SO₂ adsorption on rutile TiO₂(110): An infrared reflection-absorption spectroscopy and density functional theory study

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The removal of sulfur oxide gasses from emissions is of great environmental concern. Here TiO₂ has shown to be an effective catalyst in desulfurization reactions [1]. Furthermore, the photochemistry of TiO₂ provides alternative routes for low-temperature surface reactions, and ways to modify its surface properties [2,3]. These applications all require fundamental insight into the basic surface science of the SO₂/TiO₂ system. We will present, for the first time, a study of the interaction between SO₂ and TiO₂(110) using Infrared Reflection-Absorption Spectroscopy (IRRAS). DFT calculations of various binding configurations have also been carried out and the corresponding IRRAS spectra from these configurations have been obtained through simulation. This has enabled a unique interpretation of the experimental results, where a specific SO₃-like adsorption structure has been identified. It also enables a re-interpretation of previously reported findings.

The figure below illustrates the method by which polarized IRRAS measurements can be used in combination with theoretical simulations to not only determine the chemical state of an adsorbate, but also determine its geometrical orientation and atomic coordination to the surface. This type of measurement can only be performed on single crystals in ultrahigh vacuum, which is a system that is particularly well suited for DFT modeling.

References: