AFM with molecule modified tips: Distortions due to the lateral bending of the CO tip

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Non-contact atomic force microscopy (AFM) and scanning tunneling microscopy (STM) have become the standard tools for studying atomic scale objects on surfaces. However, in most cases neither of the techniques directly yield the true surface topography. It is well known that the STM signal depends on the local density of states (LDOS) and the work function of the surface below the tip. AFM suffers from a similar problem; the detuning signal depends on several different forces between the tip and sample. To obtain atomic resolution images, the chemical forces between the last atom of the tip and surface need to have a significant contribution to the total force. These chemical forces may also vary over the sample surface due to locally varying reactivity, which will lead to false topography in the AFM image.

When imaging single molecules on surfaces with high resolution, the AFM tip is often passivated by picking up a CO molecule to prevent the tip from moving or picking up the molecule being imaged [1]. Due to the passive nature of the CO, the attractive chemical forces between the tip and sample are diminished leaving Pauli repulsion as the primary contribution to the total force between the CO molecule and the surface. The lateral bending of the CO on the tip however introduces distortions in the recorded AFM image.

To better understand how the bending of the CO molecule affects the AFM image on samples with locally varying lateral forces, we have created a simple molecular mechanics model of the CO tip. We compare our model to AFM images of molecules on surfaces from literature and to our measurements on corrugated epitaxial graphene [2,3]. The results of our simulations show that neither the exact lateral nor the vertical positions of the surface atoms can be easily extracted from the AFM measurement with a CO tip when the sample is vertically corrugated

[1] L. Gross, et al., *Science* **325**, 1110-1114 (2009).
[2] S.K. Hämäläinen, et al., *Phys. Rev. B* **88**, 201406(R) (2013).
[3] M.P. Boneschanscher, et al., *ACS Nano* **8**, 3006-3014 (2014).