FIRST-PRINCIPLES SIMULATIONS OF THE RUBIDIUM BLUE BRONZE STM IMAGES

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The rubidium blue bronze $Rb_{0.3}MoO_3$ is one of the more intensely studied low dimensional materials because of the interesting physics it exhibits as a result of a charge density wave (CDW) instability (i.e., nonlinear conductivity, possible spin-charge separation etc). The crystal structure of $Rb_{0.3}MoO_3$ contains MoO_3 layers (with a $Mo_{10}O_{30}$ repeat unit) in between which the rubidium cations reside.

High resolution images of a cleaved (-201) surface of the $Rb_{0.3}MoO_3$ have been recently obtained using low temperature STM at high vacuum. At temperatures below the CDW transition the molecular lattice and the CDW superlattice were observed simultaneously [1]. Comparison of these images with previous first principles DFT [2] calculations for the bulk is somewhat puzzling. For instance, some of the more intense features of the STM images are associated with MoO_6 octahedra which are practically not implicated in the CDW transition because they have a minor contribution to the states near the Fermi level. This has prompted the present study in which we try to rationalize the main features of the STM images for the non-modulated phase.

The essential requirements for a successful model of the surface are considered. The contribution of the different types of octahedra to the image, as well as the possible role of the rubidium cations will be analysed. Special attention is devoted to the shift of the partially filled bands of the upper octahedral layer with respect to those of the bulk - arising from the partially non compensated nature of the surface- and the possible physical consequences of this feature are explored.

References:

[1] C. Brun et al, PRB submitted for publication (2005).
[2] J. Mozos et al, PRB **65,** 233105 (2002).