Hybrid Inorganic/Organic Systems for Opto-Electronics

Collaborative Research Centre 951

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Colloquium Announcement

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"Hybrid Inorganic/Organic Systems for Opto-Electronics"

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Hybrid Systems of 2D Materials and Organic Adlayers: Interface Properties and Challenges in Fabricating Ordered Films

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Weak and strong coupling in heterostructures with 2D semiconductors

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Hybrid Systems of 2D Materials and Organic Adlayers: Interface Properties and Challenges in Fabricating Ordered Films

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Hybrid systems of two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) and organic semiconductors (OSCs) have become a subject of great interest for future device architectures. This is because OSCs offer high optical absorption efficiency and easy tuning of their electronic properties through synthesis, while TMDs generally exhibit higher charge carrier mobility, making such hybrid systems particularly advantageous for optoelectronic applications [1,2]. Since optoelectronic properties of molecular films depend sensitively on their packing and orientation, it is of vital interest to control the microstructure of such hybrid systems – especially at the interface. Using the example of the prototypical acenes - especially pentacene (PEN) and perfluopropentacene (PFP) - I will discuss various aspects of the structure and formation of acene films grown on various 2D materials including TMDs, graphene and *h*BN. As the molecular adlayers are only weakly bound (essentially physisorbed) on the 2D materials, the mutual molecular interaction and the influence of surface defects become more important and eventually determine the film structure [3]. This seems to be particularly important for exfoliated flakes, where organic films reveal rather different growth behavior on mono- and multilayers due to defect steps and/or substrate waviness, which may require additional smoothing [4]. While sufficiently large single crystals allow in-plane X-ray diffraction for detailed structural analysis and characterization of the azimuthal film alignment, this is not possible for small flakes. Here, optical reflection anisotropy provides an easy but powerful tool to characterize the azimuthal film alignment [5].
Freshly exfoliated 2D material single crystals are best suited to investigate the film orientation and intrinsic interface structure in detail. A corresponding analysis for PFP films on different 2D substrates shows a true van der Waals epitaxy. This film order can be rationalized as an on-line epitaxy and exhibits characteristic twisting angles for each substrate. Interestingly, attempts to also prepare highly ordered monolayer films of PEN and PFP fail owing to the repulsive electrostatic interaction of the planar adsorbed molecules. While unitary films form a gas-like monolayer that prevents the condensation even at 100K, multilayers as well as mixed monolayers of PEN and PFP are stable [6]. In contrast, unilaterally fluorinated pentacene derivatives (such as F_6PEN [7]) can achieve electrostatic self-stabilization, which forms stable islands on MoS_2 even at room temperature. Interestingly, the shape of sub-monolayer islands depends on the preparations and differs if a sub-monolayer coverage is deposited or after partial desorption of a full monolayer, thereby allowing shape control of molecular nanosheets through the kinetics of their formation [8].

[1] Y. L. Huang, et al. *Chem. Soc. Rev*. **47**, 3241 (2018).
[2] S. Bertolazzi et al. *Chem. Soc. Rev.* **47**, 6845 (2018).
[3] T. Breuer et al. *Phys. Stat. Sol. RRL* **10**, 905 (2016).
[4] D. Günder et al. *ACS Appl. Mater. Interfaces* **12**, 38757 (2020).
[5] M. Dreher et al. *Chem. Mater*. **32**, 9034 (2020).
[6] S. R. Kachel et al. *Chem. Sci*. **12**, 2575 (2021).
[7] P. E. Hofmann, et al. *Angew. Chem. Int. Ed.* **59**, 16501-16505 (2020).
[8] M. Dreher et al. *Nat. Comm*. **14**, 1554 (2023).

Weak and strong coupling in heterostructures with 2D semiconductors

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Via integration of 2D semiconductors, such as transition metal dichalcogenides (TMDC) in heterostructures synergy effects are expected to arise from the coupling of the excitons in monolayer (1L) TMDCs with the excitations of a different material. In the talk I will present two examples: (1) strong coupling of 1L-WS_2 excitons with surface plasmon polaritons (SPP) propagating in a thin silver film and (2) weak coupling of 1L-WS_2 excitons with excitons in an organic dye layer. The benefits arising from the coupling will be discussed.