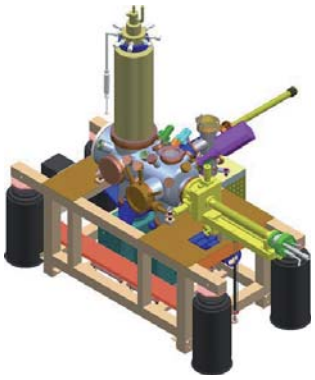
Structure-Property Relationships of Molecular Materials on Nanometer Scale

Jörg Meyer

Organic electronics research has gathered a lot interest during the last years. On one hand it is a promising approach for the miniaturisation of electronics were single molecules could act as building blocks or complete electronic circuits. On the other hand organic molecules are already in use for photovoltaic systems and light emitting diodes. In both cases, the influence of the local surrounding of the molecules plays a critical role for the functionality of the final device. To understand this influence organic molecules are investigated by Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) under ultra-high vacuum conditions at low temperatures.

Measuring principle

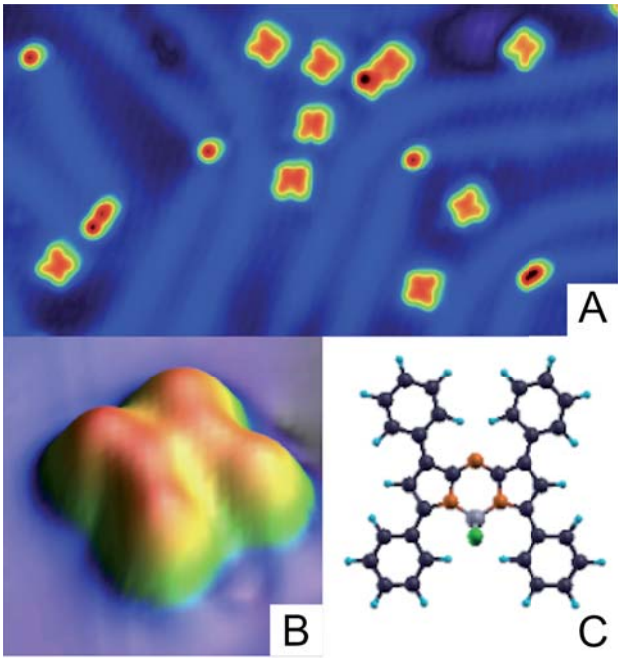
- conductive tip is scanned over conductive substrate with just a few Ångström (10^{-10} m) and a voltage is applied between tip and surface
- electrons tunnel between tip and substrate and create a measurable current
- current strongly depends on the distance between substrate and tip and the density of states near the tunnelling junction
- molecules in the tunnelling junction provide additional states and influence the tunnelling current



STM vacuum system

Investigated molecules: aza-BODIPY

Aza-BODIPY are a class of organic fluorescent dyes which have recently become interesting for organic photovoltaics because of their strong tunable infrared absorption and there high stability. Among others a tetra-phenyl derivative of aza-BODIPY (difluoro-bora-1,3,5,7-tetraphenyl-aza-dipyrromethene, Fig. C) has been measured on the Au(111) surface by low temperature STM and STS. Far less then a monolayer of aza-BODIPY has been deposited to be able to measure isolated single molecules. STS measurements of these molecules showed a broad prominent peak at a bias of 0.7 V (unoccupied state). DFT calculations indicate that the molecule forms a weak chemical bond with the Au(111) surface with significant charge transfer. Nevertheless, most likely because of the low corrugation of the Au(111) surface, diffusion of the molecule is observed for applied bias in excess of 1V. Due to the adsorption, the four phenyl groups are twisted into the molecular plane and appear as relatively flat circular protrusions in the experimental and simulated STM images.



Aza-BODIPY on Au(111): (A) overview: Aza-Bodipy appear as for protrusions representing the phenyl groups. Point-like protrusions correspond to ad-atoms. (image size: 284 Å x 152 Å) (B) 3D animation of an STM image showing a single aza-Bodipy on Au(111). (C) structure of the investigated aza-BODIPY (colour code: carbon = black; nitrogen = orange, fluorine = green; boron = grey; hydrogen = blue).

Reference

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