Contrast reversal and changing shapes of atomic adsorbates in STM

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Atomically-resolved Scanning Tunneling Microscopy (STM) images are determined by both the surface and the tip geometrical and electronic structures, and by the interactions between them. Theoretical modeling is, thus, essential for a proper understanding of the physical information actually conveyed by STM images [1]. The assignment of atomic bumps when several atomic species are simultaneously present at the surface is a difficult task. This is particularly important for oxide surfaces, whose characterization at the atomic level is essential for the microscopic understanding of supported catalysts [2]. We have chosen as model system the (2×2) superstructure of O adsorbed on Ru(0001)to carry out a quantitative comparison between STM experiment and theory. We study the role of different parameters (tip structure, sample voltage (V_s), tunneling current (I_t) and gap resistance (R_G) in the shape of the STM images and in the assignment of chemical identity to the observed atomic bumps.

When imaged with a clean W tip, the O atoms appear as depressions, whose apparent shape changes reversibly from circular (at high gap resistance) to triangular (at low gap resistance). Our ab-initio calculated STM images reproduce the experiments and confirm that the tip-sample distance dictates the shape of the STM images. After adsorption of O on the tip, we observe a contrast reversal, i.e. oxygen atoms appear bright. This is confirmed by extensive numerical simulations, which require to explicitly include the tip electronic structure. This work opens the way for a quantitative understanding of STM images of adsorbate layers and oxide surfaces [3].

References:

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Figures:

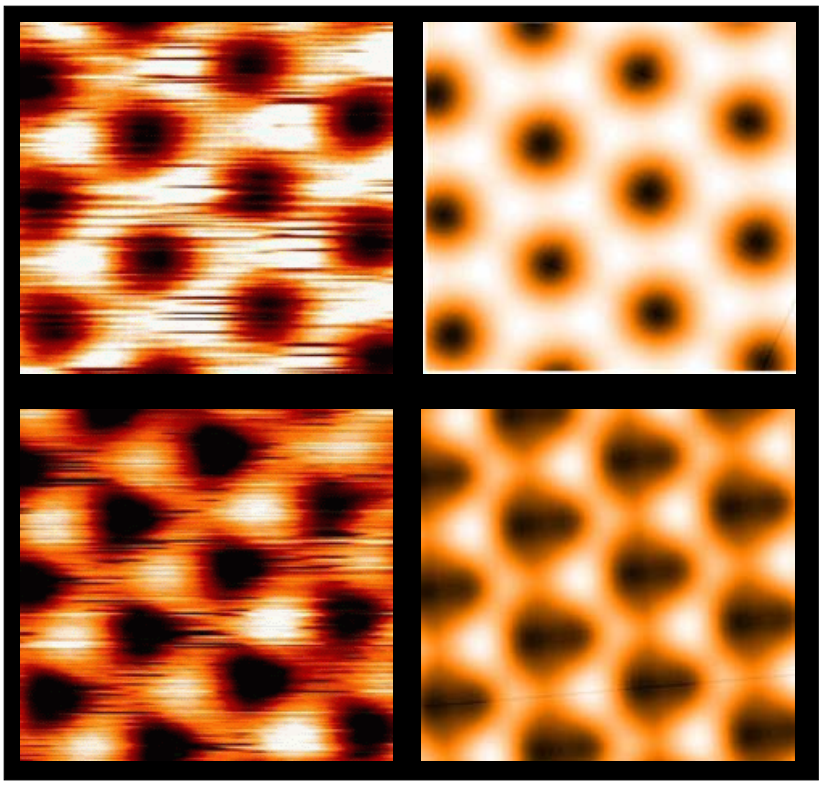

Figure 1: Comparison of experimental (left) and simulated (right) STM images of O(2×2)/Ru(0001). In both cases the sample voltage was -30 mV. The simulations have been performed with tunneling currents of 0.03 nA (above) and 0.3 nA (below) and agree with the experimental ones for 300 MΩ (above) and 30 MΩ (below) gap resistances }