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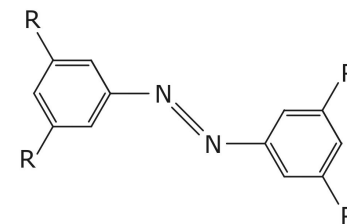
- ▶ General conclusions after one year
Where are we?
What have we learned?

- ▶ 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**

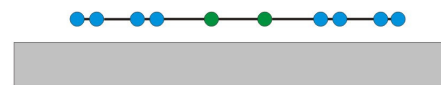
2) Planar adsorption of azobenzene derivatives

► **What have we learned:**

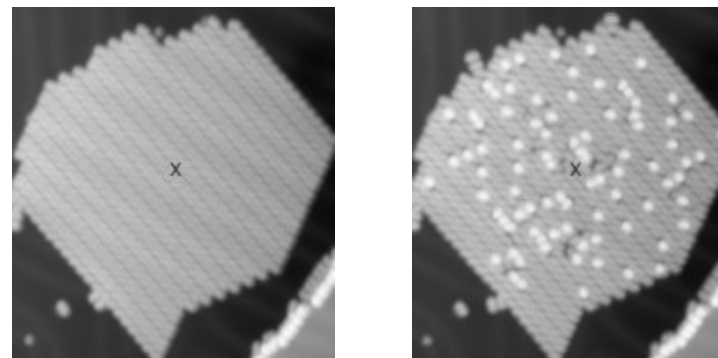
- Reversible switching on Au(111)
- Rather small yield ($\approx 10^{-8}$ events/electron)
 - sufficient for optical methods?
- Interaction with substrate and other molecules is crucial (\rightarrow substituents)
- No switching of single molecules because of low diffusion barrier
- No switching if intermolecular interaction becomes too strong

► **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

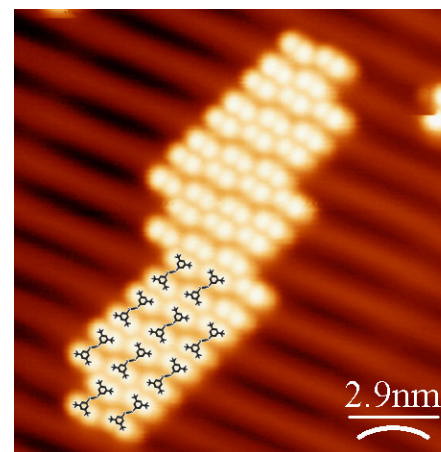


Isomerization of TBA molecules on Au(111)



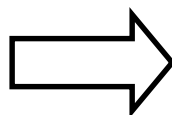
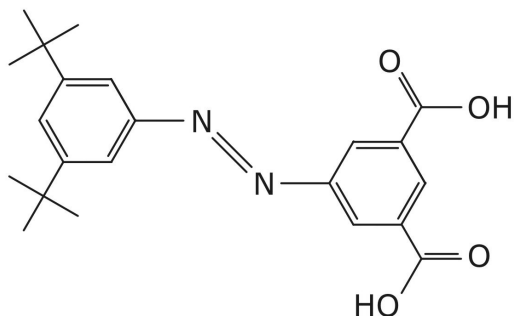
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TBA on Au(100)

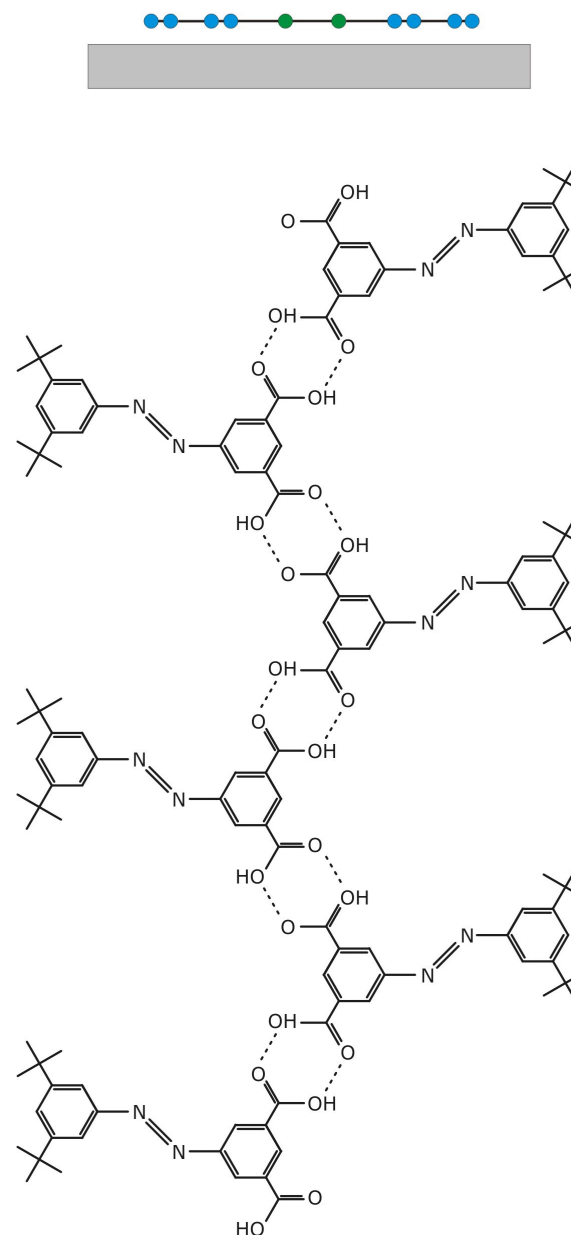


2) Planar adsorption of azobenzene derivatives

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

