

## Modeling of NC-AFM imaging of organic molecules on TiO<sub>2</sub> (110) surface

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We address the mechanism of non-contact atomic force microscopy (NC-AFM) of complex organic molecules adsorbed on the TiO<sub>2</sub> (110) surface in order to explain the contrast formation and explore the ways for manipulating these molecules with AFM tips. We have considered different tip models which simulate SiO<sub>2</sub> tip termination with either the material from the surface or silanol groups. Therefore the anatase cluster and different silanol terminated SiO<sub>2</sub> clusters were considered as tip models. The calculations demonstrate that the tip-surface interaction is electrostatic in nature. Oxygen and titanium rows can be resolved as well as the corresponding O and Ti ions inside the rows when imaged with anatase or oxygen terminated SiO<sub>2</sub> tip. We have studied the interaction of these tips with bi-benzoic acid and a prototype molecule (C<sub>52</sub>H<sub>72</sub>O<sub>3</sub>) for the NC-AFM manipulation adsorbed on the TiO<sub>2</sub> (110) surface (Fig.). Oxygen terminated silicon tip interacts strongly with both the molecules and the surface, which can be beneficial for obtaining high resolution NC-AFM images. We discuss the optimum tip structure and properties for simultaneous high resolution imaging of organic molecules and the surface.

In order to find the most favourable directions for the controlled manipulation of the C<sub>52</sub>H<sub>72</sub>O<sub>3</sub> molecule on TiO<sub>2</sub> (110) surface we have studied the barriers for its translational diffusion along the Ti rows in two orientations of the molecule with respect to the surface. Namely, the barriers were studied for the molecule oriented perpendicular to the Ti rows with the tail carboxylic group above the in-plane Ti atoms (Fig.) and for the transverse orientation with the molecules tail oriented parallel to Ti rows. Low barriers for translation of the molecule along the Ti rows, which were estimated to be less than 0.2eV, suggest that it can be a preferential direction for manipulation. The possibility for the rotation of the molecule around the carboxylic group will be also discussed.

