Structure and Dynamics of Water at Photocatalytic Interfaces

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Finding a clean and renewable energy source to replace fossil fuels has attracted much attention, the past few decades, as a step towards the sustainable development of societies. Direct hydrogen generation on TiO_2 by photocatalytic dissociation of water using sunlight was already proposed almost 50 years ago. However, despite extensive work in this area, the fundamentals of the process remain ill-understood, mainly due to the lack of a proper tool to specifically explore the interface between water and photocatalysts on ultrafast timescales. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of the water-solid interface without monitoring the bulk water. From the intensity and frequency of the static SFG signal we extract information about the different water species binding to photocatalysts.

To obtain information on the mechanism of the water splitting process, in the first part of the talk we will look into the structure of water in contact with ironoxide, both hematite and magnetite [1]. In the second part, we will put our focus on a dynamical study at the water-TiO_2 interface after excitation with a short UV pulse mimicking sun light. Subsequently, the O-H stretch vibration of the interfacial species are monitored on a subpicosecond timescale with SFG spectroscopy. Our data show that the surface charge changes on ultrafast timescales upon excitation resulting in reorientation and partly dissociation of the water molecules on 10s of ps timescales. These UV-pump SFG-probe data illustrate the first steps towards following the photo-induced dissociation of water at the TiO_2 interface in real-time. [2]

References

[1] S. Romano et al. (2024) arXiv:2410.12717.
[2] E.H.G. Backus et al. Angew. Chem. Int. Ed. (2024) **63**, e202312123.