

Intramolecular bonds studied by NC-AFM

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Various individual hydrocarbon molecules were imaged on Cu(111) and bilayer NaCl on Cu(111) by NC-AFM using a qPlus sensor at cryogenic temperatures. To achieve atomic resolution the tip was functionalized with a CO molecule [1,2]. The details and differences in contrast obtained on individual bonds within the molecules were investigated. We found that the relaxation of the CO molecule at the tip apex plays an important role in the AFM contrast formation. The relaxation leads to distortion of the images and a very sharp appearance of the bonds. DFT calculations that modelled the tip as a small Cu cluster with a CO molecule attached to it took into account the relaxations and help to understand their role for AFM imaging. The prospects of resolving details of individual bonds e.g. bond length and bond order will be discussed.

References

- [1] L. Gross *et al.* *Science* **325**, 1110 (2009)
- [2] N. Moll *et al.* *New J. Phys.* **12**, 125020 (2010)