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

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Two-dimensional (2D) epitaxial materials including hexagonal boron nitride (hBN) 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 hBN monolayers, I will report on the geometric and electronic structure of a prototypical organic/insulator/metal interface, namely tetrapyrroles on hBN/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 hBN/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 hBN/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: