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ABSTRACT:

Surface Functionalization: Organic Materials/Substrate Interactions Studied by Soft X-Ray Absorption and Core-Level Photoemission Spectroscopies

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The development of organic electronics relies strongly on the functionalization of surfaces. In general, two main categories of functionalization are distinguished: chemisorption and physisorption. Chemisorption leads to the formation of new covalent bonds between molecules and the substrate, whereas physisorption primarily involves π -conjugated systems exhibiting weaker interactions. A key interest of π -conjugated molecules lies in their ability to self-organize on metal surfaces. Molecular self-assembly results from a subtle balance between intermolecular interactions (such as hydrogen or halogen bonding) and molecule–surface interactions (including Pauli repulsion and van der Waals forces). Depending on this balance, the resulting molecular architectures can range from compact, densely packed layers to well-defined 2D porous nanostructures. These variations in surface organization greatly influence the electronic and chemical properties of the resulting nanomaterials. However, due to their nanometric dimensions, probing the electronic properties of surfaces and interfaces in such systems remains challenging.

High-resolution photoemission spectroscopy (HRPES) is a powerful technique for investigating the electronic and chemical properties of materials with high surface sensitivity [1]. Near-edge X-ray absorption fine-structure spectroscopy (NEXAFS), sensitive to the chemical environment and the orientation of molecular orbitals, enables the determination of adsorption geometries at surfaces [2]. Time-resolved photoemission spectroscopy (TRPES), performed under pulsed-laser excitation, makes it possible to determine doping type [3], measure charge-carrier lifetimes, and reveal interfacial charge-transfer processes at electrode/colloidal-nanocrystal interfaces. Using synchrotron radiation and tuning the photon energy, the combined use of HRPES, TRPES, and NEXAFS provides a comprehensive approach to elucidate molecule–substrate interactions and to probe complex interfaces in hybrid materials at the nanometric scale.

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