SO_2 adsorption on rutile TiO_2(110): An infrared reflection-absorption spectroscopy and density functional theory study

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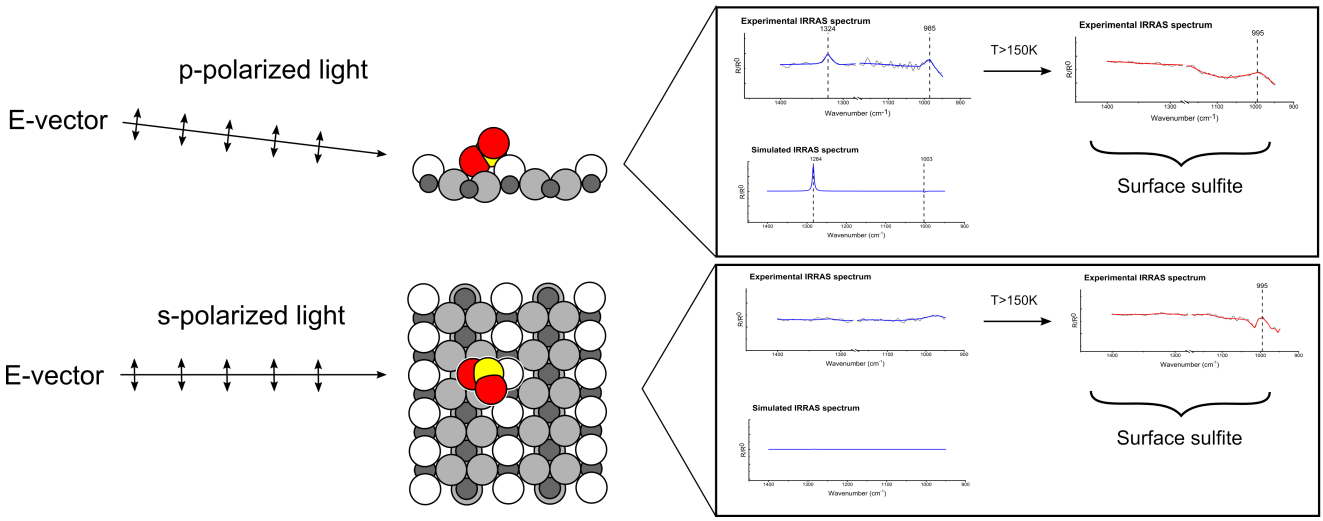
The removal of sulfur oxide gasses from emissions is of great environmental concern. Here TiO_2 has shown to be an effective catalyst in desulfurization reactions [1]. Furthermore, the photochemistry of TiO_2 provides alternative routes for low-temperature surface reactions, and ways to modify its surface properties [2,3]. These applications all require fundamental insight into the basic surface science of the SO_2/TiO_2 system. We will present, for the first time, a study of the interaction between SO_2 and TiO_2(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 SO_3-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:

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