Theoretical view on '*subatomic*' contrast on Cu adatom with CO-tip

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In 2019, F. Huber et al published work [1] reporting an unusual ring contrast observed on an adatom on Cu(111) recorded by nc-AFM with CO-functionalized SPM probe. The emergence of the characteristic ring contrast was also confirmed by DFT simulations. The origin of this 'subatomic' feature was attributed to the formation of the chemical bond between Cu adatom and CO-functionalized probe. However, a detailed understanding of the origin of the contrast was unclear.

In this contribution, we will provide an in-depth theoretical discussion of the origin of the ring contrast on Cu adatoms employing total energy DFT simulations and an extended version of the probe particle model [2]. We will demonstrate that the presence of the attractive interaction in close tip-sample distances is caused by induced charges between the CO-tip and the Cu adatom. To understand the role of the CO-functionalized tip, we also carried out DFT simulations with Xe-functionalized probe, which reveals the absence of the ring contrast on Cu adatom. These observations point out the importance of the electrostatic forces between static and induced charges [3] in the SPM junction on the imaging contrast. More details about the mechanism of the imaging contrast responsible for the ring contrast will be presented.

Reference

[1] F. Huber, et al. Science **366**, 256 (2019).

[2] P. Hapala et al. PRB **90**, 085421 (2014); P. Hapala et al. PRL **113**, 226101 (2014).

[3] B. Mallada et al Science **374**, 863 (2019).