# Quantum Chemical Investigation of $SO_2$ Adsorption and Electronic Structure on $TiO_2$ Anatase-[101] and Rutile-[110] Surfaces

**L. Gerhards, T. Klüner**

*Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany*
*luca.gerhards@uni-oldenburg.de*

The reaction of $SO_2$ on titanium dioxide has been used in industry for the production of sulphuric acid for several years. The photocatalytic activity of $TiO_2$ has also been applied in current research to react $SO_2$ with hydrocarbons to form sulfonic acids. The big advantage is the use of visible light and the resulting better efficiency than with the common UV-light process. However, the mechanism of this reaction is widely unexplained and contrasts with the postulated mechanism without catalyst (see fig 1). [1,2] Through quantum chemical investigations it is possible to gain a deeper insight into this system and clarify fundamental steps of the reaction.

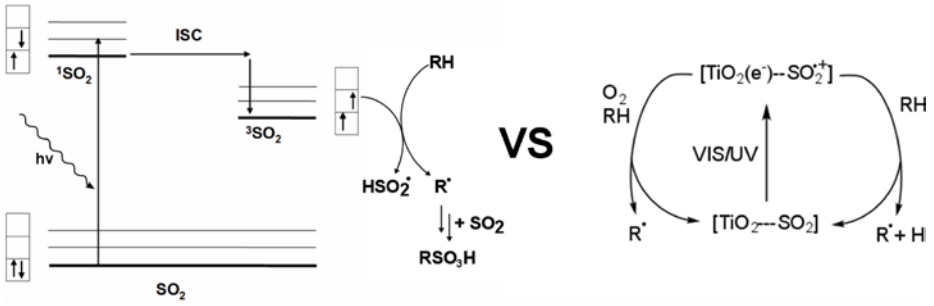


**Figure 1: Two possible mechanisms for the electronic excitation of $SO_2$ on the titanium dioxide surface. [1,2]** In this contribution, the adsorption of $SO_2$, the interaction with hydrocarbons and the resulting electronic properties on selected surfaces of different $TiO_2$ modifications are quantum chemically examined. The software package CRYSTAL17 is used to describe surface effects efficiently by means of periodic boundary conditions. [3] In addition, the differences and the behavior of $SO_2$ on anatase and rutile are contrasted and possible advantages of the individual modifications are examined.

[1] F. Parrino, A. Ramakrishnan, H. Kisch, *Angew. Chem. Int. Ed*. **47**(37), 7107-7109 (2008).

[2] F. Parrino, A. Ramakrishnan, C. Damm, H. Kisch, *ChemPlusChem* **77**(8), 713-720 (2012).

[3] R. Dovesi, et al., *WIREs Comput Mol Sci*. **8**, e1360 (2018).