Defect density dependence of partial oxidation and deoxygenation reactions of small organic compounds on rutile TiO_2 (110) surfaces

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Though titanium dioxide is among the most interesting (photo-)catalyst materials, many structural details of the occurring thermic and photo-stimulated reactions remain unclear, particularly with respect to the role of different defects.[1-3] For our mechanistic studies under ultra-high vacuum (UHV) conditions we use a rutile TiO_2 (110) single crystal surface to investigate the adsorption and reaction of small organic molecules such as methanol or methylamine with respect to the defect density.[4]

Defect states like bridging oxygen vacancies as well as Ti^{+III} interstitials can easily be introduced to this material via argon ion sputtering and subsequent annealing in UHV. Around 300 K the Ti^{+III} interstitials start to be mobile and can diffuse towards the surface.[3] We shall present our latest results illustrating the importance of such diffusive bulk defects for thermal reactions of organic molecules such as deoxygenation C-C coupling reactions or partial oxidation in different temperature regimes for alcohols in comparison to amines. Furthermore, we demonstrate the importance of different oxygen species present at the surface for these reactions, using low energy electron diffraction (LEED), temperature programmed desorption spectroscopy (TPD) and in addition Fourier-transformation polarized infrared reflection-absorption spectroscopy (FT-IRRAS).

References:
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