



Einladung zum SFB 658-Kolloquium am

Do, 18. Oktober 2012, 16.15 Uhr s.t.

Molecular dynamics at surfaces induced by inelastic electron tunnelling

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Adsorbate motions are the most fundamental steps in surface chemistry. In particular when collisions with other reaction partners or reactive surface sites are required, adsorbate motions are typically the rate-determining steps of a heterogeneously catalyzed reaction. Studying the movement of adsorbates, induced by phonons, photons, or electrons, is therefore of interest. Manipulation of single molecules at surfaces with the scanning tunneling microscope (STM) has been performed for more than a decade. However, the mechanisms of molecular excitation by electrons that inelastically tunnel through the molecule are not entirely understood. We will present results of manipulation experiments performed with single molecules of the hydrocarbon propene on Cu(211). Propene was found in two different adsorbate geometries, both appearing as two distinct enantiomorphs, i.e., in two mirror-configurations. The adsorption geometry has been identified via density-functional theory (DFT). Inelastic electron tunneling (IET) has been applied to excite molecular vibrations in the molecule. Exceeding the threshold energy for certain vibration excitations, we observe different actions of the molecule at the surface. This includes hopping, rotation, inversion of the handedness and dehydrogenation [1-3]. All actions are mode-selective, that is, only certain vibrations cause a certain action. The product of the single molecule chemical reaction has been identified in turn by IET-action spectroscopy, i.e., hopping was observed after excitation of a C-H stretching vibration in the =CH₂ group of the product molecule. Finally, I will present the activation of a chiral molecular rotor by electron attachment that leads to unidirectional rotation. A clever combination of four unidirectional rotors into one molecule leads to unidirectional translation [4].

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[2] M. Parschau, H. J. Hug, K.-H. Rieder, K.-H. Ernst, *Surf. Interface Anal.* 42 (2010) 1629.

[3] M. Parschau, K.-H. Rieder, H. J. Hug, K.-H. Ernst, J. Am. Chem. Soc. 133 (2011) 5689.

[4] T. Kudernac, N. Ruangsapichat, M. Parschau, B. Maciá, N. Katsonis, S. R. Harutyunyan, K.-H. Ernst, B. L. Feringa, Nature 479 (2011) 208

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