Simultaneous Atom-Resolved AFM and STM Studies of the Hydroxylated TiO_2 (110) Surface

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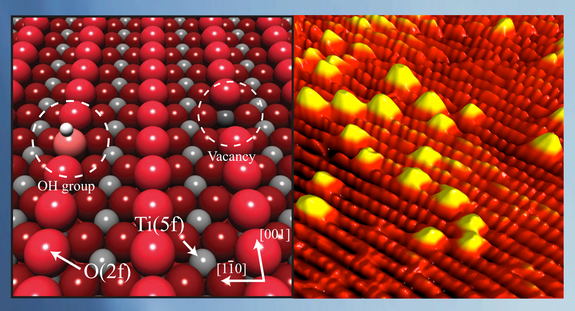
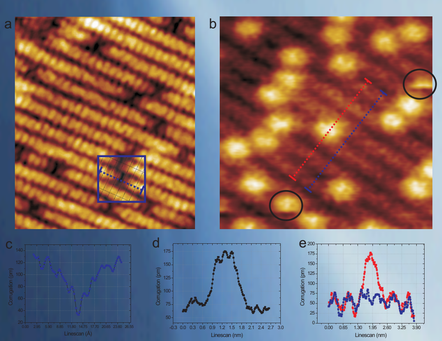
Benchmark oxide

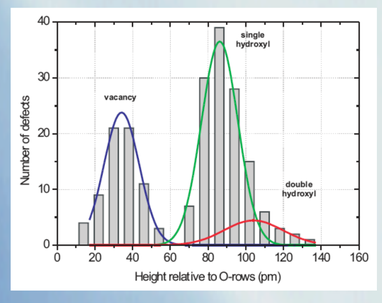


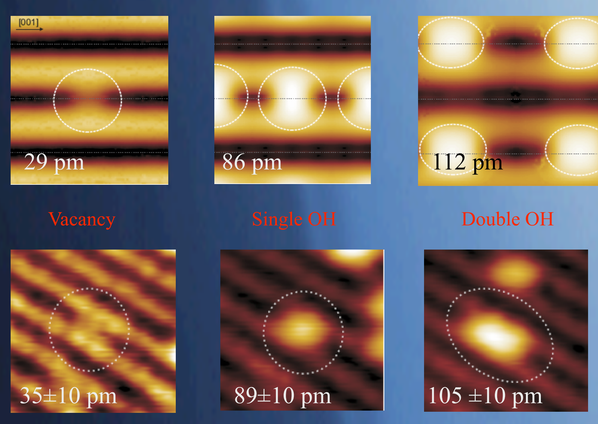
- TiO_2 remains a model oxide for many surface science studies, particularly for Scanning Probe Microscopy (SPM).

nc-AFM

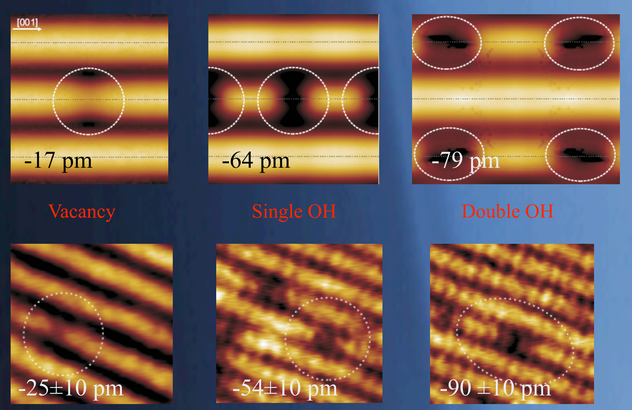


- Even in UHV, residual adsorbates can be seen on the surface after a few hours.
- Rows match TiO_2 (110) surface, but what about the atoms, defects and adsorbates?
- Statistical analysis reveals three types of defect contrast – can we prove these are linked to characteristic defects on the surface?



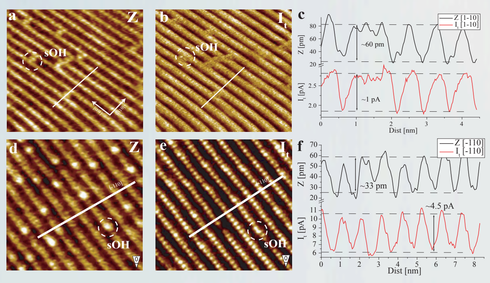


- Simulations with a negative tip match "protrusion" contrast.
- Contrast magnitude agrees with experiment for defect usual suspects.

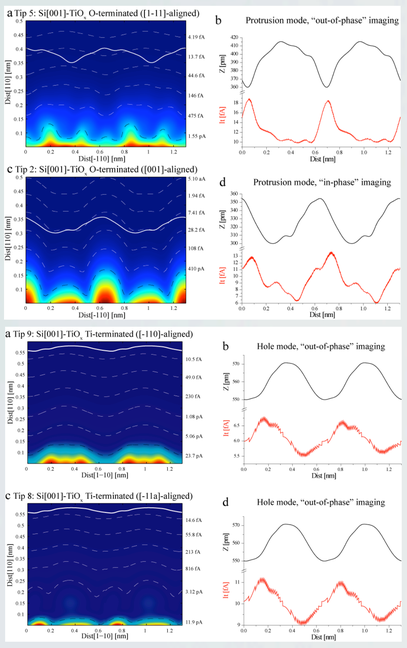


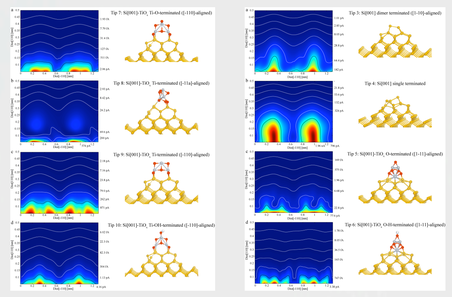
- Simulations with a positive tip match "hole" contrast.

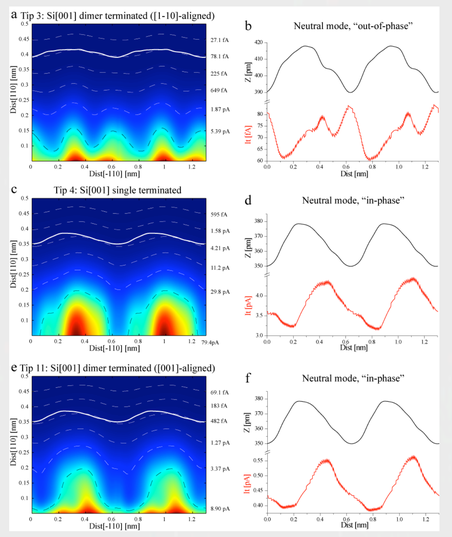
Simultaneous STM/AFM



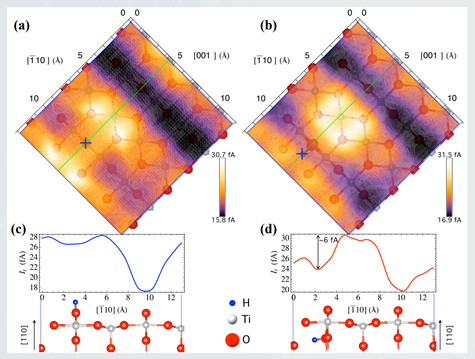
- Identification of surface species provided by AFM.
- Three modes observed.
- Registry between STM and AFM images is very sensitive to the type of tip – STM and AFM images can be in- and out-of-phase.
- Powerful tool for understanding contrast and studying further defects or adsorbates.

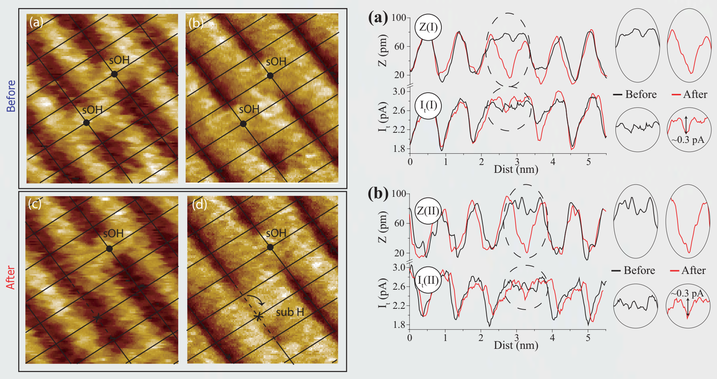


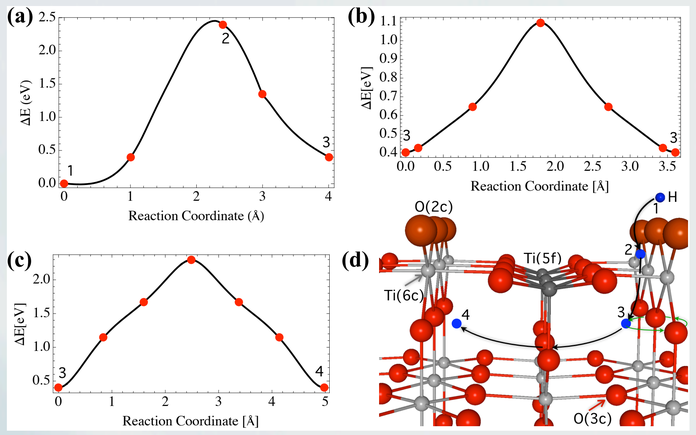




Hydrogen manipulation

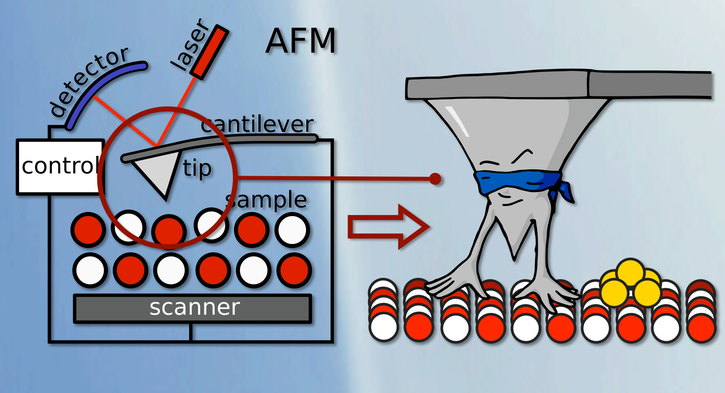






- Subsurface hydrogen invisible in AFM, but seen in STM.
- Combined STM/AFM records manipulation of H from surface to subsurface site.

Methods



- Experimental feedback loop on frequency change, while topography and current is measured.
- First principles simulations, with multiple scattering theory for tunneling.