Dye Molecules on NiO(001) Studied by Non-Contact Atomic Force Microscopy

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The properties of NiO, such as charge transport or optoelectronic characteristics, can be modified by functionalization with organic molecules. These kinds of organic/inorganic surfaces are of great interest, in particular, for the design of hybrid devices like dye sensitized solar cells [1]. However, a key parameter in the design of optimized interfaces is not only the choice of the compounds but also the properties of adsorption. Thus, fundamental studies of such hybrid systems at the nanoscale are desirable. So far, characterization of adsorbates at ambient temperature through spectroscopy techniques, such as x-ray photoelectron spectroscopy, has been limited to large agglomerates or self-assembled molecules. Recently, first studies of the adsorption properties of single molecules on NiO measured by force microscopy at low temperatures have been published [2]. This limit can be stretched to the level of individual adsorbates measured by means of non-contact atomic force microscopy at room temperature.

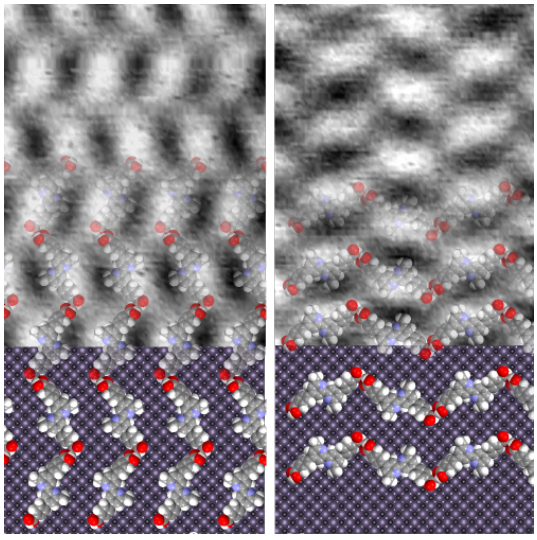

Fig. 1: High resolution topographic image of self-assembled 4,4´-di(4-carboxyphenyl)-6,6´-dimethyl-2,2´-bipyridine molecules on NiO(001). Two different island orientations (left and right image) have been observed. A model of the molecular arrangement and the NiO substrate are superimposed in the lower part of the image.

We investigated the deposition of a 2,2´-bipyridine based molecule, functionalized with carboxylic acid anchoring domains on a NiO(001) single crystal surface [3,4]. Depending on the coverage, single molecules, groups of adsorbates with random or recognizable shapes, or islands of closely packed molecules could be identified. Single molecules and self assemblies, as visible in the image on the right side, are resolved with submolecular resolution showing that they are lying flat on the surface with the 2,2´-bipyridine in a trans-conformation. Only in the close-packed form was a measurable charge transfer from the NiO to the molecular layer of 0.3 electrons per molecule observed independent on the molecular orientation of the islands.

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