* and *Prof. Ruben Costa*, Technische Universität München, Germany

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Accessible online.

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Scientific Program September 28th

Afternoon session

13.00 – 13.10: Opening address *Prof. Willi Auwärter*

13.10 – 14.00: *Prof. Irene Groot*
(Leiden University, The Netherlands)
Title: Introductory lecture UHV

14.00 – 14.50: *Prof. Petra Rudolf*
(University of Groningen, The Netherlands)
Title: Introductory lecture XPS

14.50 – 15.10: *Coffee Break*

15.10 – 16.00: *Prof. Willi Auwärter*
(Technische Universität München, Germany)
Title: Introductory lecture STM & AFM

16.00 – 16.50: *Dr. Pascal Ruffieux*
(EMPA, Switzerland)
Title: Bottom-up fabrication of nanographene-based spin chains

16.50 – 17.10: *Coffee Break*

17.10 – 18.00: Prof. *Meike Stöhr*
(University of Groningen, The Netherlands)
Title: Molecular nanostructures on metals vs. graphene: similarities and differences

All presentations will follow a unique zoom link. All times are CET.
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Scientific Program September 29th

Morning session

09.00 – 09.50: *Prof. Jonas Björk*
(Linköping University, Sweden)
Title: Atomistic insights of surface-confined reactions from theoretical modeling

09.50 – 10.40: *Prof. Carsten Busse*
(Universität Siegen, Germany)
Title: Preparation and characterization of two-dimensional transition metal dichalcogenides

10.40 – 11.00: *Coffee Break*

11.00 – 11.50: *Dr. Oleg Konovalov*
(ESRF, France)
Title: Grazing incidence synchrotron X-rays study of two-dimensional materials on liquid surfaces

11.50 – 13.00: *Lunch Break*

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Scientific Program September 29th

Afternoon session

13.00 – 14.00: *Laboratory Tour*

14.00 – 14.50: *Prof. Steven de Feyter*

(KU Leuven, Belgium)

Title: Functionalization of 2D nanomaterials: a molecular approach

14.50 – 15.40: *Prof. Zeila Zanolli*

(Utrecht University, The Netherlands)

Title: Quantum materials by design

15.40 – 16.00: *Coffee Break*

16.00 – 16.40: *Dr. Ulrike Kauscher Pinto*

(Editor at Wiley)

Title: Getting published in Wiley Advanced journals: How to present your article to survive peer review

16.40 – 17.00: *Dr. Joseph Krumpfer*

(Editor at Wiley)

Title: Diversity, Equity and Inclusion in Scientific Publishing

17.00 – 17.10: *Coffee Break*

17.10 – 17.40: *Panel Discussion*

H. Röder, as moderator;

J. Krumpfer, Editor at Wiley;

Z. Zanolli, associate professor, Treasurer and Board Member, Young Academy of Europe;

Y. Atoini, MSCA Postdoctoral Fellow

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Pascal Ruffieux, EMPA

Bottom-up fabrication of nanographene-based spin chains

Nanographenes offer a wide range of physical properties depending on their size, shape and edge structure. A deterministic control over the final properties, however, requires fabrication with atomic precision. This can be achieved using a bottom-up approach relying on the controlled colligation of molecular precursors that yield the target structure using surface-assisted reactions. This approach can be applied for the synthesis of graphene nanoribbons [1] (GNRs) with band gaps that are suitable for the fabrication of efficient switching devices or GNRs with a periodic arrangement of edge extensions giving rise to engineered topological bands [2]. More recently, we developed on-surface synthesis protocols for open-shell nanographenes where unpaired electrons give rise to magnetic moments. Covalent coupling between such molecular magnets allows to control the magnetic interaction between spins [3] and to build up extended spin structures.
Here, I will introduce bottom-up fabrication strategies in a general way and show how STM is used to characterize reaction intermediates and the final structure of nanographenes but also their electronic and magnetic properties. For instance, we apply inelastic scanning tunneling spectroscopy to triangulene chains revealing site-dependent spin excitations compatible with the Haldane phase with fractional spin excitations at the end of the spin chains [4].

[1] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, S. Blankenburg, M. Muoth, A. P. Seitsonen, M. Saleh, X. Feng, K. Müllen, and R. Fasel, *Atomically Precise Bottom-up Fabrication of Graphene Nanoribbons*, Nature **466**, 7305 (2010).

[2] O. Gröning, S. Wang, X. Yao, C. A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Mullen, P. Ruffieux, and R. Fasel, *Engineering of Robust Topological Quantum Phases in Graphene Nanoribbons*, Nature **560**, 209 (2018).

[3] S. Mishra, D. Beyer, K. Eimre, R. Ortiz, J. Fernández-Rossier, R. Berger, O. Gröning, C. A. Pignedoli, R. Fasel, X. Feng, and P. Ruffieux, *Collective All-Carbon Magnetism in Triangulene Dimers*, Angewandte Chemie International Edition **59**, 12041 (2020).

[4] S. Mishra, G. Catarina, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C. A. Pignedoli, X. Feng, P. Ruffieux, J. Fernandez-Rossier, and R. Fasel, *Observation of Fractional Edge Excitations in Nanographene Spin Chains*, ArXiv:2105.09102 [Cond-Mat] (2021).

Molecular nanostructures on metals vs. graphene: similarities and differences

Meike Stöhr
Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

To preserve the (functional) properties of either individual adsorbates or well-ordered molecular assemblies upon adsorption on solid surfaces, the molecule substrate interactions have to be generally relatively weak. This can be achieved by introducing a decoupling layer between (metallic) surface and molecules. Among others, thin insulating layers of either NaCl or hBN have been shown to be very useful to this end. The chemical inertness and the low density of states near the Fermi level also make graphene a good choice as a buffer layer to decouple adsorbed molecules from the underlying (metallic) substrate. Importantly, this holds the promise to preserve the intrinsic properties of the adsorbed species such as magnetic or catalytic properties. [1]

For three different organic molecules, the changes in both structural and electronic properties will be discussed when adsorbed on graphene compared to noble metal surfaces [2]. On the other hand, instead of reducing or even completely turning off the molecule substrate interactions, enhancing the intermolecular interactions is another possibility for preserving the adsorbates´ properties. On the basis of the self-assembly process of tetracyanophenyl porphyrins before and after coordination with either Co- or Fe-atoms on Au(111), the influence of molecular coverage on decoupling could be demonstrated [3].

References

[1] S. Maier et al., Beilstein J. Nanotechnol. 12 (2021) 950.
[2] J. Li et al., J. Phys. Chem. C 120 (2016) 18093 ; N. Schmidt et al., Chem. Eur. J. 25 (2019) 5065 ; J. Li et al., J. Phys. Chem. C 123 (2019) 12730 ; J. de la Rie, to be submitted.
[3] B.D. Baker Cortes et al., J. Phys. Chem. C 123 (2019) 19681; B.D. Baker Cortes et al., submitted.

Atomistic insights of surface-confined reactions from theoretical modeling

Jonas Björk
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Studying chemical reactions on surfaces is fascinating from several aspects, both due to the two-dimensional environment reducing the degrees of freedom of molecules and the chemical reactivity a surface may have. For example, deposition of suitable molecular precursors can result in the formation of well-defined nanostructures which are difficult to obtain by conventional wet chemistry approaches. Furthermore, working under well-defined conditions, using ultraclean monocrystalline surfaces under ultrahigh vacuum conditions, together with high resolution scanning probe microscopy and a variety of spectroscopic techniques, makes it possible to study the mechanisms of chemical reactions at a fundamental level. However, experiments are most often limited to provide information about reactants and products and sometimes intermediate states.

Theoretical modeling –in terms of density functional theory (DFT) – has become increasingly popular for studying the atomistic details of chemical reactions on surfaces. In this lecture, the DFT-based methods for computationally studying molecules on surfaces will be presented, with particular attention to on-surface reactions. We will demonstrate the abilities of DFT to provide complementary support for the interpretation of experimental data as well as insights into actual reaction pathways. The intention of the lecture is to give an overview of the information that theoretical modeling can provide but also some of the difficulties we need to have in mind. This will be achieved by focusing on specific systems of molecules undergoing chemical reactions on surfaces for which theoretical modeling has played an important role.

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Tailored materials for Sustainable Technologies: programming functional molecular components through Boron-Nitrogen doping

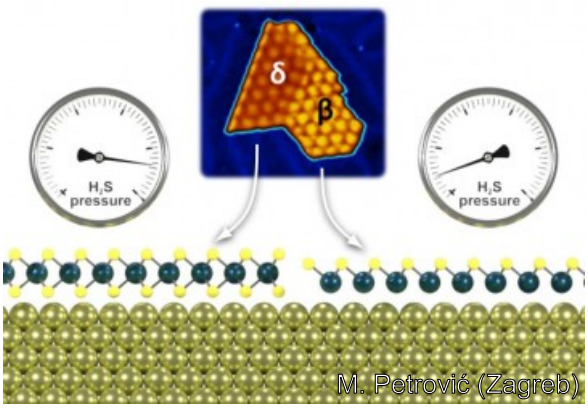
(H2020 Innovative Training Network)

Surface-Confined Synthesis and Advanced Surface Characterization Tools

(I. Groot, P. Rudolf, W. Auwärter)

Preparation and characterization of two-dimensional transition metal dichalcogenides

(C. Busse, Universität Siegen)



Epitaxial growth is a versatile method for the preparation of two-dimensional materials. In this talk I focus on the growth of monolayers of transition metal dichalcogenides (TMDCs) by reactive molecular beam epitaxy (MBE). These materials consist of a layer of a transition metal sandwiched between two layers of a chalcogen. We prepare MoS_2, WS_2, and TaS_2 by sulfurization of evaporated metal atoms, either by exposure to H_2S or co-evaporation of elemental S from a valved cracker cell. The resulting ultrathin films are studied using surface science methods, foremost scanning tunneling microscopy and spectroscopy (STM/STS).

We compare the interaction of semiconducting MoS_2 and metallic TaS_2 with the Au(111) surface used as the substrate and find that although the geometric structure is very similar, far fewer sulfur atoms of the lower layer participate in the bonding to gold atoms for the case of MoS_2. This localized bonding also causes local variations in the electronic structure. For sulfur-poor growth conditions, a novel phase of tantalum sulfide is found that corresponds to TaS_2 without the lower sulfur layer. This structure is stabilized by the Au(111) surface and has no known bulk analogue. Finally, we study lateral heterostructures of different TMDCs (e.g. MoS_2-WS_2). Decoupling from the metallic substrate by a graphene layer allows us to determine the band banding across this ultrathin semiconductor heterojunction.

STiBNite school

Grazing incidence synchrotron X-rays study of two-dimensional materials on liquid surfaces.

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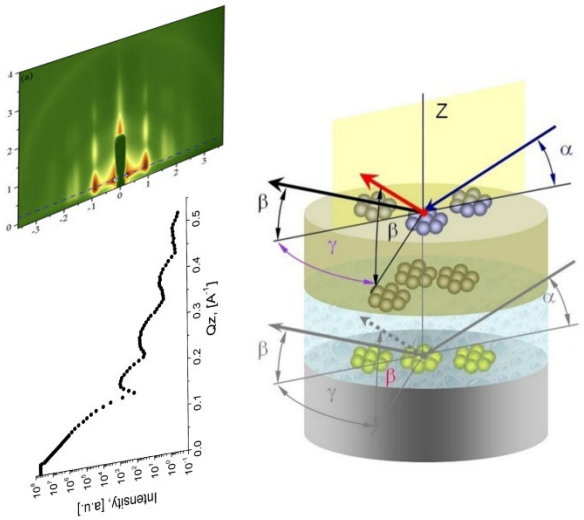
The growing over last decades interest to the study of the surfaces and interfaces using grazing incidence geometry techniques leads to the consistent development of both the theory and the experimental instrumentation. These techniques are used for a comprehensive study of the structure of a wide class of the hard and soft condensed matter. The latter comprise such systems as liquids, polymers, gels, self-organized mono- and multi-molecular layers of organic molecules on the water surface (for example, models of cell membranes), colloids, micelles, polymer films, two-dimensional crystals of proteins and nanoparticles.

The presentation gives an overview and theoretical basis of such surface sensitive synchrotron X-ray methods as the X-ray reflectivity (XRR), the Grazing Incidence Wide Angle Scattering (GIWAXS), the Grazing Incidence Small Angle Scattering (GISAXS) and the Grazing Incidence X-ray Fluorescence (GIXF). These techniques will be illustrated by examples of scientific research of 2D materials (2DMs) performed at the state-of-the-art the ESRF ID10 beamline optimized for soft surfaces and interfaces studies. In situ synchrotron study of 2DMs formation such as graphene and ordered arrays of nano-particles (NPs) will be presented more detailed.



Generic illustration of X-ray scattering on air-liquid, liquid-liquid and solid liquid interfaces with XRR (bottom left) and GISAXS (top left) signals.

Functionalization of 2D nanomaterials: a molecular approach

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In this presentation, I will focus on the functionalization of graphite and graphene using molecules, at the liquid-solid interface, though the concepts can be applied to other 2D materials too.

Nanostructuring is at the heart of all functionalization protocols that we develop, because it opens new possibilities of control and functionality.

A first approach of surface functionalization is based on molecular self-assembly at the interface between a liquid or air, and graphite or graphene. I will discuss concepts of nanostructuring emphasizing the effect of solvent, solute concentration and temperature, stimulus-driven self-assembly and self-assembly under nanoconfinement conditions.

A second approach is based on grafting molecules on graphite or graphene via covalent chemistry. It will be demonstrated how in addition to bottom-up strategies that in addition to control on the density and layer thickness also provide submicron to nanoscale nanostructuring, also top-down nanolithography can be used to nanostructure such covalently modified surfaces.

A third approach does not focus on the functionalization of the surface, but uses the surface as a support for the in-plane covalent stitching of molecules, leading to the formation of on-surface 2D polymers.

Advanced interface specific methods such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM) provide, at the liquid-solid interface, structural, dynamic, and other types of information, at the nanoscopic level.

Figure: Combined nanolithographic, covalent and non-covalent functionalization

Quantum Materials by design

Zeila Zanolli
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Major advances in human civilization are driven by developments in materials. This is such a remarkable feature that historical eras are named after the material (and the related technology) that dominated that time. Today we live in the silicon era: Silicon technology enables our modern way of life via mobile phones, computers, automation. However, we are reaching the limits of silicon technology, as the related energy demand is not sustainable. It is time to move forward. As a scientist, we work to answer the question: what is the material that will enable the next revolution?

In this talk, I will present my personal perspective to answer this general question. Using the predictive power of first-principles techniques, I will show that a possible way forward is to design new materials, exploiting the quantum effects emerging at reduced dimensionality and at interfaces. By looking at the intersection of topological materials, interfaces, and spin-based electronics, we will see that it is possible to understand and, hence, control key parameters for next-generation devices as spin injection [1], topological (dissipationless) carrier transport [2] or spin lifetime [3] in 2D layered materials.

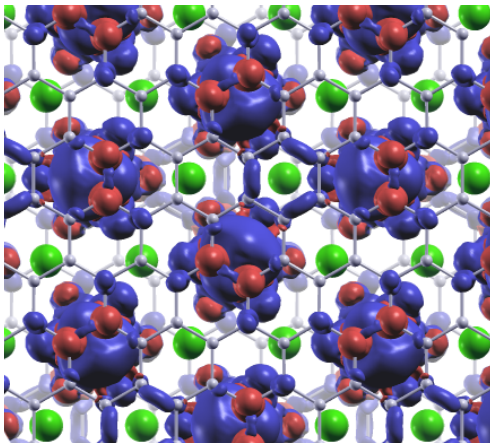

Figure 1. Spin density induced in non-magnetic graphene by proximity interaction with a magnetic substrate

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Dr. Ulrike Kauscher Pinto,

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Diversity, Equity and Inclusion in Scientific Publishing

Dr. Josef Krumpfer

As the scientific community continues to grow and change to meet and solve the increasingly complex demands facing our global society, so too must scientific publishers strive to create an ever inclusive research ecosystem for our diverse group of readers, authors and reviewers. Across the last several years, a great number of initiatives have begun to intentionally and proactively reflect our values and the values of our communities in our day-to-day work internally, with our partners, and with our publishing practices. This talk gives an overview of the efforts towards greater diversity, equity and inclusion across all scientific publishers, as well as recent progress and policies made through Wiley's Research DEI team.