

STM-experiments on aza-BODIPY

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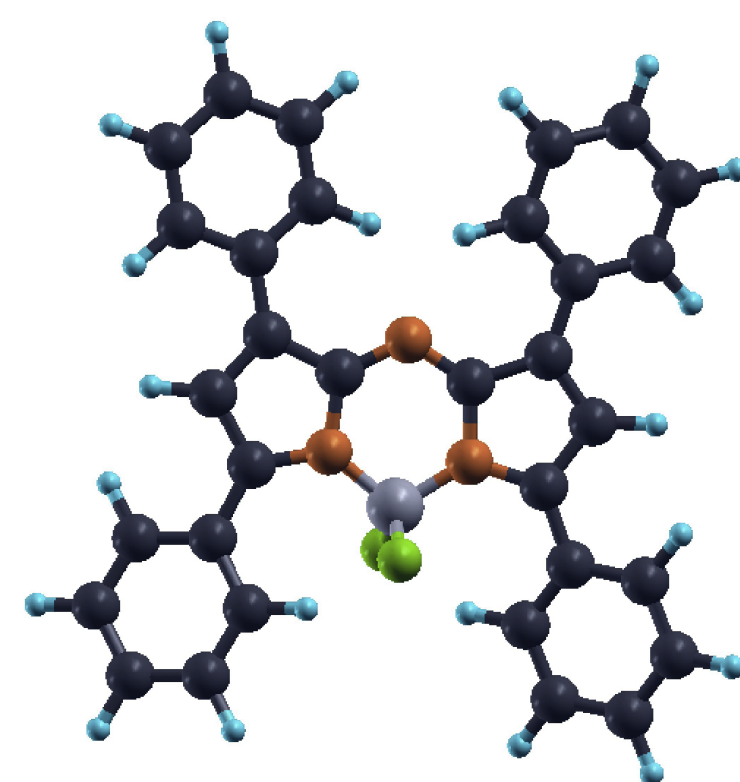
Abstract

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 enable 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

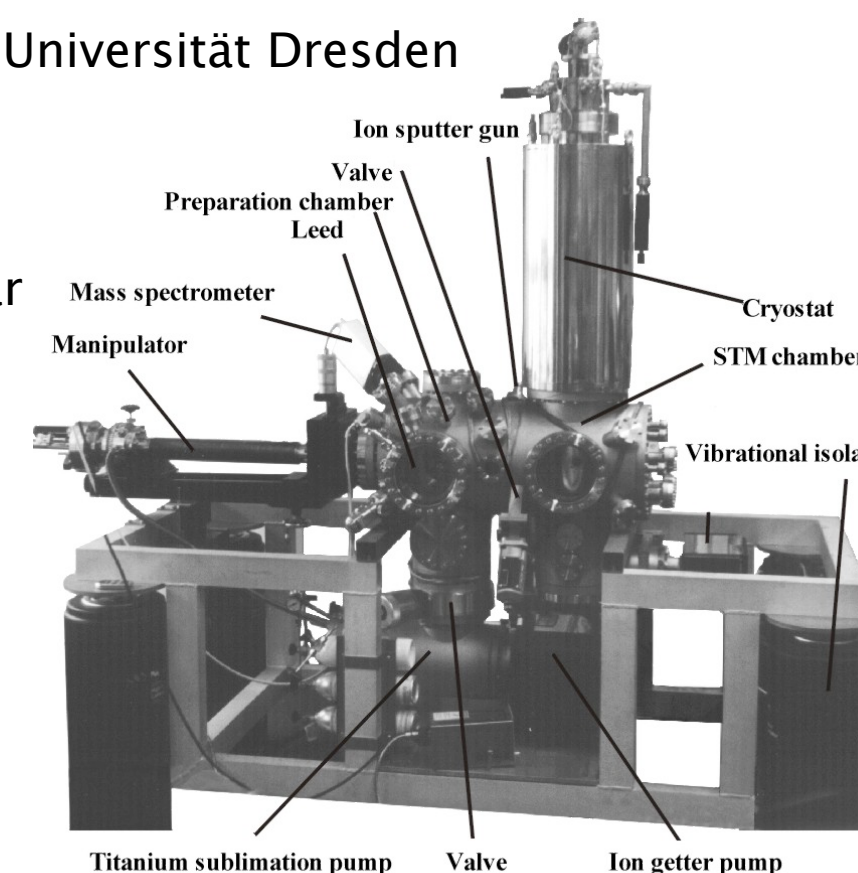
Aza-BODIPY

- 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
- λ_{abs} up to 800 nm with varying side groups
- Currently used in immunostaining, PDT and OPVs
- B = grey; C = black; F = green; H = blue; N = orange
- Synthesis by Institute for Applied Photophysics, Technische Universität Dresden



Createc LT-STM/AFM system

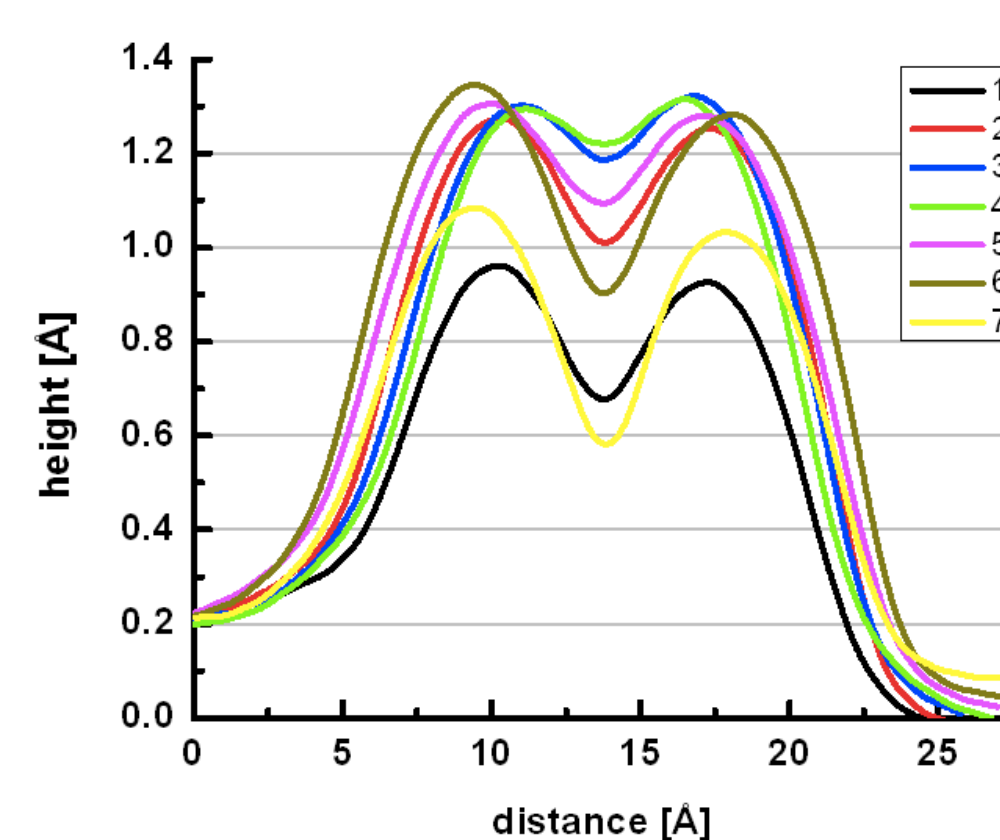
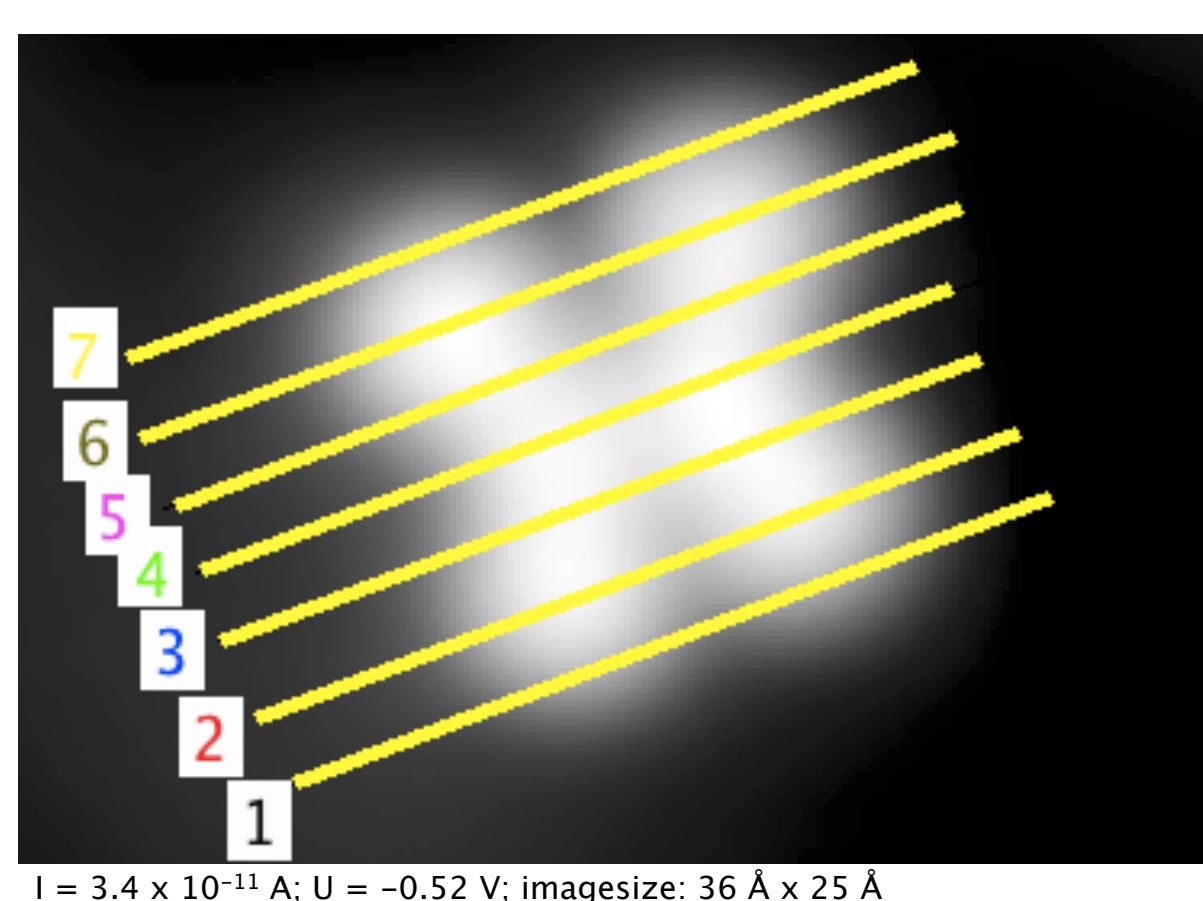
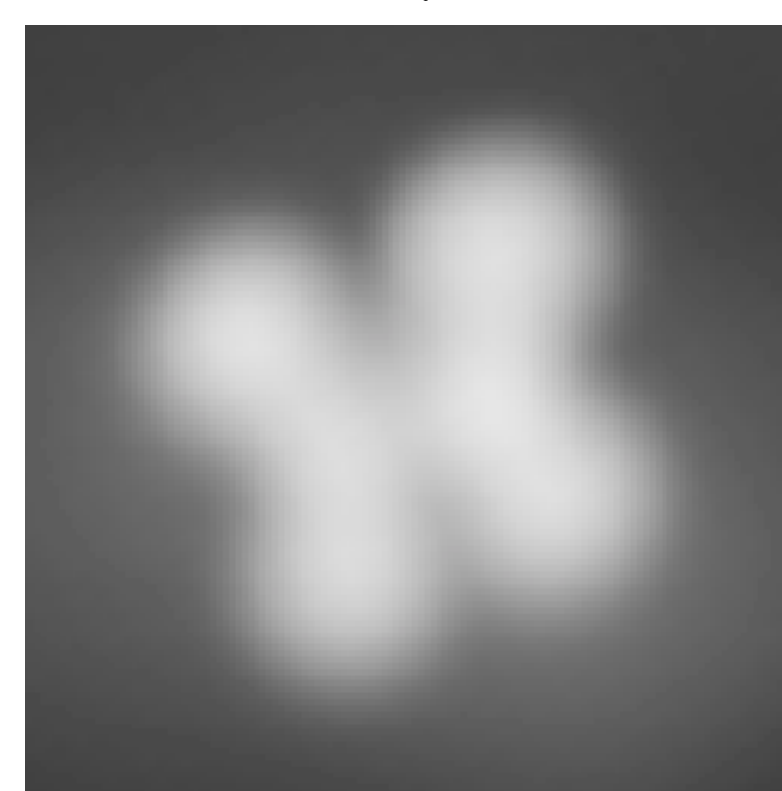
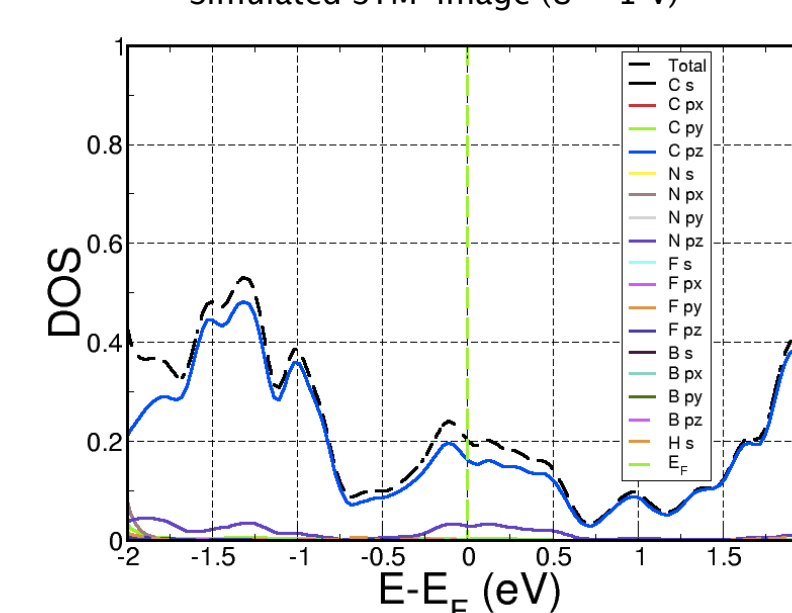
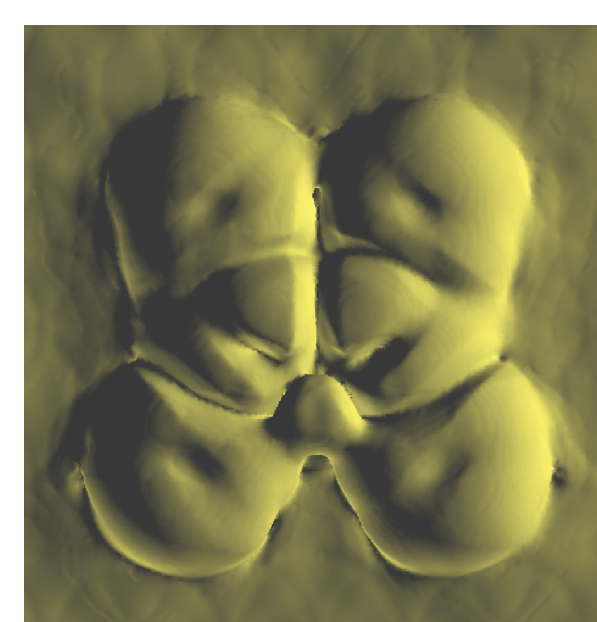
- 3 chamber UHV system with base pressure of $5 \times 10^{-11} \text{ mbar}$
- Operated at 5 K
- Molecular beam epitaxy
- Tuning fork AFM



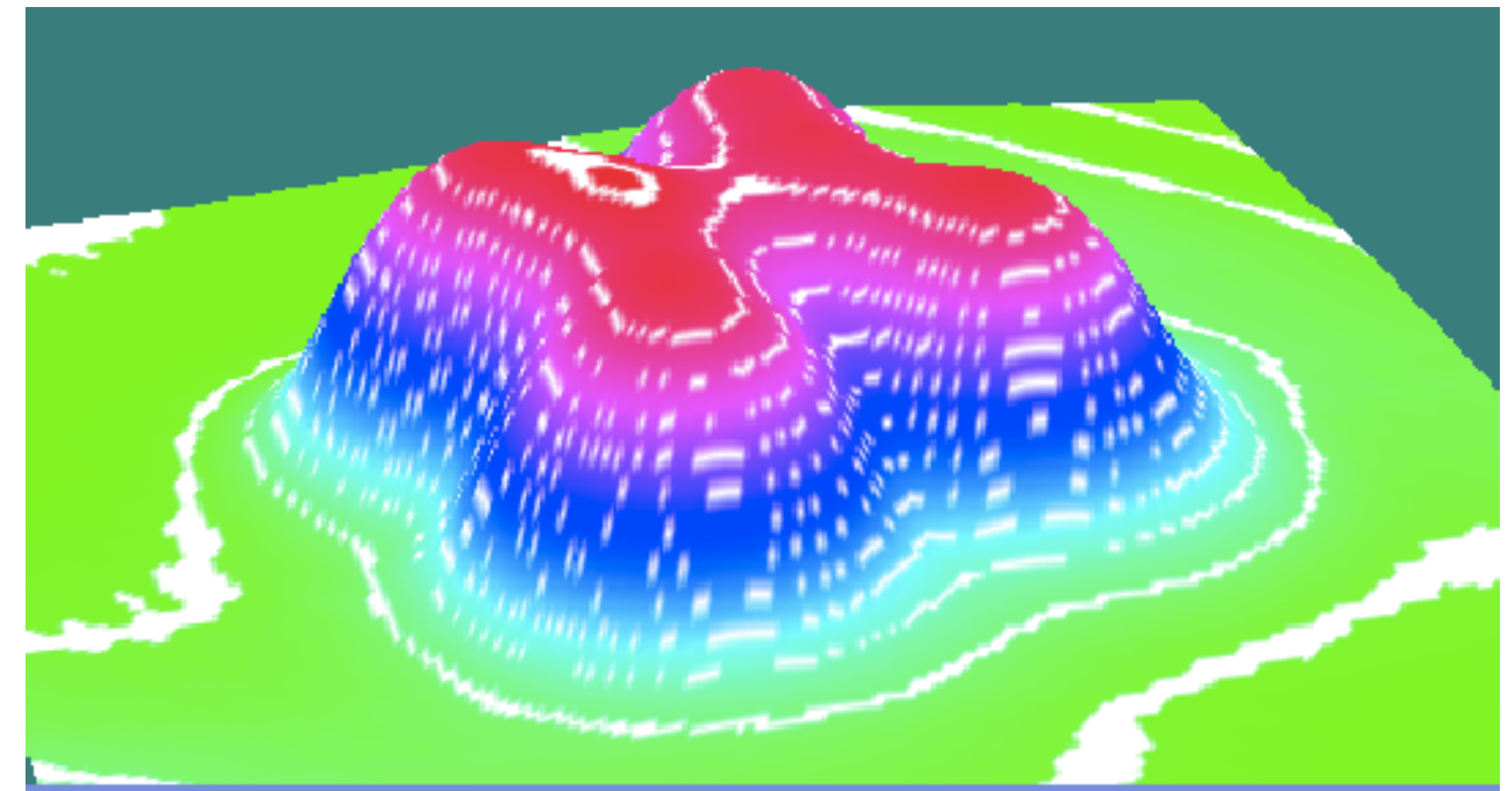
Imaging

Simulations (Cormac Toher)

- Relaxed state on Au(111) 5 eV lower than unrelaxed
- Molecule flattens on surface
- Various orientations with minor energy differences
- Phenyl groups flatten on surface
- LDOS mainly contributed by C_{π}



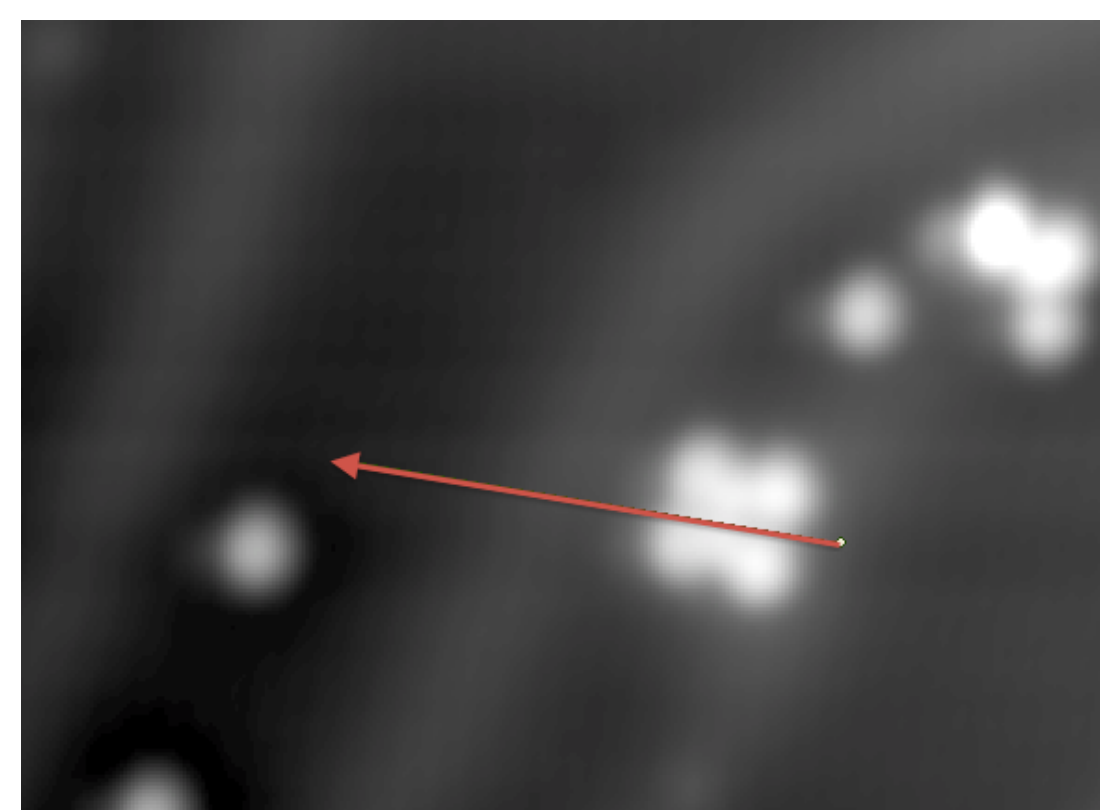
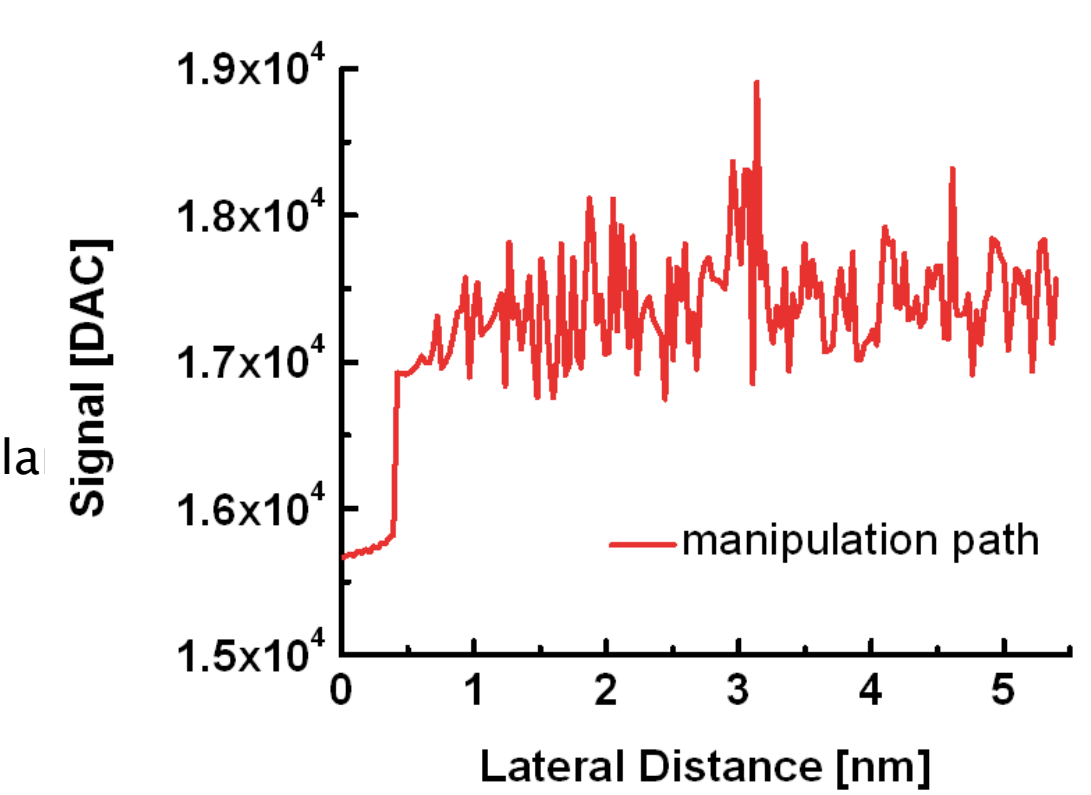
3D picture



Manipulation

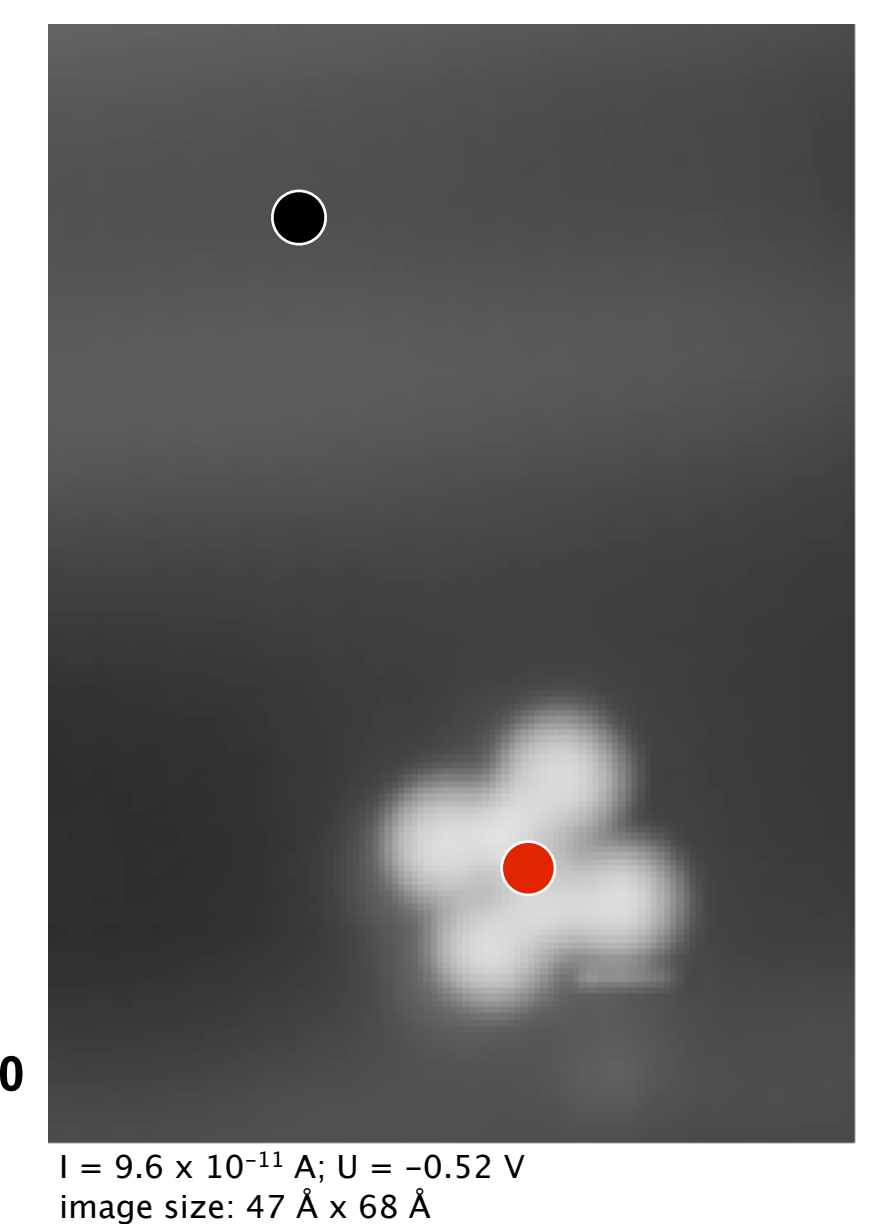
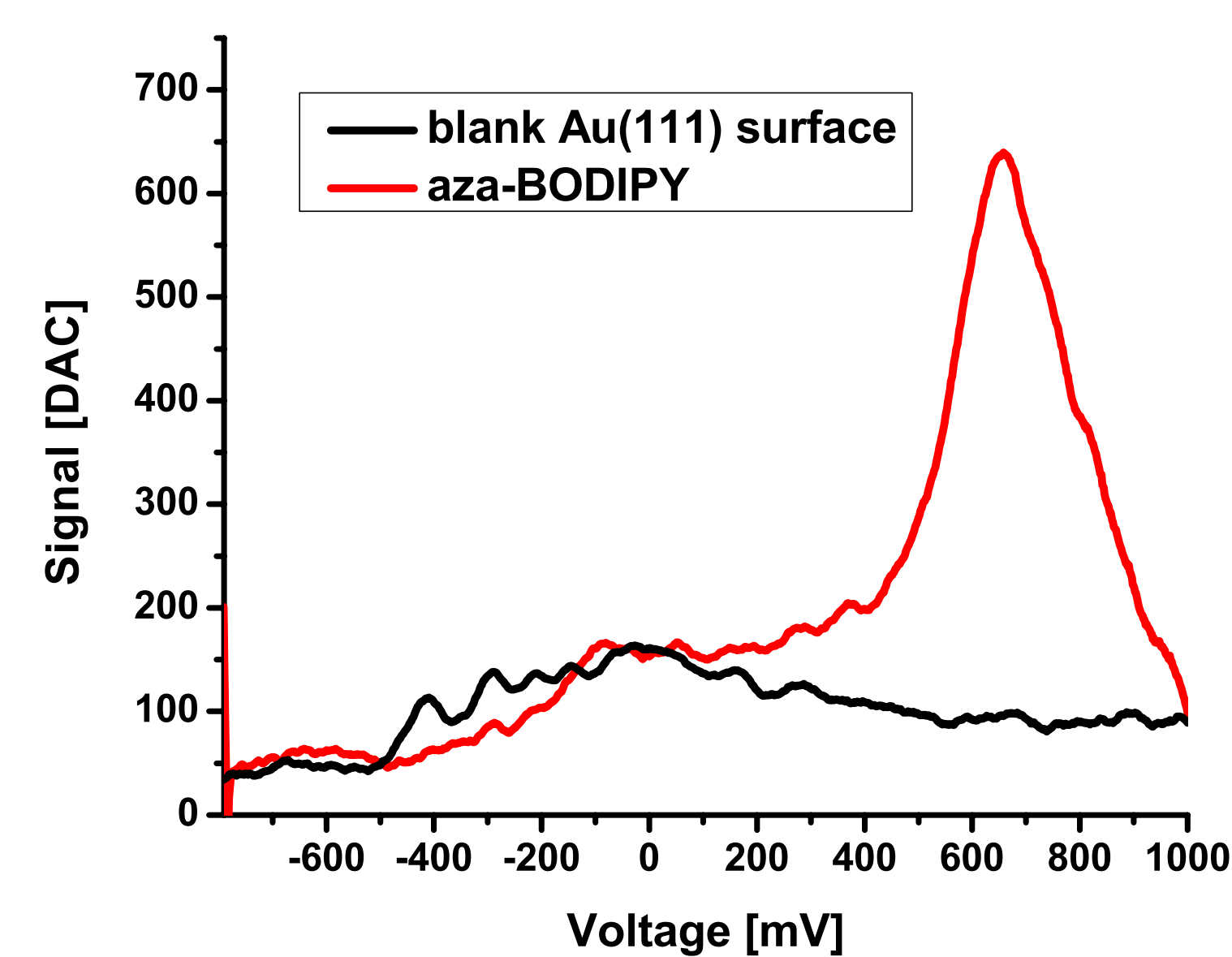
Lateral Manipulation

- 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



Spectroscopy

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



Acknowledgment

- ECEMP – European Center of Emerging Materials and Processes (project A2) for funding
- InnovaSens for funding
- IAPP (TU Dresden) for synthesis