Electron Spin Resonance Spectroscopy in Catalysis: Setup for In-Situ Studies and Characterization of Catalysts

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Overcoming the ongoing climate crisis is most likely one of the biggest hurdles of the current century. It is important to decrease the emissions caused by human hand, but also to make room for additional and attractive options, for example the chemical reduction of CO2 to useful carbon-based resources. Modern catalysis approaches, such as mimicking natures enzymatic reactions are an attractive option for succeeding in this mammoth task.1 The use of immobilized catalysts in confined geometries could improve selectivity and catalyst stability, allowing the tailored reduction of CO2 to C2 and higher products, mitigating the effects of global warming.

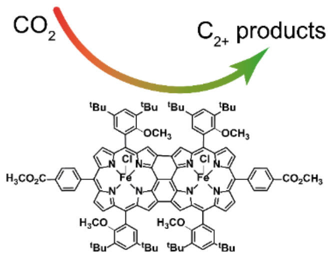

Figure 1: Triply fused iron porphyrin scaffold as a potential photo-/ electro-catalyst for the reduction of CO2

This work is focused on novel metal porphyrins and their fused species as potential catalysts to reduce CO2. Initial characterization of the electronic ground state by means of HF-EPR (320 GHz) and SQUID is important to understand these possible photo /electro-catalysts. Another principal tool to investigate such catalytic systems is In-situ EPR.2 The development of this method allows to study catalysis in realistic environments, becoming more important than ever with the recent focus on first row transition metal catalysts favoring single electron transfers. The ultimate goal is to confirm the effects of confinement on catalysis by comparing the homogenous catalyst with the in mesoporous silica immobilized species.

[1] Buchmeiser, M. R., ChemCatChem, 2021, **13**, 785, doi.org/10.1002/cctc.202001941

[2] Bonke, S. A., et. al., Nat Rev Methods Primers, 2021, **1**, 33, doi.org/10.1038/s43586-021-00031-4