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

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On-surface chemistry is a powerful tool for building covalent molecular structures such as chains, networks, or graphene nanoribbons [1, 2]. In particular, the catalytic properties of the metal substrate as well as the 2D confinement 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 (see Fig. 1). Due to different molecule-substrate interactions these adsorption configurations differ significantly from each other for the two substrate materials. Hence, the adsorption position can be actively controlled by the choice of substrate material.

References

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[2] Cai, J. et al. Nature 466, 470–473 (2010)
[3] Zhong, Q. et al. J. Am. Chem. Soc. 141, 7399–7406 (2019)
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Figures

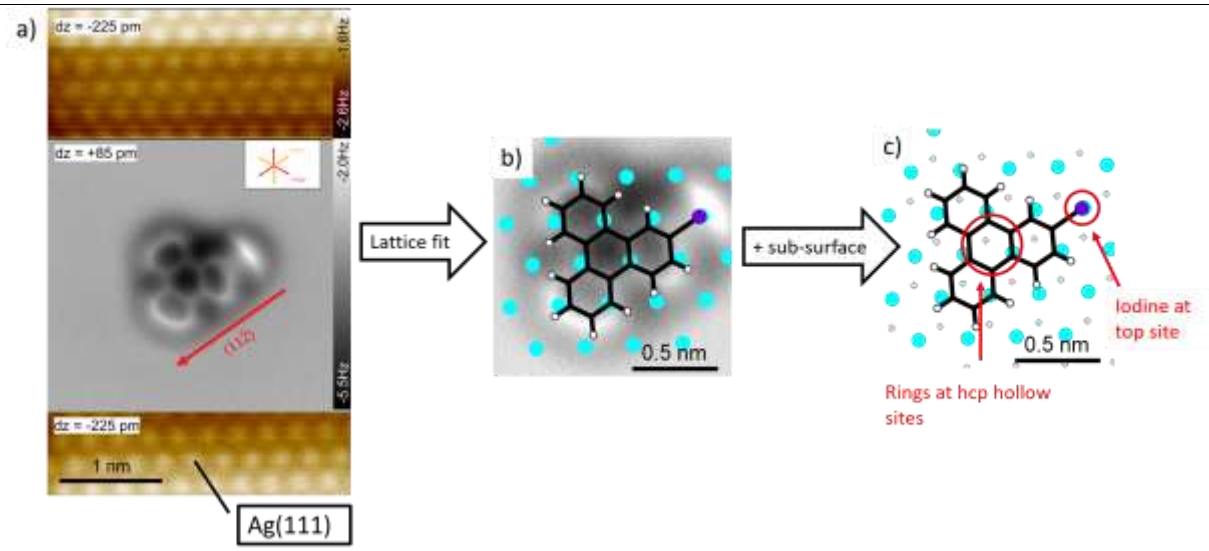

Figure 1: Adsorption configuration of 2-iodotriphenylene on Ag(111). **(a)** AFM constant height scan at two different tip-sample distances to resolve both the lattice and molecule. **(b)** Zoom-in of (a) showing the fitted atom positions of the Ag lattice (light blue) and a fitted structural model of iodotriphenylene (black: aryl backbone; purple: iodine) **(c)** Fit of the lattice and sub-lattice reveals the rings being adsorbed at hcp hollow sites and the iodine adsorbing at top sites.