

A comparison of pyrocatechol on anatase (101) and rutile (110) surfaces of TiO₂ using photoelectron and NEXAFS spectroscopy

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TiO₂ is of technological interest due to its photocatalytic properties, biocompatibility and use in photovoltaic solar cells. Many of these applications use TiO₂ in a nanoparticulate form, which adopt the anatase structure. However, single crystals of anatase TiO₂ are difficult to grow so rutile single crystals, which are readily available, have been studied more widely. Pyrocatechol is of interest as a potential light harvesting molecule, which could be used in photovoltaics since adsorption of the catechol on titania nanoparticles shifts the absorption from 370 nm to 420 nm [1,2]. It has been suggested that this is due to a direct catechol to TiO₂ conduction band charge transfer process [2]. In addition, dopamine, a related molecule, is being studied as a functionalising molecule on TiO₂ nanoparticles for pharmaceutical applications [3].

This work investigates the adsorption of pyrocatechol on TiO₂ rutile and anatase surfaces to determine the adsorption geometry using NEXAFS spectroscopy. In addition photoelectron spectroscopy is utilised to investigate the effect on the electronic structure of the surface and adsorbate following deposition of 1ML pyrocatechol. It is found that following adsorption O-vacancies on the clean surfaces are removed, as evidenced by the reduction of the so-called defect state in valence band photoemission. This in turn leads to band-bending at the surface. Finally experimental data are compared to DFT cluster calculations in order to interpret the experimental data in terms of the stability of the adsorbate.

References

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