O 33: Graphene: Growth, structure and substrate interaction (joint session O/HL)

Time: Tuesday 10:30–12:30 Location: HSZ/0201

Invited Talk O 33.1 Tue 10:30 HSZ/0201
During-synthesis functionalization of graphene layers — •Cristina Africh — CNR-IOM, Trieste, Italy

Introducing heteroatoms into graphene is a powerful way to modulate its catalytic, electronic, and magnetic properties. During the last decade, we developed a clean and scalable functionalization strategy that exploits the sponge-like properties of nickel substrates as well as the catalytic role played by transition metal (TM) single atoms at graphene edges during Chemical Vapor Deposition synthesis [1]. Following this route, it is possible to grow N-doped, B-doped and TM-doped graphene as well as co-doped layers [2,3,4]. The potential of the functionalized networks for sensing and, as a perspective, for catalysis, was evaluated by monitoring their response upon gas exposure [5,6].

[1] C. Africh, M. Peressi and G. Comelli, Surf. Sci. 753, 122652 (2025). [2] S. Fiori et al., Carbon 171, 704-710 (2021). [3] S. Patil et al., Surf. Interfaces 51, 104700 (2024). [4] V. Chesnyak et al., Sci. Adv. 10, eado8956 (2024). [5] D. Perilli, S. Fiori et al., J. Phys. Chem. Lett. 11 8887-8892 (2020). [6] D. Perilli, V. Chesnyak et al., Angew. Chem. Int. Ed. 64, e202421757 (2025).

O 33.2 Tue 11:00 HSZ/0201
Heterotriangulene Kagome Graphene Films: Growth and Effect of Kinetic Reaction Parameters — •Wyatt Behn[1], Simon Briesenick[1], Chang Wan Kang[2], Manuel González-Lastre[3], Pablo Pou[3], Rubén Pérez[3], Dmytro Perepichka[2], and Peter Grutter[1] — [1]Dept. of Physics, McGill — [2]Dept. of Chemistry, McGill — [3]Universidad Autónoma de Madrid

Nanoporous graphenes featuring Kagome lattices formed by heterotriangulene units continue to attract interest for their correlated electronic properties. Their symmetry gives rise to flat bands and Dirac cones [1,2]. Covalent organic frameworks (COFs) like these are often synthesized by surface-assisted Ullmann coupling, and are susceptible to defects such as voids, irregular-sided linkages, and limited grain sizes of around 100 nm [3,4]. We perform a series of polymerizations over a range of sample temperatures (180-250 C) for tribromo- and triiodotrioxaazatriangulene precursors on the Au(111) surface. Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) we interrogate how deposition conditions and choice of halogen affect the final polymer film quality, which we quantify using minimum spanning tree and persistent homology approaches. We also investigate the prevalence of halogenated edge terminations and of undesired organometallic intermediates. Experimental results are complemented by simulated STM and nc-AFM analyses. [1] C. Steiner, et al. Nat. Commun. 8, 14765 (2017). [2] G. Galeotti, et al. Nat. Mater. 19 (2020). [3] M. Lackinger, Chem. Commun. 53 7872 (2017). [4] T. Qin, et al. Commun. Chem. 7 154 (2024).

O 33.3 Tue 11:15 HSZ/0201
Defect-Driven Formation of Distinct 2D-Ag Phases at the Graphene/SiC Interface — •Sawani Datta[1], Boyang Zheng[2], Arpit Jain[2], Vibha Reddy[1], Kathrin Küster[1], Joshua A. Robinson[2], Vincent H. Crespi[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalation of two-dimensional (2D) materials at the graphene/SiC interface is important for improving environmental stability of the intercalant and tuning graphene's electronic properties. However, the underlying mechanisms remain complex and are still not fully understood. In this study, we show that by modifying the intercalation process, specifically through defect engineering, it is possible to selectively stabilize two distinct phases of intercalated silver (Ag). The previously established phase (Ag_1) aligns with nearly (1×1) registry of SiC [1, 2], while the second phase (Ag_2) develops a denser $(3\sqrt{3}\times3\sqrt{3})R30^\circ$ superstructure on a (5×5) SiC unit cell, producing a 6.25×6.25 Moiré pattern with respect to graphene, as seen in the low energy diffraction (LEED) pattern [2]. Angle-resolved photoemission spectroscopy (ARPES) reveals a striking kaleidoscopic modulation of the Ag_2 and graphene bands, absent in Ag_1, along with notable differences in charge transfer between the two phases. These results demonstrate that defect-controlled, phase-selective intercalation offers a promising pathway to design and explore exotic 2D electronic states at graphene/SiC interfaces. [1] PRB 101, 201407(R) (2020). [2] arXiv:2511.07151v1 (2025).

O 33.4 Tue 11:30 HSZ/0201
Strain-Induced 2D Pb phases confined between graphene and SiC — •Sergii Sologub[1,2], Markus Gruschwitz[1], Zamin Mamiev[1], Chitran Ghosal[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The intercalation of metals beneath graphene offers a powerful route to stabilizing and protecting novel 2D phases. We performed a detailed intercalation study of Pb beneath the ZLG on SiC(0001) using low-energy electron diffraction (at the temperatures from 70 to 600° C) as well as scanning electron and tunneling microscopy [1]. Our analysis reveals the formation of different 2D Pb monolayer phases, such as stripes and hexagons, which emerge due to the interplay between substrate pinning and strain within the Pb layer, depending on local coverage. The interface reconstruction of Pb was shown can be tuned by varying the details of the intercalation protocol. Based on our experiments combined with recent simulations [2], an intercalation model, accounting for the different periodicities observed in the interface layer, was proposed. These findings provide new insights into the strain-driven stabilization of intercalated metal layers and highlight the potential of graphene as a versatile platform for engineering low-dimensional materials.

[1] Adv. Mater. Interfaces 12, no. 21: e00617 (2025); [2] Appl. Surf. Sci. 681, 161572 (2025).

O 33.5 Tue 11:45 HSZ/0201
Strain engineering in graphene on Ru(0001) — Paula García-Mochales[1] and •Antonio J. Martínez-Galera[1,2,3] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

The ability to induce and characterize strain in the atomic lattice of 2D materials, localized within only a few nanometers around specific positions, is a major challenge for the development of straintronics. In this work, the interaction between Si nanoparticles and the surface of graphene/Ru(0001) is employed to induce local strain in the latter. The strain field has been mapped at the nanoscale by scanning tunneling microscopy (STM), using the moiré pattern intrinsic to graphene/Ru(0001) surfaces as a magnifying lens. The induced strain is found to be confined within only a few nanometers around each nanoparticle. To achieve more accurate control, strain engineering at the nanometer scale was successfully performed by manipulating nanoparticles through the STM tip. This approach to controlled strain could provide a key tool for exploring new physics arising by strain in 2D materials.

Reference:

P. García-Mochales and A. J. Martínez-Galera, Nano Lett. 25, 16097-16103 (2025).

O 33.6 Tue 12:00 HSZ/0201
Subsurface carbon controls graphene growth on Ir(111) — •Smruti Ranjan Mohanty, Lothar Brendel, Marko Kriegel, Niels Ganser, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

The CVD growth of 2D materials is governed by a balance between adsorption, surface diffusion, and nucleation. For transition metal substrates, dissolution into the bulk acts as an additional parameter. By employing in-operando low-energy electron microscopy (LEEM) to monitor graphene growth on Ir(111), the effect of the growth temperature and the precursor pressure on the nucleation behavior is studied. The island nucleation density exhibits two distinct regimes, described as separate cases within Venables nucleation theory [1]. For a critical nucleus size $i^* = 5$, low dosing pressures yield a low nucleation density that is governed by incomplete condensation with a scaling exponent of 2.5. At higher-dosing pressures, adsorptions at island edges dominate over the adatoms loss into the substrate, resulting in a higher nucleation density and a strongly reduced scaling exponent. Kinetic Monte Carlo simulations that incorporate bulk dissolution reveal both nucleation regimes and find a universal, temperature-independent scaling law. The results indicate a universal nucleation behavior for 2D materials with finite, non-negligible solubility in the supporting metal substrate.

[1] J A Venables et al 1984 Rep. Prog. Phys. 47 399

O 33.7 Tue 12:15 HSZ/0201

Thermodynamics of heteroatom-doped graphene: Brute forcing the partition function — •Lukas Hörmann[1,2], Benedict Saunders[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, United Kingdom — [2]University of Vienna, Austria

The introduction of dopants into graphene can be used to tune material properties for specific applications, such as electronics, sensors, or catalysis. Achieving such tunability requires precise control over the composition and concentration of dopants within the lattice. This demands a fundamental understanding of the thermodynamics that govern the phase space of heteroatom superstructures in the two-dimensional graphene framework. We present a comprehensive approach to determining dopant structures that enables the near-exhaustive enumeration of all relevant heteroatom superstructures. The approach combines Density Functional Theory and machine learning to build a transferable energy model for dopant formation. Our method's efficient data handling and fast inference enable the evaluation of more than 150 million possible structures, allowing us to effectively brute force the partition function and derive all thermodynamic properties from it. We show the capabilities of our approach for free-standing graphene doped with nitrogen atoms, establishing a thermodynamic model to investigate how temperature affects the configuration space of doped graphene. Our analysis yields physical insights into defect interactions. We observe a characteristic peak in the heat capacity, indicating an order-to-disorder transition, and present a mechanistic understanding of how this peak arises.