DEPARTMENT OF CHEMISTRY AND PHYSICS OF MATERIALS

ANNOUNCEMENT

PARIS LODRON UNIVERSITÄT SALZBURG

Vortragsankündigung

Mittwoch, 29. Jänner 2025, 11.15 Uhr im SR I

Prof. Dr. Laerte L. PATERA

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"Investigating molecular processes at surfaces: from dynamic covalent chemistry to dihydrogen bonding"

Combining structural tunability, chemical stability with a crystalline structure, covalent organic frameworks (COFs) are promising material platforms for a wide range of applications in (photo-) catalysis. Two-dimensional COFs, composed of a single atomic layer, exhibit peculiar opto-electronic properties, making them suitable platforms for light-induced up-conversion of chemicals. However, despite the growing interest in such 2D polymers, their synthesis is still a major challenge. A proposed approach relies on dynamic covalent chemistry, where the chemical equilibrium is tuned to enable reversible bond formation, allowing the polymer networks to overcome kinetic limitations and reach the crystalline configuration. Here, I will describe the application of near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) to elucidate the reversible formation of a two-dimensional boroxine framework. By controlling the water partial pressure and the sample temperature, the chemical equilibrium can be tuned, leading to the formation or dissolution of the framework.

In the second part of the talk, I will focus on the characterization of dihydrogen bonding (DHB). This represents a peculiar intermolecular interaction, arising from hydrogen atoms acting as both proton acceptors and donors. Despite its significance, the manifestation of DHB in molecular assemblies on surfaces has remained elusive. Here, I will present evidence of DHB within borazine assemblies on Au(111) surfaces. By means low-temperature scanning tunneling microscopy (LT-STM), distinct configurations have been unveiled, exhibiting single and double DHB motifs. Complementary density functional theory (DFT) calculations shed light on the delicate interplay between substrate adsorption and intermolecular interactions, elucidating the stabilization mechanisms driving the formation of borazine clusters on Au(111).