Seminář odd. 26
Tenkých vrstev a nanostruktur

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TÉMA

Structure and Dynamics of Functional Molecules on Surfaces

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A fundamental understanding of molecular structure and chemical reactivity at complex interfaces is key to many technological applications ranging from single molecule electronics to hybrid materials. The central aim hereby is to control the function of single molecules in well-defined chemical environments. Using predictive quality Density-Functional Theory simulation, we study prototypical example systems such as azobenzene and porphyrine derivatives adsorbed on single crystal metal surfaces. Hereby the focus lies on the effects of molecule functionalization, substrate reactivity, finitetemperature, and surface coverage on measurable structural and electronic properties of adsorbates. Through detailed discussion of the chemical interactions and thermal fluctuations that govern the adsorbate structure and stability we establish the reliability of our approach in comparison to Temperature Programmed Desorption and X-ray Spectroscopy measurements. On the example of photo-induced isomerization of azobenzene, key. parameters and molecular design principles will be discussed that govern molecular function on metallic surfaces. Finally, the intrinsically non-adiabatic mechanistic details of molecular reactions on metal surfaces are addressed using recently developed excited-state simulation methods.

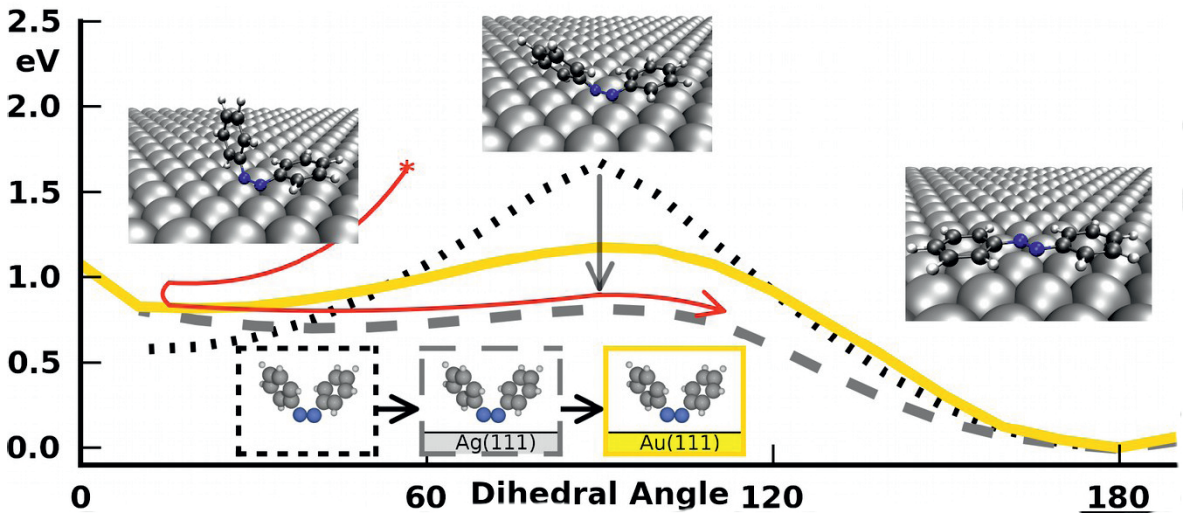

Figure: Loss of molecular bistability is a central reason the behind loss of molecular function for azobenzene isomerization on metal surfaces.

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