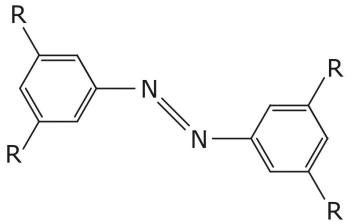
Index:

- General conclusions after one year
  Where are we?
  What have we learned?
- Next steps
- Possible improvements

Teilprojekte:
A1 Pascual/Grill
B1 Tegeder/Wolf
B2 Weinelt
B3 Kuch/Wende
B6 Rück-Braun
B7 Haag
B8 Hecht
C2 Saalfrank/Klamroth
C3 Reuter/Scheffler

1) Optimization of the chemical properties for efficient switching:



- ***Different molecules:***
  - Azobenzene
  - Stilbene
  - Imine
- ***Role of the substituents R:***
  - Decoupling from the surface
  - Acceptor/Donor groups
  - Modify the electron density at the N=N bond
- ***Surfaces:***
  - Less reactive surfaces (Graphite, NaCl/Cu(111))

NEXT STEPS

1) Search for best candidates

2) Calculation of the switching efficiency of the best candidates

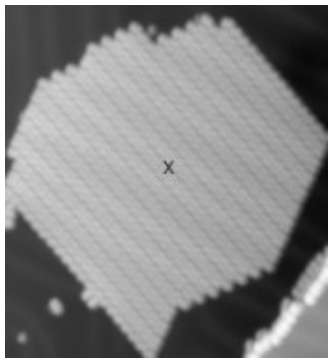
3) Calculation of the isomerization barriers

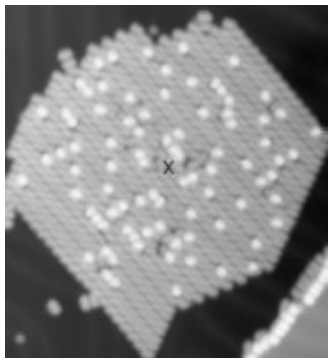
→ Ideal molecules for experiments

2) **Planar** adsorption of azobenzene derivatives

- ***What have we learned:***
  - Reversible switching on Au(111)
  - Rather small yield (≈10^{-8} events/electron) - sufficient for optical methods?
  - Interaction with substrate and other molecules is crucial (→ substituents)
  - No switching of single molecules because of low diffusion barrier
  - No switching if intermolecular interaction becomes too strong

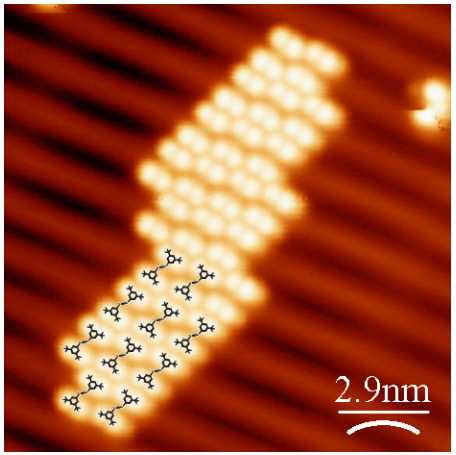
Isomerization of TBA molecules on Au(111)





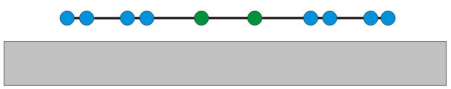
J. Am. Chem. Soc. 128, 14446 (2006)

TBA on Au(100)

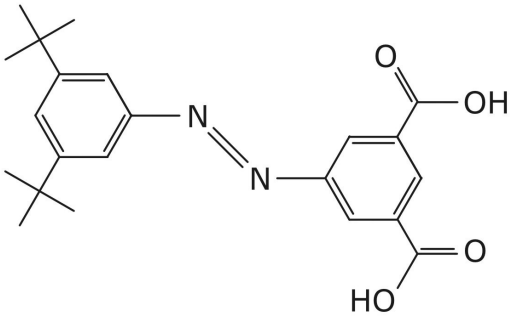


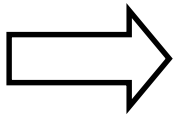
- ***Next steps:***
  - Optimize molecule and substituents for higher efficiency (theory)
  - Less reactive substrates
  - Change the position of *tert*-butyl groups at TBA (from meta- to ortho-)
  - Anchoring of molecules on one end

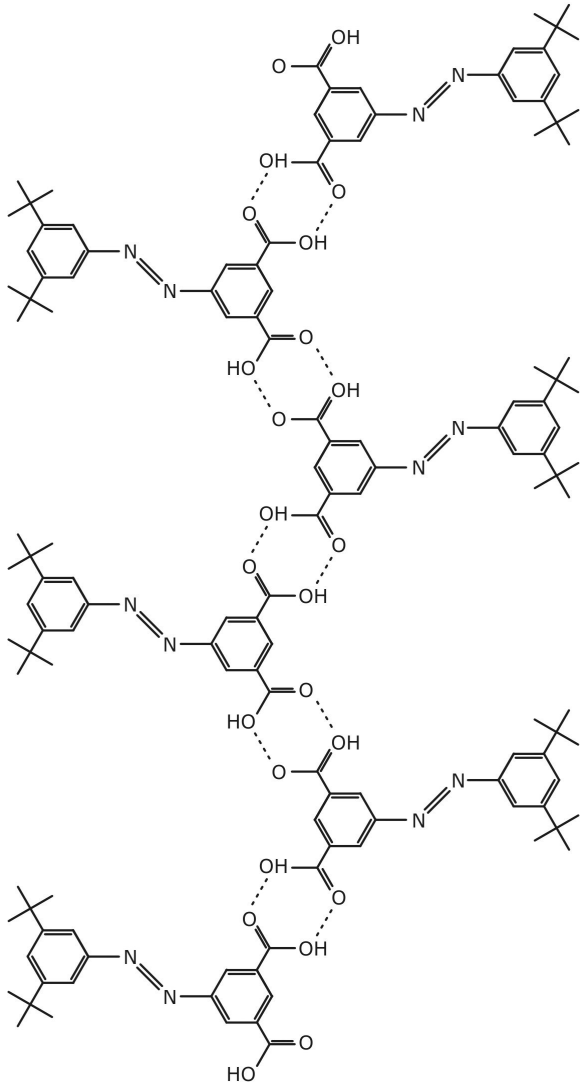
2) **Planar** adsorption of azobenzene derivatives



Use of different substituents

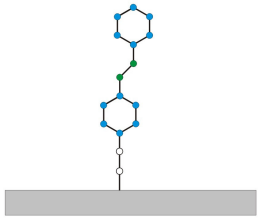




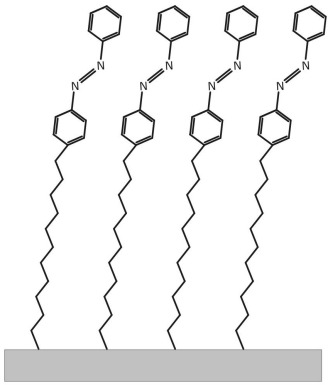


- ***Formation of chains via H-bonds at carboxyl groups***
- ***Controlling (and using) intermolecular interactions***
- ***Fixing of the molecules on one end and switching on the other (free) end***

3) **Vertical** adsorption of azobenzene derivatives: SAMs



- ***What have we learned:***
  - Azobenzene chains adsorb closely packed (π stacking)
  - Conformational change by x-rays was observed, but no isomerization
  - Neighbour molecules hinder isomerization process



- ***Next steps:***
  - Adsorb molecules at larger distances
  - Preparation in two steps (with azobenzene-amide)
  - Maximum density of 50% on the surface