

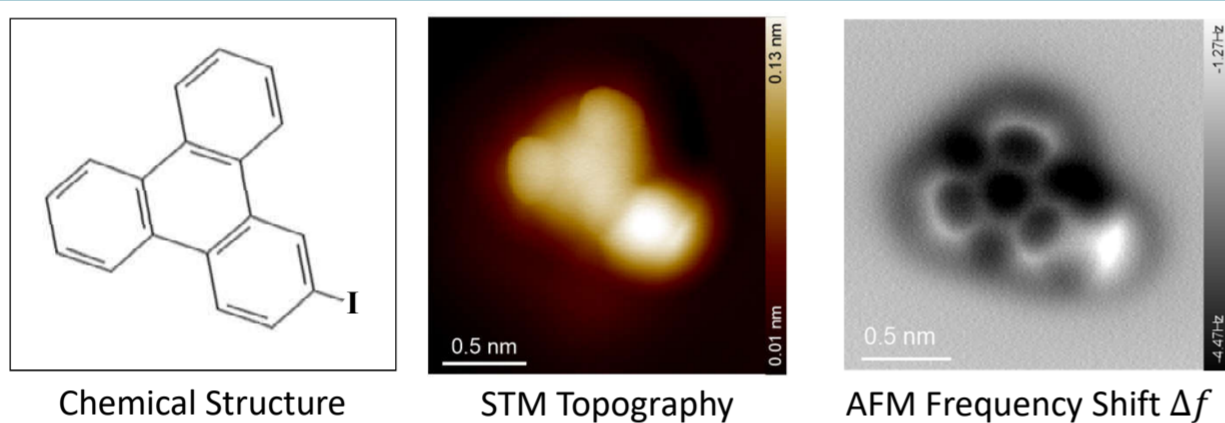
Adsorption Geometry of 2-Iodotriphenylene on Ag(111) and Cu(111)

Alexander Ihle¹, Sebastian Ahles², Tobias Schlöder³, Doreen Mollenhauer³, Hermann A. Wegner², Andre Schirmeisen¹, and Daniel Ebeling¹

Motivation

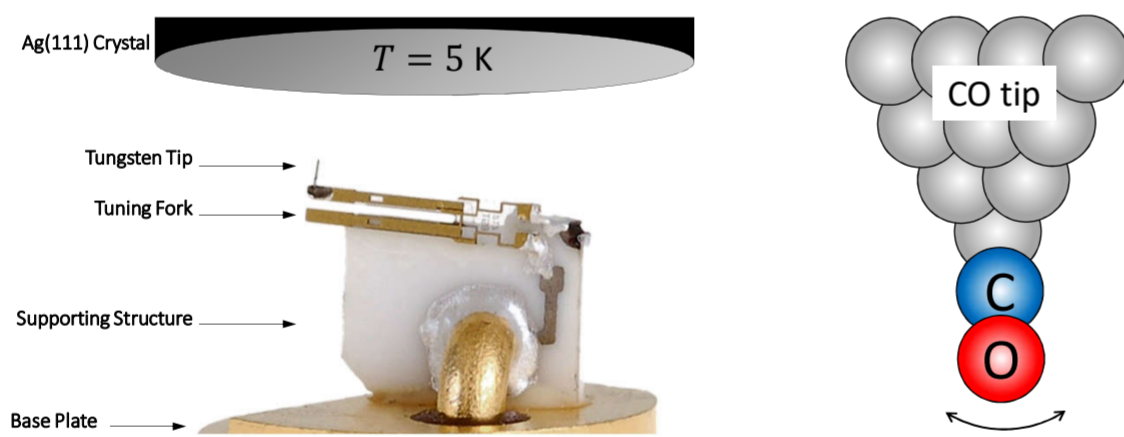
On-surface chemistry is a powerful tool for building covalent molecular structures such as chains or graphene nanoribbons [1, 2]. In particular, the catalytic properties of the metal substrate facilitate the synthesis of new structures that are not accessible via solution chemistry [3]. In order to control the bottom up formation process precise knowledge about the adsorption geometry of the molecular precursors is needed since this will help to understand the reaction mechanisms in detail [4]. Here we studied the adsorption geometry of 2-iodotriphenylene on Ag(111) and Cu(111). By using low temperature atomic force microscopy with CO-functionalized tips we are able to identify the precise adsorption position of the molecules and their orientation with respect to the substrate lattice. On both substrates we find one preferred and one less preferred adsorption configuration. Depending on the substrate material, these are either directed by metal atoms in the surface and the sub-surface layer or the halogen group. Hence, the adsorption position can be actively controlled by the choice of substrate material.

Model System



Methods

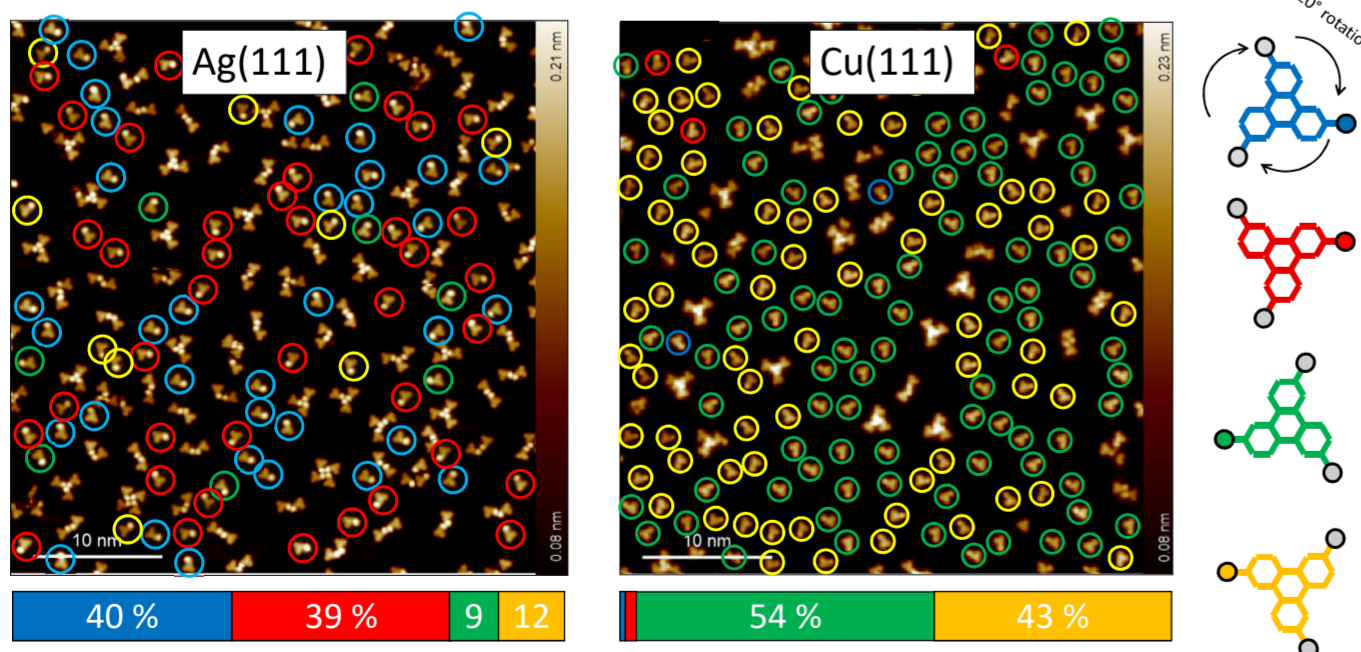
STM/AFM in UHV and low T ($p < 10^{-10}$ mbar, $T = 5.2$ K)



Adsorption Structure is determined by STM / AFM

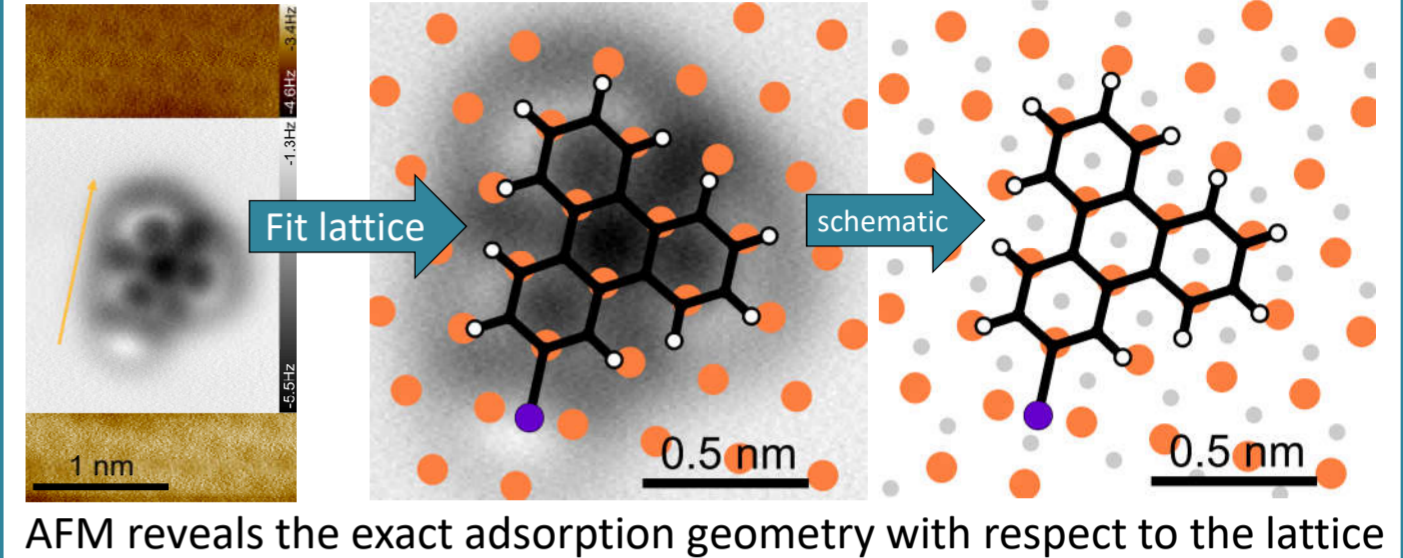
We analyze individual 2-iodotriphenylene molecules on the surface by high-resolution STM.

We observe four different adsorption configurations (blue, red, green, yellow)

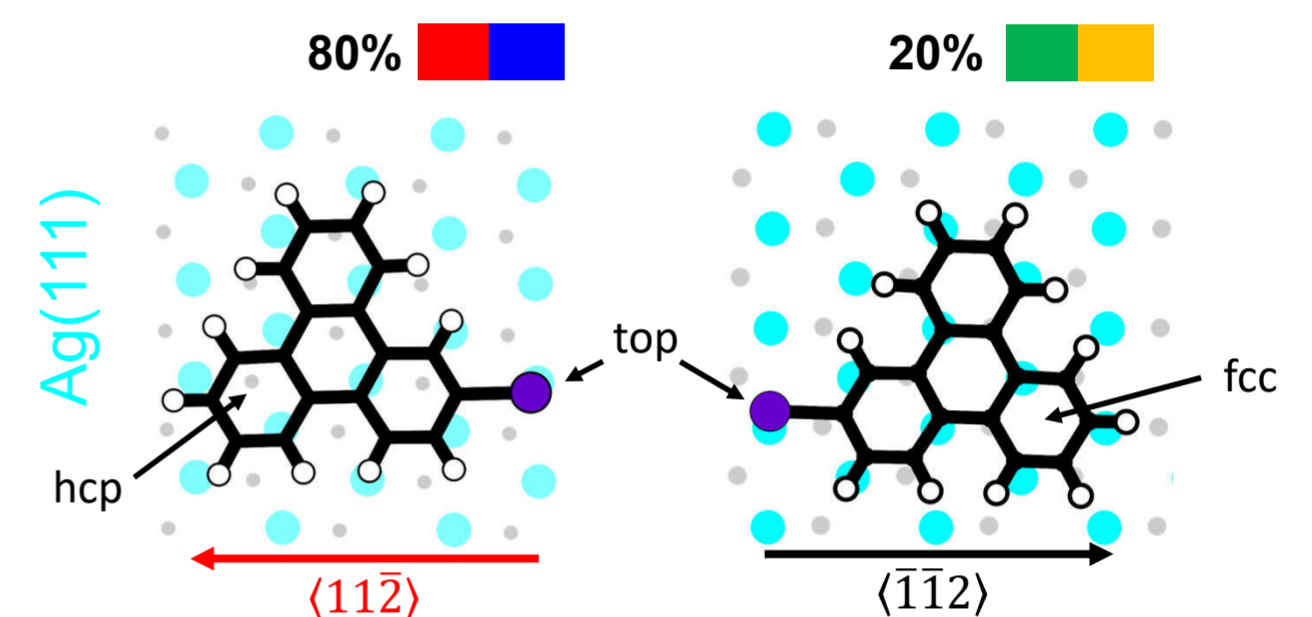


STM overview scans reveal different preferred and un-preferred adsorption geometries of iodotriphenylene on Ag(111) (left) and Cu(111) (right).

Adsorption Geometry

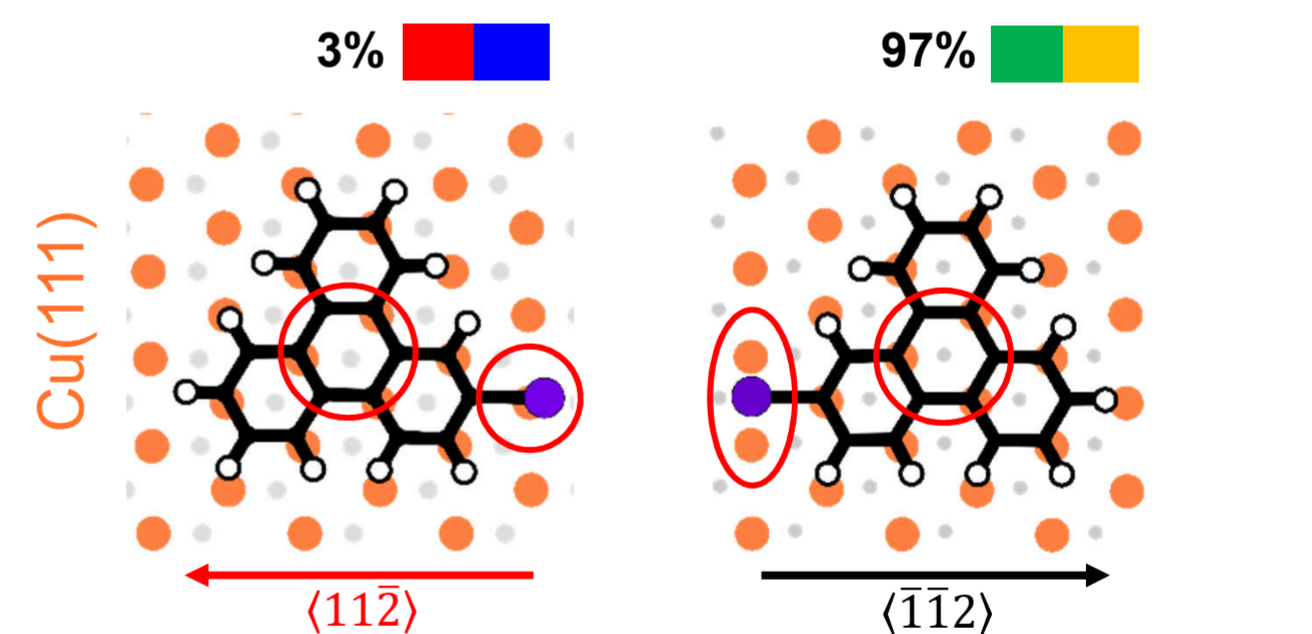


Substrate Material Directs Adsorption Geometry



Ag(111):

- Iodine always at **top** site.
- Centers of carbon rings either at **hcp** or at **fcc** hollow sites.
- **80 %** preferred and **20 %** unpreferred states



Cu(111):

- Iodine either at **top** or **bridge** site.
- Centers of carbon rings always at **hcp** hollow sites.
- **97 %** preferred and **3 %** unpreferred states

Conclusions

- **On Ag(111):**
 - Weaker interaction between the triphenylene backbone and the substrate atoms than on Cu(111)
 - Iodine seems to direct the adsorption position
 - **On Cu(111):**
 - Strong interaction between the triphenylene backbone and the substrate atoms
 - Molecular backbone seems to direct the adsorption position
- Adsorption positions on Ag(111) and Cu(111) differ significantly due to different molecule-substrate interactions
- Interactions with **subsurface** atoms are not negligible

CONTACT PERSON

Alexander IHLE
Institute of Applied Physics
Justus-Liebig-University Giessen
alih@physik.jlug.de

REFERENCES

- [1] Grill, L. et al. Nature Nanotechnology 2, 687–691 (2007)
- [2] Cai, J. et al. Nature 466, 470–473 (2010)
- [3] Zhong, Q. et al. J. Am. Chem. Soc. 141, 7399–7406 (2019)
- [4] Ebeling, D. et al. ACS Nano 13, 324–336 (2019)

AFFILIATIONS

- 1 Institute of Applied Physics, Justus Liebig University Giessen, Germany
- 2 Institute of Organic Chemistry, Justus Liebig University Giessen, Germany
- 3 Institute of Physical Chemistry, Justus Liebig University Giessen, Germany