STM-experiments on aza-BODIPY

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Abstract

Scanning Tunnelling Microscopy (STM) is a powerful experimental technique in surface science. It combines atomic resolution imaging with the opportunity to perform nanoscale manipulations. Additionally, STM enables the mapping of the density of states of materials. Here we report first experiments on aza-BODIPY adsorbed on metal surfaces with a newly commissioned low-temperature STM/AFM-System. Aza-BODIPY are a class of organic fluorescent dyes characterised by the same molecular core. These molecules exhibit strong chemical stability and highly tuneable, sharp absorption wavelength. Aza-BODIPY has previously been used for immunostaining and photodynamic therapy during the last few years. Recently, electron donor materials for organic photovoltaics (OPVs) has emerged as another field of application, due to aza-BODIPYs strong infrared absorption. In this work single aza-BODIPY molecules adsorbed on Au(111) were investigated by STM at 5 K. The adsorption configuration and geometry were determined and found to be in qualitative agreement with theoretical simulations.

Introduction

Aza-BODIPY
• Class of organic fluorescent dyes
• Characterized by azadipyrromethene boron complex
• 1,3,5,7-tetraphenyl-8-azadipyrromethene
• \[\lambda_{\text{abs}} = 650 \text{ nm in CHCl}_3\]
• \[\lambda_{\text{abs}} \text{ up to } 800 \text{ nm with varying side groups}\]
• B = grey; C = black; F = green; H = blue; N = orange
• Synthesis by Institute for Applied Photophysics, Technische Universität Dresden

Create: LT-STM/AFM system
• 3 chamber UHV system with base pressure of \[5 \times 10^{-11} \text{ mbar}\]
• Operated at 5 K
• Molecular beam epitaxy
• Tuning fork AFM

Imaging

Simulations (Cormac Toher)
• Relaxed state on Au(111) 5 eV lower then unrelaxed
• Molecule flattens on surface
• Various orientations with minor energy differences
• Phenyl groups flatten on surface
• LDOS mainly contributed by C

Experiments
• Constant current mode
• Imaging parameters: \[I = 0.5 \text{ to } 1.2 \times 10^{-11} \text{ A}\]
• \[U = -0.3 \text{ to } -0.7 \text{ V}\]
• Molecule flattens on surface
• Adsorption regardless of herring bone structure
• No distinct surface orientation
• Bright spots correspond to phenyl groups
• No visible features from N or F atoms

Spectroscopy
• Au(111) surface state at \(-510 \text{ meV on blank Au surface}\)
• Additional broad peak at 650 meV on molecule

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• Innovations for funding
• IAPP (TU Dresden) for synthesis

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Preview

3D picture

Manipulation

Lateral Manipulation
• At 5 K on Au(111)
• Parameters: \[I = 4 \text{ nA}; U = -0.4 \text{ V}\]
• Manipulation path influenced by complex molecule
• Manipulation across herring bones

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