In_2O_3(111): Surface Structure and Adsorption of Small Molecules

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Indium oxide, a transparent conductive oxide (TCO), is widely used in semiconductor industry but it also displays promising performance in electro- and photo catalytic reactions. As the interface is central in all these applications, understanding the fundamental properties is critical, especially when going to nanoscopic dimensions in novel device architectures.

As a model system we investigate the non-polar In_2O_3(111) surface[1] experimentally with low temperature scanning tunnelling microscopy and atomic force microscopy (STM, AFM), temperature programmed desorption (TPD) and x-ray photoelectron spectroscopy (XPS), and with density functional theory (DFT) calculations. This talk gives an overview on our current investigations on In_2O_3(111) including the adsorption of water and the interaction with small organic molecules.

In_2O_3(111) has an intrinsically large unit cell composed of a hydrophilic and a hydrophobic area. We test the reactivity of these areas by unravelling the interfacial water structures for the whole range of water coverages in UHV, from single dissociated molecules[2,3] to multilayers. Even at high coverages we clearly see hydrophilicity and hydrophobicity within the unit cell, both in experiments and calculations[4]. Comparison with methanol and acetylene shows common adsorption preferences.

The interaction of conjugated organic molecules with surfaces is of great fundamental interest and important in many applied areas. Surface science investigations have significantly contributed to understand the organics/metal interface, but the second electrode in such devices – the one that is optically transparent – is unknown territory. Our studies aim at closing this gap: Starting with the smallest aromatic molecule, benzene, we expand to more complex organic molecules including phthalocyanines and study the interaction with the In_2O_3(111) surface and the condensation into 2dim structures.

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[2] M. Wagner, et al. Direct assessment of the acidity of individual surface hydroxyls. Nature 592, 722–725 (2021).

[3] M. Wagner, et al. Resolving the Structure of a Well-ordered Hydroxyl Overlayer on In_2O_3(111): Nanomanipulation and Theory. ACS Nano 11, 11531–11541 (2017).

[4] H. Chen et al. A locally hydrophobic oxide surface: In_2O_3(111). ACS Nano, 16, 12, 21163–21173 (2022).