Dissociation of formic acid on anatase TiO_2 (101) probed by vibrational spectroscopy

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The role of metal oxides is central in many technological areas such as gas sensing, solar energy conversion, water splitting and environmental treatments. It is known that most TiO_2 nanoparticles show the anatase form, which exhibits generally a substantially higher photocatalytic activity than that of rutile TiO_2 (110) [1]. In last decades numerous Infrared (IR) investigations of metal oxide powders, including the different modifications of TiO_2, 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.

Here, the interaction of formic acid with anatase TiO_2(101) has been monitored by infrared reflection absorption spectroscopy (IRRAS) using a novel ultrahigh vacuum (UHV) system[2]. It was found that the formic acid molecules do not adsorb intact on TiO_2(101), as proposed previously, but dissociate yielding different formate species. The IR-bands observed in the IRRAS-data indicate the presence of a mono- and a bidentate species. It is proposed that the formation of the bidentate form could be present only with of oxygen vacancies[3].

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