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Hydrogen Bonding Controls the Dynamics of Catechol Adsorbed on a TiO_2(110) Surface ULRIKE DIEBOLD[1], SHAO-CHUN LI, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, USA, LI-NA CHU, XUE-QING GONG, Labs for Advanced Materials, Research Institute of Industrial Catalysis, East China University of Science and Technology, Shanghai, P. R. China — Direct studies of how organic molecules diffuse on metal oxide surfaces can provide insights into catalysis and molecular assembly processes. We studied individual catechol molecules, $C_6H_4(OH)_2$, on a rutile TiO_2(110) surface with scanning tunnelingmicroscopy. Surface hydroxyls enhanced the diffusivity of adsorbed catecholates. The capture and release of a proton caused individual molecules to switch between mobile and immobile states within a measurement period of minutes. Density functional theory calculations showed that the transfer of hydrogen from surface hydroxyls to the molecule and its interaction with surface hydroxyls substantially lowered the activation barrier for rotational motion across the surface. Hydrogen bonding can play an essential role in the initial stages of the dynamics of molecular assembly.

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