

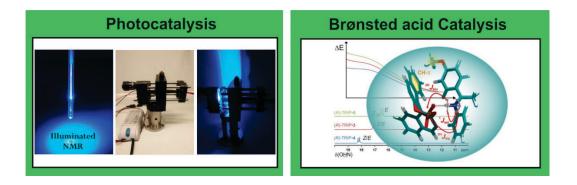
IN-7

## NMR IN CATALYSIS AND PHOTOCATALYSIS PUSHING THE FRONTIERS

Ruth M. Gschwind

Institute of Organic Chemistry, University of Regensburg, 93040 Regensburg, Germany ruth.gschwind@chemie.uni-regensburg.de

The detection and characterization of intermediates in catalytic reactions is crucial for the rational optimization of reaction conditions. However, in many rapidly expanding fields of asymmetric catalysis, mechanistic studies as well as structural investigations on intermediates or intermolecular interactions are scarce. In this talk I will present techniques and methods to extend the application of NMR in catalysis and photocatalysis and explain their impact on examples. First our LED based NMR illumination device<sup>[1]</sup> will be introduced together with the new triple combination illumination/NMR/UV<sup>[2]</sup> and an NMR access to intermediates below the detection limit.<sup>[3]</sup> These methods allow for new insights into one- versus two-electron processes usually inaccessible to UV/Vis,<sup>[4]</sup> the inclusion of radical species into NMR reaction profiles,<sup>[2]</sup> the structure elucidation of thermally labile photoswitches<sup>[2]</sup> and the sequencing of tiny intermediates.<sup>[5]</sup> Last, the extension of the NMR time scale to µs is demonstrated using relaxation dispersion methods. In a catalyst substrate complex taken from Brønsted acid catalysis even the switching of a single hydrogen bond can be detected experimentally.<sup>[6]</sup>



## REFERENCES

- [1] C. Feldmeier, H. Bartling, E. Riedle, R. M. Gschwind, J. Magn. Res., 2013, 232, 39.
- [2] A. Seegerer, P. Nitschke, R. M. Gschwind, Angew. Chem. Int. Ed. 2018, 57, 7493-7497.
- [3] L. Nanjundappa, A. Seegerer, J. Hioe, R. M. Gschwind, JACS 2018, 140, 1855-1862.
- [4] C. Feldmeier, H. Bartling, K. Magerl, R. M. Gschwind, Angew. Chem. Int. Ed., 2015, 54, 1347.
- [5] S. Wang, L. Nanjundappa, J. Hioe, R. M. Gschwind, B. König, Chem. Sci., 2019, 10, 4580.
- [6] L. Nanjundappa, J. Hioe, J. Gramueller, R. M. Gschwind, submitted.