ON DATA, DISCOVERY & SENSITIVITY IN (PHOTO)CATALYSIS

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Catalysis is a key technology, since it allows for increased levels of selectivity and efficacy of chemical transformations. While significant progress can be made by rational design or engineered step-by-step improvements, many pressing challenges in the field require the discovery of new and formerly unexpected results. Arguably, the question "How to discover?" is at the heart of the scientific process. In this talk, (smart) screening strategies for accelerated discovery and improved reproducibility will be presented,[1] machine learning for chemistry will be discussed,[2] together with new photocatalytic transformations.[3,4] In addition, two other exciting areas will be addressed briefly:

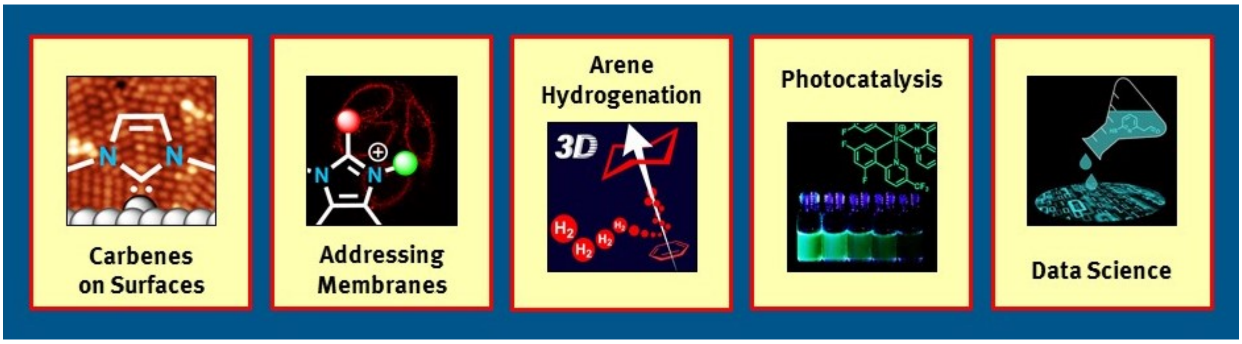

Figure 1. Graphical teaser for the work presented.

N-Heterocyclic Carbenes (NHCs)[5] are powerful ligands in catalysis due to their strong electron-donating properties and their ability to form very stable bonds to transition metals. In addition, they can stabilize and modify nanoparticles or flat metals surfaces, outperforming established phosphine or thiol ligands regarding structural flexibility, electron-donating properties and stability. Current research is highly interdisciplinary and focusses on the basic understanding of the binding mode, mobility and the elucidation of the impact on the surface properties. Exciting applications in materials science, heterogeneous catalysts and beyond are within reach.[6]

Biological membranes and their constituents are some of the most important and fundamental building blocks of life. However, their exact role in many essential cellular processes as well as in the development of diseases such as cancer or Alzheimer's is still not very well understood. Thus, we design, synthesize and evaluate imidazolium-based lipid analogs that can integrate into biological membranes and can be used as probes for live cell imaging or to manipulate membranes.[7]

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References

1. L. Pitzer, F. Schäfers, F. Glorius, *Angew. Chem. Int. Ed.* **2019**, *58*, 8572-8576. M. L. Schrader, F. R. Schäfer, F. Schäfers, F. Glorius, *Nat. Chem.* **2024**, *16*, 491-498.
2. F. Strieth-Kalthoff, F. Sandfort, M. H. S. Segler, F. Glorius, *Chem. Soc. Rev.* **2020**, *49*, 6154-6168. F. Strieth-Kalthoff, F. Sandfort, M. Kühnemund, F. R. Schäfer, H. Kuchen, F. Glorius, *Angew. Chem. Int. Ed.* **2022**, *61*, e202204647. D. Rana, P. M. Pflüger, N. P. Hölter, G. Tan, F. Glorius, *ACS Cent. Sci.* **2024**, *10*, 899-906.
3. J. Ma, S. Chen, P. Bellotti, R. Guo, F. Schäfer, A. Heusler, X. Zhang, C. Daniliuc, M. K. Brown, K. N. Houk, F. Glorius, *Science* **2021**, *371*, 1338-1345. R. Kleinmans, T. Pinkert, S. Dutta, T. O. Paulisch, H. Keum, C. G. Daniliuc, F. Glorius, *Nature* **2022**, *605*, 477-482. H. Wang, H. Shao, A. Das, S. Dutta, H. T. Chan, C. Daniliuc, K. N. Houk, F. Glorius, *Science* **2023**, *381*, 75-81.
4. F. Strieth-Kalthoff, M. J. James, M. Teders, L. Pitzer, F. Glorius, *Chem. Soc. Rev*. **2018**, *47*, 7190-7202. S. Dutta, J. E. Erchinger, F. Strieth-Kalthoff, R. Kleinmans, F. Glorius, *Chem. Soc. Rev*. **2024**, *53*, 1068-1089.
5. M. N. Hopkinson, C. Richter, M. Schedler, F. Glorius, *Nature* **2014**, *510*, 485-496. P. Bellotti, M. Koy, M. N. Hopkinson, F. Glorius, *Nat. Rev. Chem.* **2021**, *5*, 711-725.
6. M. Koy, P. Bellotti, M. Das, F. Glorius, *Nature Catal.* **2021**, *4*, 352-363.
7. T. Wegner, R. Laskar, F. Glorius, *Curr. Opin. Chem. Biol.* **2022**, *71*, 102209.