

# X-ray emission spectroscopy to understand photochemical reactions and mechanisms

M. Bauer

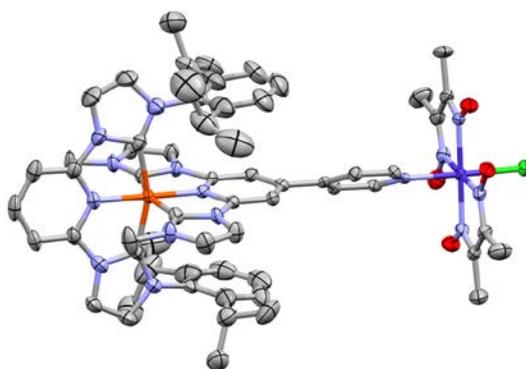
University of Paderborn, Chair for Inorganic chemistry, Warburger Str. 100, 33098 Paderborn, Germany,  
**matthias.bauer@upb.de**

The conversion of sunlight into fuels or chemicals gains lots of attention by the so-called Sun-to-X approach. The conversion of protons in water to hydrogen using sun light is the standard reaction of this type. In particular with the renaissance of fuel cells as alternative to batteries, sustainable hydrogen production becomes even more important.

Using base metals instead of noble metals increases the sustainable character of photocatalytic proton reduction. Both in photosensitizers and photocatalysts metals like iron and cobalt can be used. However, achieving competitive activity requires major efforts in photosensitizer and catalyst design. Due to the very limited knowledge about the properties and functionality of base metal compounds in this context, fundamental insights into their working principle are required.

X-ray emission based spectroscopy provides unique details about the electronic and geometric structure of iron and cobalt photosensitizers and photocatalysts [1]. This will be demonstrated with selected examples of two-component systems, where photosensitizer and catalyst are independent compounds. One focus here will be the identification and investigation of hydride ligands, which play a dominant role in proton reduction reactions [2].

The contribution will close with the presentation of dyads (figure 1), that connect photosensitizer and catalyst in a bimetallic complex.[3] Cutting edge two-colour emission experiments at X-ray free electron lasers, that record the emission lines of both metal sites simultaneously, show unprecedented new insights into the excited state behaviour of this new compound class.



**Figure 1:** Example of a bimetallic dyad using iron as photosensitizer and cobalt as catalyst

## References

- [1] - M. Bauer, *Phys. Chem. Chem. Phys.* **16**, 13827 (2014).
- [2] - L. Burkhardt, M. Holzwarth, B. Plietker, M. Bauer, *Inorg. Chem.* **56**, 13300 (2017).
- [3] - P. Zimmer, L. Burkhardt, R. Schepper, K. Zheng, D. Gosztola, A. Neuba, U. Flörke, C. Wölper, R. Schoch, S.E. Canton, M. Bauer, *Eur. J. Inorg. Chem.* 5203 (2018).