

Infrared reflection absorption spectroscopy on metal oxide single crystals

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Infrared Reflection Absorption Spectroscopy (IRRAS) studies of molecule adsorption on metal oxide single crystals are extremely scarce due to the fact that the reflectivity of such samples is two orders of magnitude lower than of metal single crystals. Moreover, for metal surfaces vibrational modes with a transition dipole moment orientated parallel to the surface cannot be seen in IR spectra, because the s-polarized light is annihilated at grazing incidence (the surface selection rule). Otherwise, for dielectric surfaces the situation is more complicated, since both s- and p-polarized light couples with adsorbate vibrations.

In this presentation I outline our results of IRRAS studies carried out under UHV conditions on metal oxide single crystals. The measurements have been done at different azimuths both with s- and p-polarized light. That allowed to determine the orientation of the functional groups on the different metal oxide single crystal surfaces, in particular, the mixed-terminated ZnO(10-10), anatase TiO₂ (101)^[1] and rutile TiO₂ (110). These surfaces were chosen, because they are the dominating surface for powder particles and energetically most favorable. The adsorption of small molecules like CO and CO₂, which are used in catalytic reactions, as well as the adsorption of some carboxylic acids, will be discussed in a detail.

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[1] M. C. Xu, H. Noei, M. Buchholz, M. Muhler, C. Wöll, Y. M. Wang, *Catalysis Today* **2012**, *182*, 12-15.