

Substrate configuration effects on large organic molecule adsorption

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ABSTRACT

The role of the configuration of metal surface atoms in the interaction between individual large, planar organic molecules and a metal substrate was investigated by low-temperature scanning tunneling microscopy and density functional theory calculations, including a semi-empirical correction scheme to account for dispersion effects. As test case, we used the adsorption of the oligopyridine derivative 2-phenyl-4,6-bis(6-(pyridine-2-yl)-4-(pyridine-4-yl)pyridine-2-yl)pyrimidine (2,4'-BTP) on a stepped Ag(100) surface. Both experiment, via statistical evaluation of the adsorption site and orientation of 2,4'-BTP ad molecules, and theory indicate distinct structural effects. The results are compared with the adsorption behavior of pyridine derivatives and benzene on metal surfaces. Consequences on the understanding of the interaction between heteroatoms or functional groups in large organic adsorbates and metal atoms in surface defects and hence of the interaction with more realistic metal surfaces are discussed.

Keywords: Adsorption, Adsorption site configuration, Structure, Large organic molecules, Molecule-surface interactions, Scanning tunneling microscopy, Density functional theory, Ag(100)

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