Abstract template:

**Title**
Surface Characterization of Nanoscale TiO$_2$ Film by Sum Frequency Generation Using Methanol as a Molecular Probe

**Reference**

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**Abstract**

Sum frequency generation (SFG) vibrational spectroscopy is applied to study the surface characteristics of a film composed of nanoscale TiO$_2$ particles, in which methanol is employed as a molecular probe. The SFG signal from methanol adsorbed on the TiO$_2$ film surface in the CH region consists of four primary peaks located at 2828, 2855, 2935, and 2968 cm$^{-1}$. The peaks at 2855 and 2968 cm$^{-1}$ arise from molecular methanol; the other two are attributed to methoxy produced by dissociative chemisorption of methanol on TiO$_2$. Changes in the SFG features with methanol pressure and with surface temperature provide the first direct proof of methoxy generation on nanoparticulate films. In comparison with molecular methanol, methoxy sits more perpendicularly on the surface. The chemisorption is barrierless, and a Langmuir constant of $2.13 \pm 0.14 \times 10^3$ is derived from the adsorption isotherm. Moreover, UV pretreatment of the TiO$_2$ film substantially increases the methoxy signal. Changes in SFG intensity are in good agreement with the current models for surface active sites and face specificities on TiO$_2$. 