# Manipulation of Benzene on Cu(110) by Atomic Force Microscopy: The Last Atom Matters

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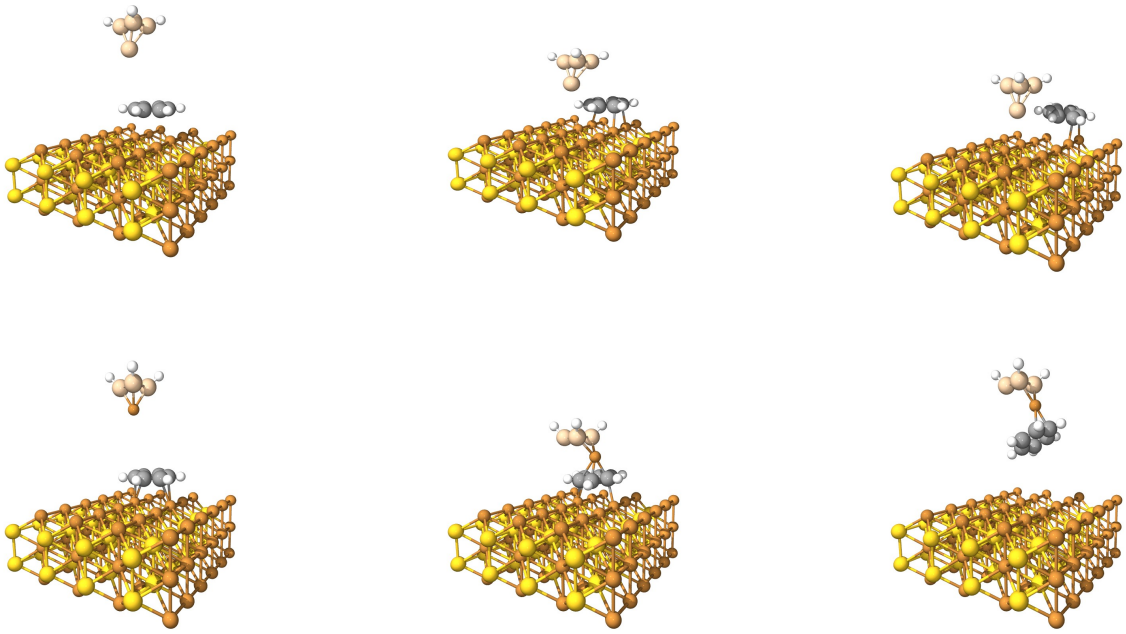
The imaging and manipulation of single molecules adsorbed on clean surfaces by scanning tunnelling microscopy (STM) has been the topic of research for several years. Although non-contact atomic force microscopy (NC-AFM) should give equivalent results, its application to single molecules is very limited. Based on *ab initio* calculations we simulated how an aromatic organic molecule like $C_6H_6$ adsorbed on a Cu(110) surface can be mechanically manipulated in non-contact atomic force microscopy. Using two different kinds of tips we simulated several approach and retraction curves on different positions of the carbon ring. Interestingly, the overall behaviour of the molecule is independent of the actual approach position. The most important factor is the atom at the tip-apex. For a pure silicon tip the benzene molecule can be pushed over the sample surface. This behaviour is comparable to the results obtained with tungsten tips in scanning tunnelling microscopy. A quite different behaviour is found for a cupper terminated tip where the apex atom of the silicon tip is replaced by a cupper atom. In this case the benzene is picked up by the tip and can be completely retracted from the surface.



Ball and stick model of the atomic configurations obtained by *ab-initio* simulations. The images shows the approach of the silicon (upper panel) and cupper (lower panel) terminated tips.