



# STM-investigations on aza-BODIPYs at low temperatures

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### motivation: heterojunction solar cells

- exciton created in electron donor
- separation of electron-hole pair at donor acceptor interface
- current standard materials lag infrared adsorption (ZnPc/C60)
- aza-BODIPY as electron donor material
  - tuneable infrared absorption



Gong et.al. Sol. En. Mat. & Sol. Cells **94** (2010) 114 Riede et. al. Nanotechnology **19** (2008) 424001





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- class of organic fluorescent dyes
- characterised by azadipyrromethene boron complex
- 1,3,5,7-tetraphenyl-8-azadipyrromethene
- first synthesised in 1993
- no single molecule investigations so far







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  - STM-experiments:

aza-BODIPY on Au(111)







### experimental setup

- low temperature STM
- base pressure 5 x  $10^{-11}$  mbar
- experiments at liquid helium temperature (5 K)
- Au(111) sample with herringbone reconstruction
- aza-BODIPY evaporated from a Knudsen cell at ca. 220 °C





#### complex nano materials

### imaging

- aza-BODIPY preferentially adsorb on fcc domains
- no distinct surface orientation
- molecule flattens on surface (app. height 1.4 Å)
- molecules move at  $U_{\text{bias}} \ge \pm 1 \text{ V}$



image size: 152 Å x 284 Å





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- molecules can be manipulated to hcp domains
- molecule changes orientation
- no conformation changes observed
- manipulation parameters:

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- DFT-LDA simulations
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experiment image size: 25 Å x 25 Å

theory image size: 22.5 Å x 22.5 Å





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#### spectroscopy

- dI/dV measurements (range -1 V  $\leq$  U < 1 V)
- surface state observed for bare Au(111)
- single peak at U = 0.7 V (unoccupied state)





image size: 54 Å x 88 Å





spectroscopy

- single peak at U = 0.2 V
- consists mainly of delocalised  $C\pi$  states
- discrepancy due to DFTlimitations







### conclusion and outlook

- experiments and simulation agree well
- phenyl rings flatten on surface
- low diffusion barrier restricts STS measurements
- stronger binding surface would increase STS range but also increase hybridisation
- investigation of other aza-BODIPY derivatives to analyse structural reasons for electronic property changes





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#### Europa fördert Sachsen.









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SACHSEN

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# Thank you for your attention

further theory details:

poster session TUE 18:30 WIL 036.27