

## Carboxylic acids on metal oxide surfaces - UHV-IR-spectroscopy study

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The role of metal oxides is central in many technological areas such as gas sensing, catalysis and thin film growth. In last decades numerous IR investigations of metal oxide powders, including the different modifications of TiO<sub>2</sub>, have been reported, however an unambiguous assignment of the features in the complex IR spectra recorded for molecules bound to the oxide powders is quite complicate. Otherwise, it could be possible on the basis of data recorded for well-defined reference systems, e.g. surfaces of single crystals, but, unfortunately, studies on oxide single crystals are extremely scarce due to the fact that the sensitivity of reflection IR-spectroscopy for molecular adsorbates is two orders of magnitude lower for oxides than for metal single crystals.

Owing to the fact that many Dye Sensitized Solar Cells (DSSCs) consist of dyes grafted to the oxide support via carboxylate groups determining and controlling the adsorption of carboxylic acids on oxidic substrates is fundamental to understanding the energy transfer from the molecule to the substrate.

The adsorption of benzoic and terephthalic acids<sup>[1]</sup> was studied with the highly sensitive UHV IRRAS<sup>[2]</sup> system. The obtained data were compared with the results of DFT-Slab-calculations and the theoretical calculated reflectivity of these molecules on r-TiO<sub>2</sub> (110). The IR-spectra allow, in particular, answering the question whether the carboxylic acid group is still protonated, a question which could not be answered by the results from x-ray absorption spectroscopy<sup>[1]</sup>.

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- [1] P. Rahe, M. Nimmrich, A. Nefedov, M. Naboka, C. Woll, A. Kuhnle, *Journal of Physical Chemistry C* **2009**, *113*, 17471-17478.  
[2] Y. Wang, A. Glenz, M. Muhler, C. Wöll, *Rev. Sci. Instrum.* **2009**, *80*, 113108-113106.