The prototypical organic-oxide interface: Adsorption and monolayer formation of sexiphenyl on In_2O_3(111)

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The interaction of large organic molecules with surfaces is of great fundamental interest and important in many applied areas, most prominently in organic electronics. 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 study closes this gap: This work focuses on the prototypical organic molecule para-sexiphenyl (6P) and the thermodynamically most stable surface of the most-common transparent conducting oxide, indium (tin) oxide, In_2O_3(111).

The onset of nucleation and the formation of the first monolayer are followed with scanning tunnelling microscopy (STM) and constant-height non-contact atomic force microscopy (nc-AFM). We find that the molecules adsorb in a flat lying geometry, adopting the high-symmetry directions of the support. From the adsorption site of the single molecules on the complex oxide surface it is clear that the 6P prefers the interaction with the 5-fold coordinated indium In(5c) atoms, and avoids the oxygen-terminated regions. At higher coverage the molecules reorient into a densely packed first monolayer with a distinct pattern that is also based on the atomic configuration: half the molecules are able to maintain their preference for adsorbing on In(5c) atoms, while the other half are stabilized by molecule-molecule interaction in a less favored adsorption site; in the images this is manifested in white and dark stripes. The structure has a (1×2) symmetry with one 6P per In_2O_3(111) substrate unit cell.