Molecules on 2D Templates: Interface Characterization and On-Surface Reactions

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Two-dimensional (2D) epitaxial materials including hexagonal boron nitride (*h*BN) are frequently employed as templates for self-assembled molecular films and nanostructures, opening perspectives both to tune molecular properties and to modify 2D sheets and interfaces [1]. A quantitative structural characterization of the respective interfaces and adsorbate geometries however is largely missing. After reviewing some examples of molecular self-assembly on metal-supported *h*BN monolayers, I will report on the geometric and electronic structure of a prototypical organic/insulator/metal interface, namely tetrapyrroles on *h*BN/Cu(111), investigated by combining X-ray photoelectron spectroscopy, X-ray standing waves, and scanning tunneling microscopy (STM) [2]. The gating and charge state control by the template, the STM tip, and the molecular environment will also be discussed (see Fig. 1). In a second part of my presentation, I address on-surface chemical reactions that are operational on *h*BN/Cu(111), covering the formation of polycyclic aromatic chains via intermolecular cyclization as well as the synthesis of actinide- and lanthanide-complexes [3].

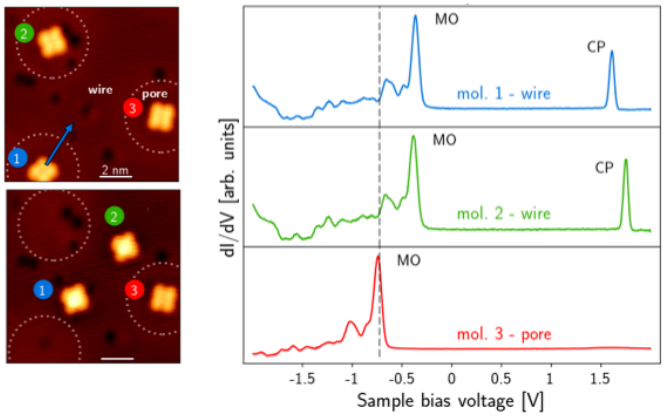

Fig. 1: STM images of F_{16}CoPc molecules on *h*BN/Cu(111) before (top left) and after manipulation (bottom left) with spectroscopic signatures (right panel) showing features related to molecular orbitals (MO) and charging (CP).

References:

[1] W. Auwärter, "Hexagonal boron nitride monolayers on metal supports: Versatile templates for atoms, molecules and nanostructures", *Surf. Sci. Rep.,* 74, 1, (2019), pp. 1-95.
[2] M. Schwarz *et al.*, "Quantitative Determination of a Model Organic/Insulator/Metal Interface Structure", *Nanoscale,* 10, 41, (2018), pp. 21971-21977.
[3] D. Ecija *et al.*, "Lanthanide-Directed Assembly of Interfacial Coordination Architectures – From Complex Networks to Functional Nanosystems", *Acc. Chem. Res.,* 51, 2, (2018), pp. 365-375.