## Titanium-based catalysts for CO2 activation: Experimental modelling of hybride (photo-)catalysts

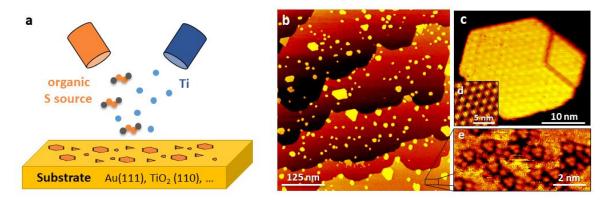
Niko Kruse, Justin Klimek, Celina Groothuis, and Lars Mohrhusen

Institute of Chemistry, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany. Contact: lars.mohrhusen@uol.de

Conversion of greenhouse gases and especially CO<sub>2</sub> into useful hydrocarbons via a low-cost route is among the major challenges of the current energy transition. For this purpose, photocatalysis may be a relevant technology, as sunlight is a free and unlimited energy source, and photoreactions usually do not require high temperatures. Oxide-based photocatalysts usually consist of a semiconducting oxide support with nanostructured (noble) metal particles.<sup>1</sup> Unfortunately, these metals are often expensive and have limited lifetimes due to for example sintering, coking or poisoning with carbon monoxide. Thus, for several reasons, it is attractive to develop strategies to replace noble metal in such systems.<sup>2</sup>

Titanium is one of the few elements, that are attractive in terms of its natural availability and considering various economic and ecological aspects. Titanium dioxide  $(TiO_2)$  for example offers a broad platform, as e.g. defects such as  $Ti^{3+}$  interstitials can boost the photocatalytic activity towards oxygen containing molecules.<sup>3,4</sup> TiO<sub>2</sub> also readily forms hybrid systems with other oxides (e.g. WO<sub>3</sub> clusters)<sup>4</sup> or sulfides such as MoS<sub>2</sub>.<sup>5</sup> Thus, we investigate titanium-based hybrid photocatalytic systems using well-defined model catalysts under ultrahigh-vacuum conditions.

Herein, we present selected results from well-defined model catalysts en route to the desired Ti-based hybrid materials, for example, nanostructured combinations of  $TiS_2$  and  $TiO_2$ .  $TiS_2$  has a broad light absorbance throughout the visible range, is easily reduceable and widely inert to CO poisoning, rendering it an attractive material. Our multi-method approach involves combinations of spectroscopy (esp. photoelectron spectroscopy (XPS)), microscopy (scanning tunneling microscopy (STM)) and reactivity studies (temperature-programmed desorption (TPD)). As one example, nanoparticles of  $TiS_2$  as a classic 2D TMDC can be fabricated and studied on various substrates to derive an atomic-level understanding of structure-reactivity relationships (figure 1).



**Figure 1:** a) schematic representation of the synthesis of  $TiS_2$  nanoparticles. b-c) STM images of  $TiS_2$  particles on Au(111). d) high-resolution image of a  $TiS_2$  basal plane on Au(111). e)  $TiS_3$  and TiS clusters in the Au(111) background as nucleates of bigger  $TiS_2$  particles. <sup>6</sup>

## References

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