

High-Resolution STM and TPD Studies of Surface Reactions on Rutile TiO₂(110)

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In this talk, we summarize recent surface science studies on a prototypical model oxide system – the rutile TiO₂(110)–(1 × 1) surface. We present clear-cut identification of surface defects such as oxygen vacancies, hydroxyl groups, and near surface defect such as Ti interstitials. Based on these assignments we discuss the complex oxygen–TiO₂(110) interaction. Specifically, the role of bulk defects in the oxygen chemistry on reduced rutile TiO₂(110) is studied by means of scanning tunnelling microscopy (STM) and temperature-programmed desorption (TPD) measurements. An ionosorption model is proposed to explain the obtained STM and TPD results. In addition, we show that these results help to improve our understanding of the use of TiO₂ as photo-catalyst. By means of high resolution STM and TPD/TPR spectroscopy, we studied the desorption and thermal decomposition of ethanol and ethoxide groups on differently prepared TiO₂(110) surfaces. Furthermore, direct evidence for ethanol dissociation at bridging O vacancies will be presented. Accompanying density functional theory calculations support the assignments made in the STM studies and rationalize the observed distinct diffusion behaviors of molecularly and dissociatively adsorbed ethanol species. Finally, we discuss the photo-reaction of ethanol on differently prepared TiO₂(110) surfaces.