

Bulk Defect Dependent Adsorption of Acetone on Rutile TiO₂(110)

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In chemical industry acetone is produced by the Cumene Process using homogenous catalysis. However, this process causes many problems like the handling of peroxides, acids, the by-product phenol and a difficult heat treatment.[1] To get rid of these problems a heterogeneously catalysed process is considered. Cao et al. already showed production of acetone by photo oxidizing *i*-propanol adsorbed on MnO₂. Here, only a conversion of 8 % can be achieved.[2] That is why, we want to elucidate the potential of TiO₂ as alternative photo catalyst. An important part of the reaction is the interaction of acetone with titania itself. Therefore, the adsorption of acetone on rutile TiO₂(110) was studied as model system.

Recently, an influence of the temperature dependent mobility of bulk defects has been proven by own work to be important in thermal reactions on titania as apparent from reductive coupling of benzaldehyde.[3] We further indicated that the reduction state of titania strongly influences the population of different reaction paths.[3] In previous coverage dependent studies on acetone and coadsorbed molecular oxygen the occurrence of a diolate species has been identified on a medium reduced single crystal by Henderson and cooperation partners.[4,5] Therefore, we considered the adsorption of acetone and coadsorption with molecular oxygen and oxygen adatoms on a lower and stronger reduced rutile TiO₂(110) single crystal to elucidate the impact of defects by means of Temperature Programmed Reaction Spectroscopy (TPRS) and polarized FT-Infrared Reflection Absorption Spectroscopy (FT-IRRAS). For a low reduction degree an adsorption behaviour as described by Henderson for a medium reduced single crystal is proposed. Besides diolate a possible β -hydroxy ketone formation enhanced by oxygen adatom coadsorption is found at stronger reduced single crystals.

References:

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