STM Simulations As A Structural Tool

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Despite the Scanning Tunneling Microscope (STM) routinely provides atomic scale images of surfaces, it has been long recognized the difficulty to determine the surface atoms' location directly from the experimental images. The reason is well understood after the pioneering work of Tersoff and Hamann[1], who provided the first theoretical interpretation of the STM contrast: the features (bumps or holes) appearing in the images should not be assigned to atomic sites but, instead, should be correlated with the electronic local charge density around the Fermi level and at a distance of a few Angstroms (5-10 A) away from the surface. Furthermore, the STM signal is the convolution of the tip and sample electronic states and thus, the actual tip structure often plays a major role in determining the final aspect of the images. Hence, it is not surprising that several STM modeling formalisms have been developed during the last two decades in order to enhance the STM structural sensitivity via the comparison of experimental images against simulated ones.

In this talk we will review the main ingredients for STM modeling[2] and show, via several examples -e.g. Figs. 1 and 2, how it can help experimentalists to understand what they are "seeing". We will address issues such as STM depth sensitivity[3] or the limitations of this procedure for solving complex surface structural models or reproducing IV spectra.

References:

[1] J. Tersoff and D.R: Hamann, Phys. Rev. B, 31 (1985) 805.
[2] J. Cerdá, M.A. Van Hove, P. Sautet and M. Salmeron, Phys. Rev. B 56 (1997) 15885.
[3] C. Rogero, J.A. Martín-Gago and J.I. Cerdá, Phys. Rev. B 74 (2006) 121404.

Figures:

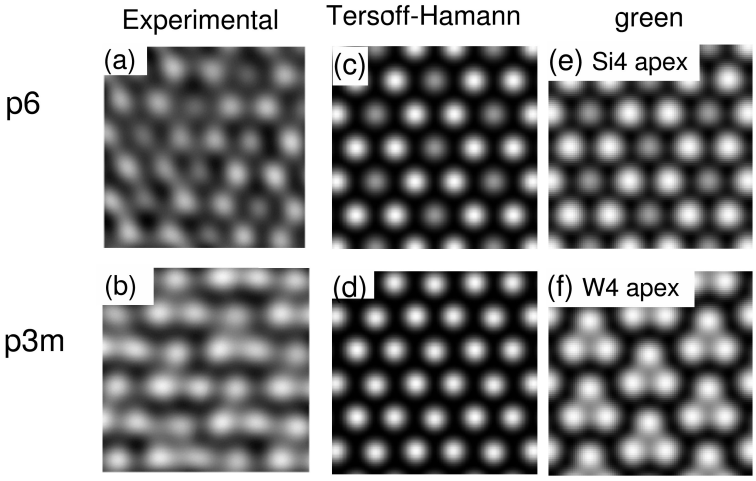

Figure 1. STM images for the Y3Si5(0001) surface. (a), (b) Experimental topographic images exhibiting p6 and p3m symmetry; I=1 nAmp, V=-50 mV. (c),(d) Tersoff-Hamann images evaluated 3 A above the surface for the p6 and p3m models. (e),(f) Theoretical topographic images calculated with a tip (GREEN code)

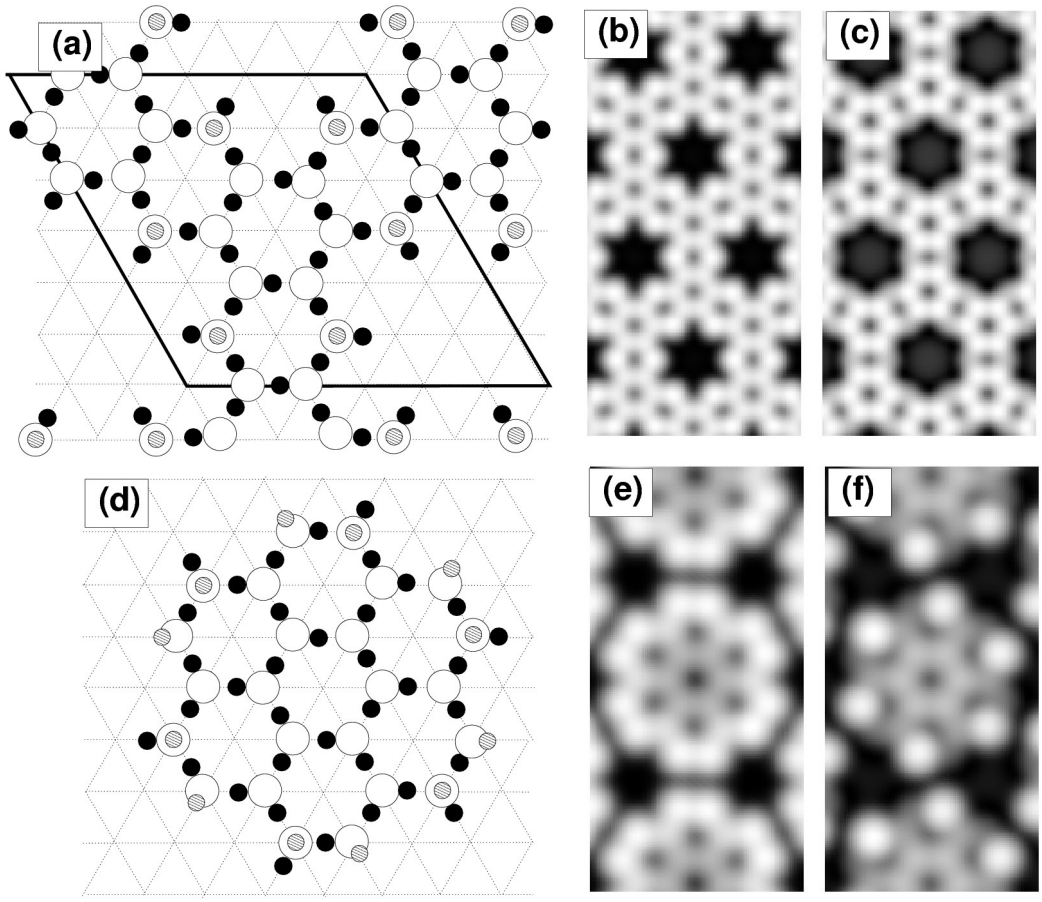

Figure 2: Optimized 2D water structures on Pd(111) for (a) lace and (d) rosette patterns. (b), (e) STM topographic image simulations for each model. (c),(f) Same as (b) and (e), but for models where the bridging species are OH species.