O 28: Graphene: Electronic Structure and Excitations (joint session O/HL)

Time: Tuesday 10:30–12:15 Location: H6

O 28.1 Tue 10:30 H6

Doping of epitaxial graphene by proximitized 2D quantum islands — •Julian Koch[1], Sergii Sologub[1,2], Chitran Ghosal[1], Dorothee Boesler[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The effects of 2D quantum islands on the transport properties of monolayer graphene/SiC(0001) were investigated by magnetotransport. Two types of adsorbates are compared, Bi(110) and Pb(111) islands with average coverages of up to 3.6 bilayers (BL) and 3 monolayers (ML), respectively. The analysis is supported by structural investigations using SPA-LEED and STM. The doping behaviour of both materials is fundamentally different. In the case of Bi, the carrier concentration determined from the SdH oscillations remains at 1×10^{13} cm^{-2} independent of the Bi coverage, although photoemission spectroscopy revealed a strong doping of the graphene by Bi [1]. This strongly indicates a highly anisotropic carrier concentration across the surface and is confirmed by a positive, temperature independent contribution to the magnetoresistivity. The Bi islands rather behave as antidots and reduce the charge carrier mobility slightly from around 2250 cm^2/(Vs) for MLG to 1920 cm^2/(Vs) at 2.4 BL Bi. In contrast, there are no signs of an anisotropic carrier concentration or mobility when Pb is adsorbed. The electron concentration increases uniformly by approximately 5×10^{11} ML^{-1}cm^{-2}. The mobility is reduced from around 1400 cm^2/(Vs) for MLG to 1200 cm^2/(Vs) at 3 ML Pb.

[1] Gierz et al. *Nano Lett.* **8**, 12, 4603 (2008)

O 28.2 Tue 10:45 H6

Photocurrent control in a graphene-based Floquet topological insulator — •Weizhe Li[1], Daniel Lesko[1], Tobias Weitz[1], Simon Wittigschlager[1], Christian Heide[1,2], Ofer Neufeld[3], and Peter Hommelhoff[1,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel — [4]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Topological insulators offer unique opportunities for novel electronics and quantum phenomena. However, intrinsic material limitations often restrict their applications and practical implementation. A circularly-polarized laser pusle can generate topologically non-trivial non-equilibrium states known as Floquet topological insulators (FTIs) which host a variety of topological phenomena. Floquet engineering with strong optical fields opens routes to optically tunable band structures and devices for petahertz electronics.

Here we demonstrate coherent control of photocurrents in light-dressed graphene. Circularly-polarized laser pulses dress the graphene into an FTI, and phase-locked second harmonic pulses drive electrons in the FTI. This approach allows us to measure all-optical anomalous Hall currents and photocurrent circular dichroism, which put FTIs on equal footing with equilibrium topological insulators. The coherent control of photocurrents in graphene-based FTI connects optics tools to condensed matter physics.

O 28.3 Tue 11:00 H6

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], Philip Schädlich[1], Bharti Matta[3], Philipp Rosenzweig[3], Kathrin Küster[3], Ulrich Starke[3], Thomas Seyller[1], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Two-dimensional materials such as graphene are fascinating because they combine unique mechanical and electronic properties. The next level of complexity, however, comprises the assembly of various stacked 2D materials to generate structures with desired properties. Intercalation of epitaxial graphene systems is an effective method to tailor the electronic, optical, and transport properties of graphene while keeping its honeycomb lattice on SiC. Furthermore, intercalation facilitates the synthesis of otherwise unstable 2D layers. A wide range of elements have been used as intercalants below a graphene sheet, forming often well-defined heterobilayers with different functionalities. In particular, intercalation of heavy elements such as Pb and Bi are specially promising since they can introduce additional effects such as spin-orbit coupling to the electron gas of graphene and Rashba spin polarization. Using first-principles methods, we investigate the modifications in the electronic structure of epitaxial graphene due to proximity effects induced by intercalation.

O 28.4 Tue 11:15 H6

Accelerated Exploration of Defective Graphene Superstructures — •Benedict Saunders[1], Lukas Hörmann[1,2], and Reinhard Maurer[1,2] — [1]Department of Chemistry, University of Warwick, Coventry — [2]Department of Physics, University of Warwick, Coventry

Graphene has been meticulously studied due to its remarkable mechanical, electrical, and thermal properties. It is well documented that introducing various dopants and defects to the lattice can be used to tune the material's properties for a specific application, such as in electronics, sensors, or catalysis. In order to design graphene with specific properties, one must achieve precise control over the composition and concentration of defects. This requires a fundamental understanding of the stability of defects and their interaction in a given superstructure. We present a comprehensive method for exploring the configurational space of defective 2D superstructures. We have extended the SAMPLE structure search code to defects in 2D materials. SAMPLE uses Bayesian learning based on sparse Density Functional Theory data for structure exploration. We show the capabilities of our approach for a proof-of-principle application on free-standing graphene with heteroatom defects. Finally, we use the SAMPLE code to gain physical insight into the interactions between these defects, paving the way for effective and rational growth models of topologically designed defective graphene.

O 28.5 Tue 11:30 H6

Polymorphism of a two-dimensional Pb layer underneath charge neutral graphene on SiC — •Markus Gruschwitz, Sergii Sologub, Zamin Mamiyev, Chitran Ghosal, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Germany

Since the first studies on graphene, researchers strive to implement its unique properties in industrial relevant processes. The intercalation of epitaxially grown buffer layers on SiC results in high quality, quasi-freestanding graphene, which allows the electronic properties to be modified by varying the intercalants and their arrangement. Pb recently sparked a great interest by reliably providing almost perfectly charge neutral graphene. The Pb layer effectively screens the substrate induced doping. In a novel approach using differential phase contrast in cross-sectional scanning transmission electron microscopy we reveal their vertical charge density distribution. Surprisingly, the charge neutrality is robust against variations in the Pb interface reconstruction. Depending on the preparation, a Pb monolayer often reconstructed in two coexisting phases, the so-called stripe [1] or bubble [2] phase. Intercalated multilayers reveal a similar striped phase arising from two twisted plumbene layers [3]. Here we combine structural investigations by scanning tunneling microscopy and high-resolution low-energy electron diffraction in a model of flexibly arranged grain boundaries releasing lattice mismatch stress.

[1] Materials 14, 7706 (2021), [2] Adv. Mater. Interfaces 10, 2300471 (2023), [3] Phys. Rev. Lett. 129, 116802 (2022)

O 28.6 Tue 11:45 H6

Facet-dependent growth and properties of graphene on Al_2O_3 surfaces from first principles — •Armin Sahinovic and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The direct growth of graphene on functional substrates such as sapphire (Al_2O_3) enables the use in optoelectronic devices without the necessity of sample transfer. We explore the role of the surface orientation of Al_2O_3 on the growth of graphene [1] using density functional theory. The stoichiometric terminations are identified as the most stable surface terminations of the C-, R- and A-plane facets in the framework of *ab initio* thermodynamics. Next, we consider the adsorption of carbon atoms on the different surface facets, varying their position and concentration. The adsorption energy shows the weakest binding

at the R-plane and the most favorable at the A-plane. We associate this with the more unsaturated oxygen bonds at the A-plane compared to the R- and C-plane. Furthermore, we explore the graphene - Al_2O_3 interaction and its impact on the electronic properties of graphene. Our results provide a deeper understanding of the role of the surface facets of the substrate in the scalable graphene growth on Al_2O_3.

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[1] Y. Ueda et al., Appl. Phys. Lett. 1, 115 (1), 013103 (2019)

O 28.7 Tue 12:00 H6

Enhanced light-matter interactions via Sn nanoislands on epitaxial graphene — •Zamin Mamiyev, Narmina Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Surface-enhanced Raman scattering (SERS) is an advanced technique for coupling light into quasiparticle excitations in low-dimensional materials, offering promising applications in trace detection, enhanced light-matter interactions, photonic energy harvesting, and catalytic processes. Recent studies in this field have focused on integrating noble metal nanostructures with graphene.

In this study, we investigate a novel SERS platform utilizing tin (Sn) nanoislands to enhance graphene Raman signals by up to two orders of magnitude. We examine the SERS performance on Sn-intercalated charge-neutral and intrinsically doped epitaxial monolayer graphene (MLG) on SiC(0001). The increase in the Raman cross-section and enhanced intensity is accompanied by spectral shifts, which may be correlated with the localized surface plasmons (LSPs) of Sn nanoislands as well as dynamic charge transfer between the Sn particles and graphene. This dynamic charge redistribution, primarily determined by the doping concentration and interface interactions, enables control over the SERS response. Additionally, plasmonic and thermalization-induced carrier density propagation across μm ranges indicates efficient coupling between localized and propagating plasmons.

[1] Z. Mamiyev and C. Tegenkamp, 2D Materials. 11, 025013 (2024)
[2] Z. Mamiyev and C. Tegenkamp, Surf. & Int. 34, 102304 (2022)