Hybrid Inorganic/Organic Systems for Opto-Electronics

Collaborative Research Centre 951

Colloquium Announcement

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"Hybrid Inorganic/Organic Systems for Opto-Electronics"

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Proximity coupling in epitaxial graphene on SiC(0001) by intercalation: Doping, strong correlation, interface electronic structure

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Electronic structure of hybrid materials: some dilemma and some solutions

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Proximity coupling in epitaxial graphene on SiC(0001) by intercalation: Doping, strong correlation, interface electronic structure

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Wafer scale epitaxial graphene (EG) grown on Silicon Carbide (SiC) is regarded as a suitable candidate for carbon based electronics. Homogeneous graphene layers can be prepared with atomic thickness definition on a wafer scale. The functionalization of the graphene/SiC interface on an atomic scale enables tuning of the electronic and structural properties of the graphene layer.

Intercalation under the first carbon layer relieves its covalent bonds to the SiC(0001) substrate and the π-band structure can be manipulated in a large range of aspects [1]. In addition, the structure of the intercalated layer can be precisely defined. Au intercalation generates a highly ordered graphene/intercalant/substrate system with many-body interactions renormalizing the graphene bands. A sharp 2D band structure can be resolved for the gold layer [2]. By varying the Au thickness a semiconductor to metal transition is induced in the interface layer. By proximity coupling, the dielectric constant of the graphene layer is tuned. High doping regimes can be reached by the intercalation of rare earth elements, such as Gd or Yb. As a result, the Van-Hove singularity (VHS) of the π*-bands reaches the Fermi level. The doping is accompanied by a strong bending of the bands at E_F, which is attributed to strong electron-electron interaction [3]. By a combination of Yb intercalation and K adsorption, the EG layer can be n-doped even past the VHS. Thereby a Lifshitz transition is completed, where the Fermi surface topology changes from two electron pockets into a giant hole pocket [4]. Crossing the VHS in this way allows access to potential exotic phases where unconventional superconductivity or charge and spin density waves are predicted.

By starting with a patterned SiC surface with mesas and trenches of 200 nm periodicity, EG nanoribbons (GNRs) can be grown on the mesa facets. High-resolution ARPES demonstrates the 1-dimensional behaviour of graphene on these facets: while the whole facet has a width of about 40nm, it contains an array of mini-GNRs (≈ 2 nm wide) separated by nano-basal stripes. The subbands of these mini-ribbons reveal a sharp distribution of ribbon widths of around 18 dimers [5]. On the mesas, a conventional graphene buffer layer develops. By H-intercalation, both graphene types, on mesa and facet, are decoupled and transform into a single two-dimensional graphene sheet rolling over the mesa structures. Due to the different surface terminations of the basal and vicinal SiC surfaces, different types of charge carriers are locally induced into the graphene layer leading to two symmetrically n- and p-doped phases. Thus a regular array of of graphene pn-junctions develops [6].

Recently we have started to grow highly ordered epitaxial layers of transition metal dichalcogenides (TMD) on high-quality large-scale graphene substrates grown epitaxially on SiC. The good epitaxial order allows to assess in high resolution the electronic properties of the TMD layers and elucidate e.g. precise values of spin-orbit splitting, doping and band alignment in WS_2 and WSe_2 [7,8].

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Electronic structure of hybrid materials: some dilemma and some solutions

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Organic/inorganic hybrid systems are fascinating materials as various interactions may happen on the same energy scale. With the examples of pyrene and pyridine on MoS_2, we show that predicting the level alignment at the interface is challenging as in both cases semi-local density-functional theory (DFT) finds type-II alignment that changes to type I when including dynamical screening effects [1]. Hybrid metal halide perovskites (HaPs) are other critical examples, being governed by the interplay between strong electron-electron interaction and spin-orbit coupling (SOC). By assessing various methodologies for computing their electronic structure, comprising DFT and many-body perturbation theory (MBPT), we demonstrate the difficulties of finding a trustworthy quantitative approach [2] that allows for comparison with experiments.

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