

## Simulating imaging of organic adsorbates on oxide surfaces

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As atomic resolution on plain surfaces in noncontact atomic force microscopy (NC-AFM) experiments becomes almost routine, the focus has shifted to imaging of more complex systems such as defects and adsorbed molecules. In particular, the combination of adsorbed organic molecules on insulating oxide surfaces provides an application-rich area. Here, we focus on the MgO (001) and TiO<sub>2</sub> (110) surfaces as general benchmarks in surface science, and also systems which have been imaged in atomic resolution with NC-AFM. We use theoretical simulations of the AFM imaging process as a tool to understand current, and predict future, experimental results.

We study the adsorption of acid molecules onto characteristic oxide surfaces - formate (HCOOH) on MgO and formate, acetate (CH<sub>3</sub>COOH) and trifluoroacetate (CF<sub>3</sub>COOH) on TiO<sub>2</sub>. The acid molecules all dissociate on TiO<sub>2</sub>, with the proton bonding to a bridging oxygen. On the ideal MgO surface the formate ion exhibits rich dynamic behaviour despite the nominal strength of the ionic bond and significant adsorption energy. The two-site structure of the molecule can be revealed at low temperatures. However, the mobility makes AFM detection of a single species at higher temperatures unlikely. Calculations of the TiO<sub>2</sub>-based systems with a reactive silicon tip demonstrate that the molecules are very inert, and atomic resolution would not be possible – the strongest interaction is between molecules, and Ti ions would actually appear as bright. However, it is possible to see the difference between H and F in a simulation of the mixed monolayer on TiO<sub>2</sub>, as in experiments on the same system [1]. Finally, we consider how a more realistic, oxidized silicon tip model affects the interaction, and whether it explains the differences between theory and experiment.

[1] A. Sasahara, H. Uetsuka and H. Onishi, Phys. Rev. B 64 (2001) 121406