

Freie Universität



Berlin

AG Sarkar: Where Catalysis and Switching meet (Spectro)electrochemistry

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15.11.24

Research and Drinks



Research Topics: Sarkar Group

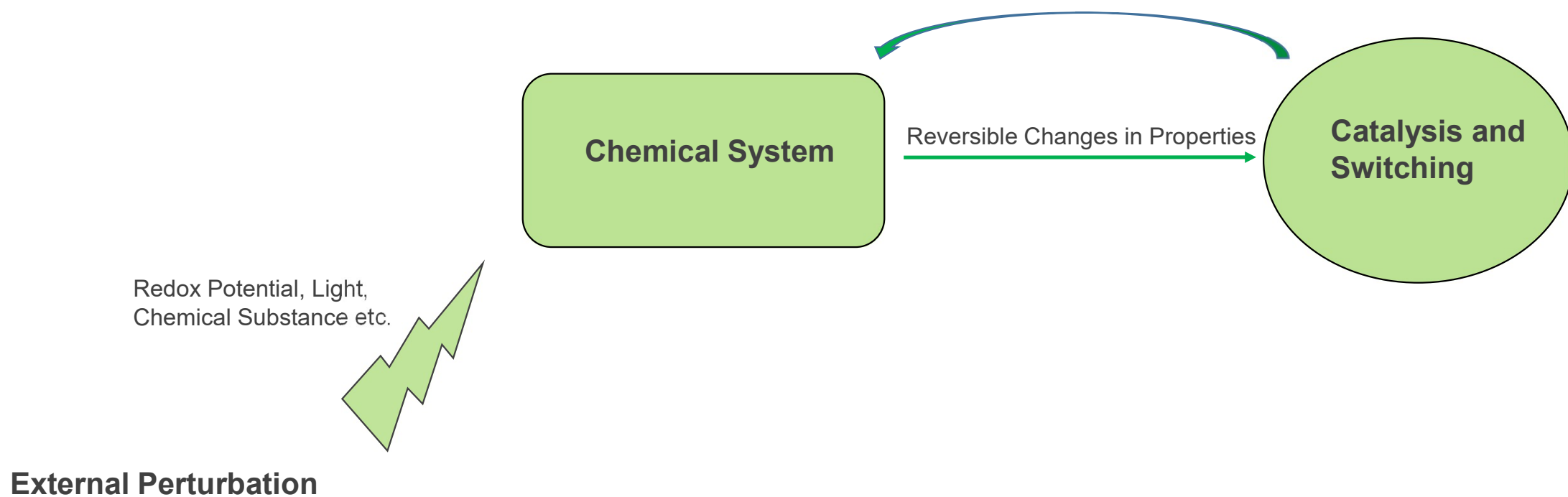
- ✓ **Switchable Systems for Magnetic and Optoelectronic (Near-IR, Electrochromic) Molecular Materials**

- ✓ **Metal Complexes for Activation and Production of H₂ and Activation of O₂, CO₂ and (H₂O)**

- ✓ **Stimuli Responsive Homogenous Catalysis**
 - (Transfer)hydrogenation of various functionalities
 - C-H Functionalization, Oxidation Catalysis
 - Cyclization reactions, (Polymerization Catalysis)

- ✓ **Reagents for Bioorthogonal Chemistry**

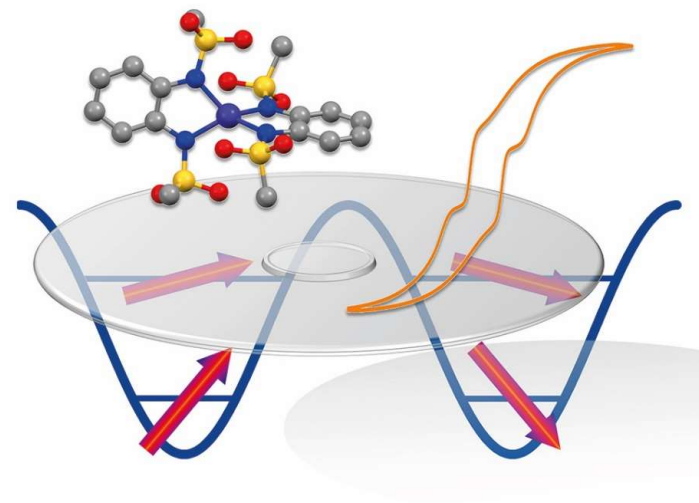
Binding Theme: Sarkar Group



Relevance of the Topics: Sarkar Group



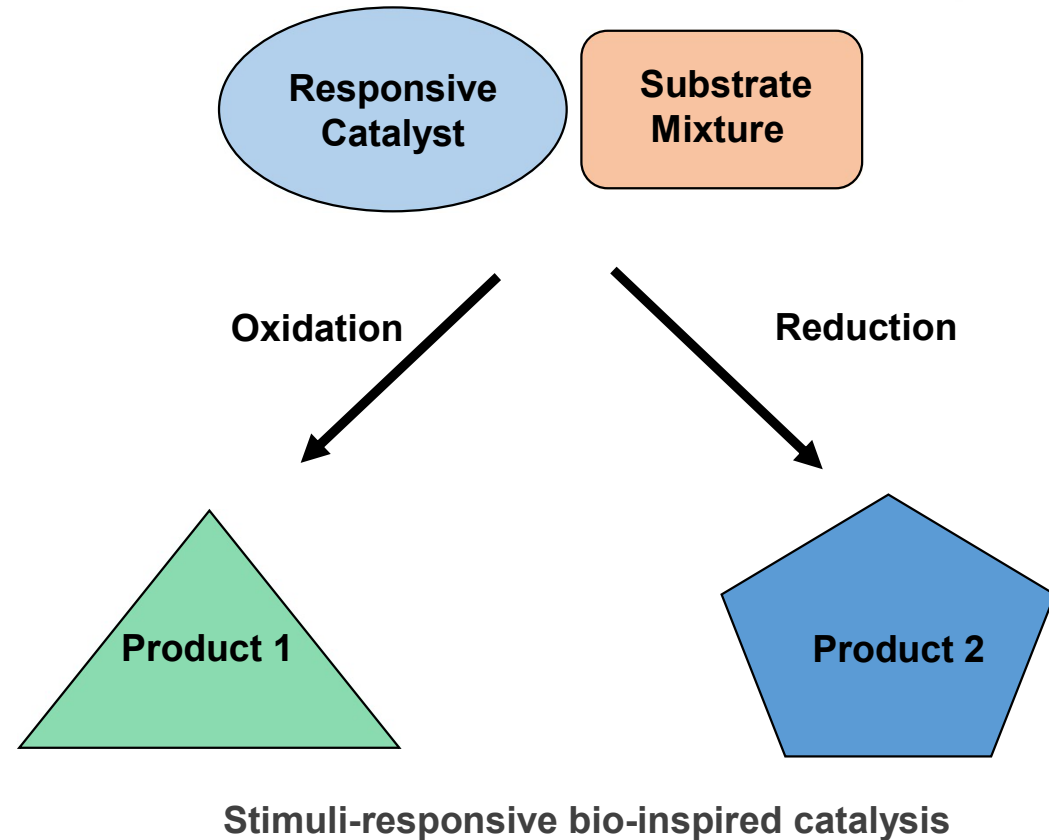
Electrochromism in Smart Windows



Single Molecule Magnets for Data Storage

Picture credits: MIT Research and Sarkar/van Slageren

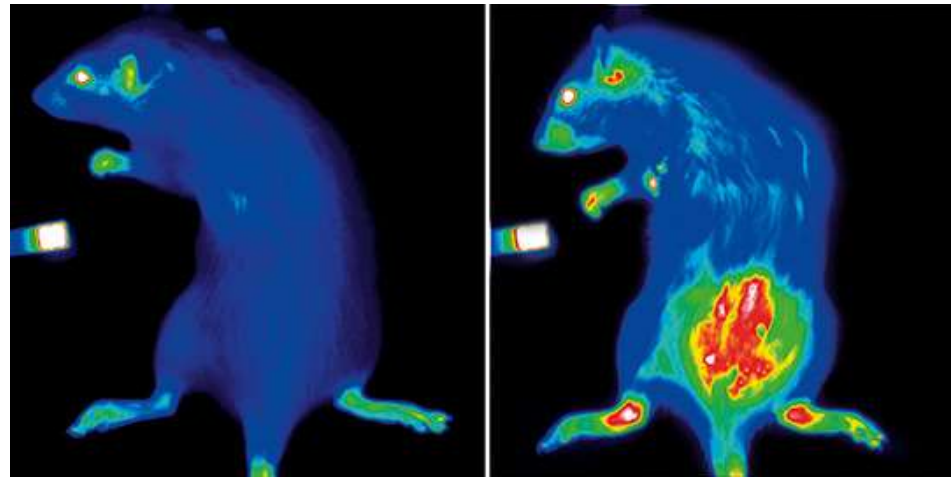
Relevance of the Topics: Sarkar Group



Energy-related research and sustainability:

Reduce CO_2 to CO and proton to H_2 and use as syngas.
Reduce CO_2 to formic acid/oxalic acid/methanol

Relevance of the Topics: Sarkar Group



Medicinal diagnostics: Imaging

Finding bio-compatible fluorescent markers

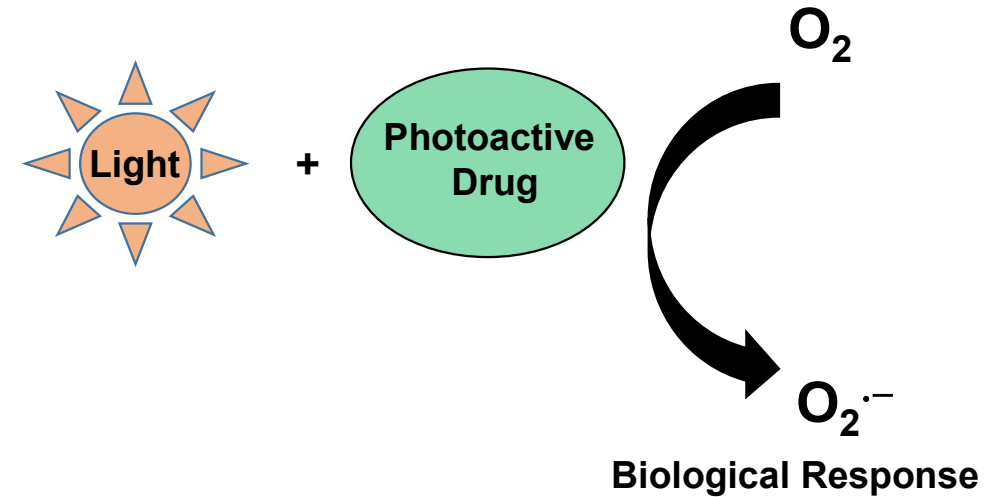


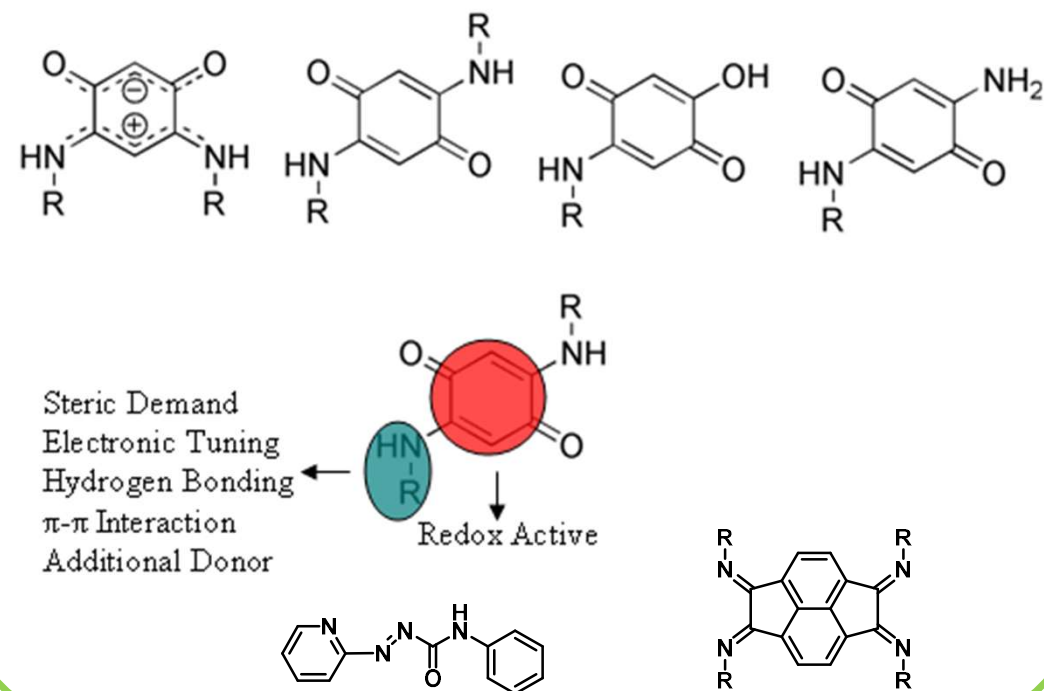
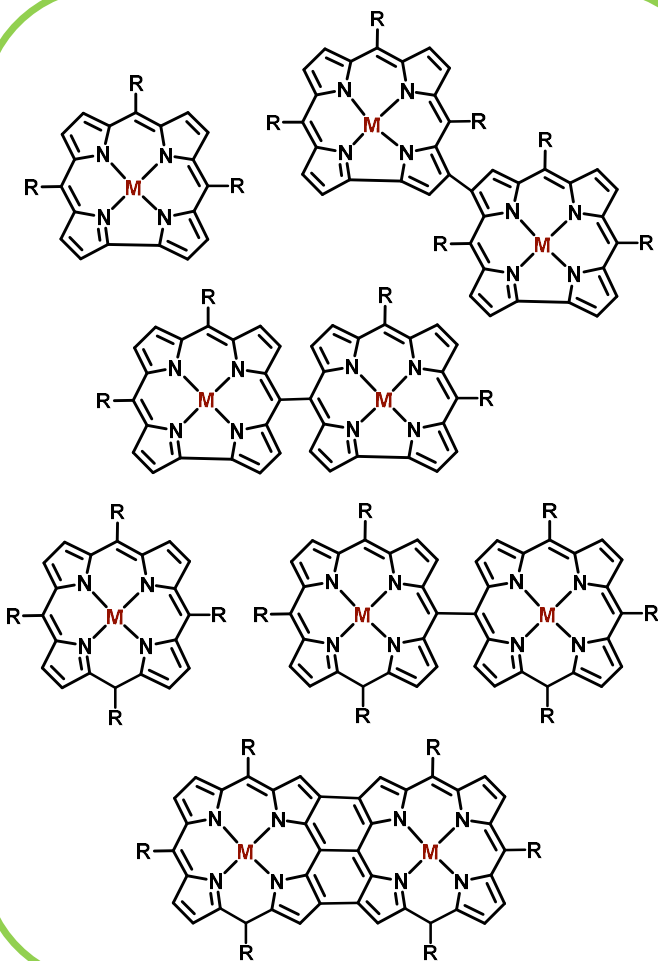
Photo Dynamic Therapy

Reactive oxygen species / free radicals
PDT for anti-tumor therapy

Medicinal therapeutics:
Finding „non-toxic“ substitutes for porphyrinoid systems

Image credit: www.kerafest.com

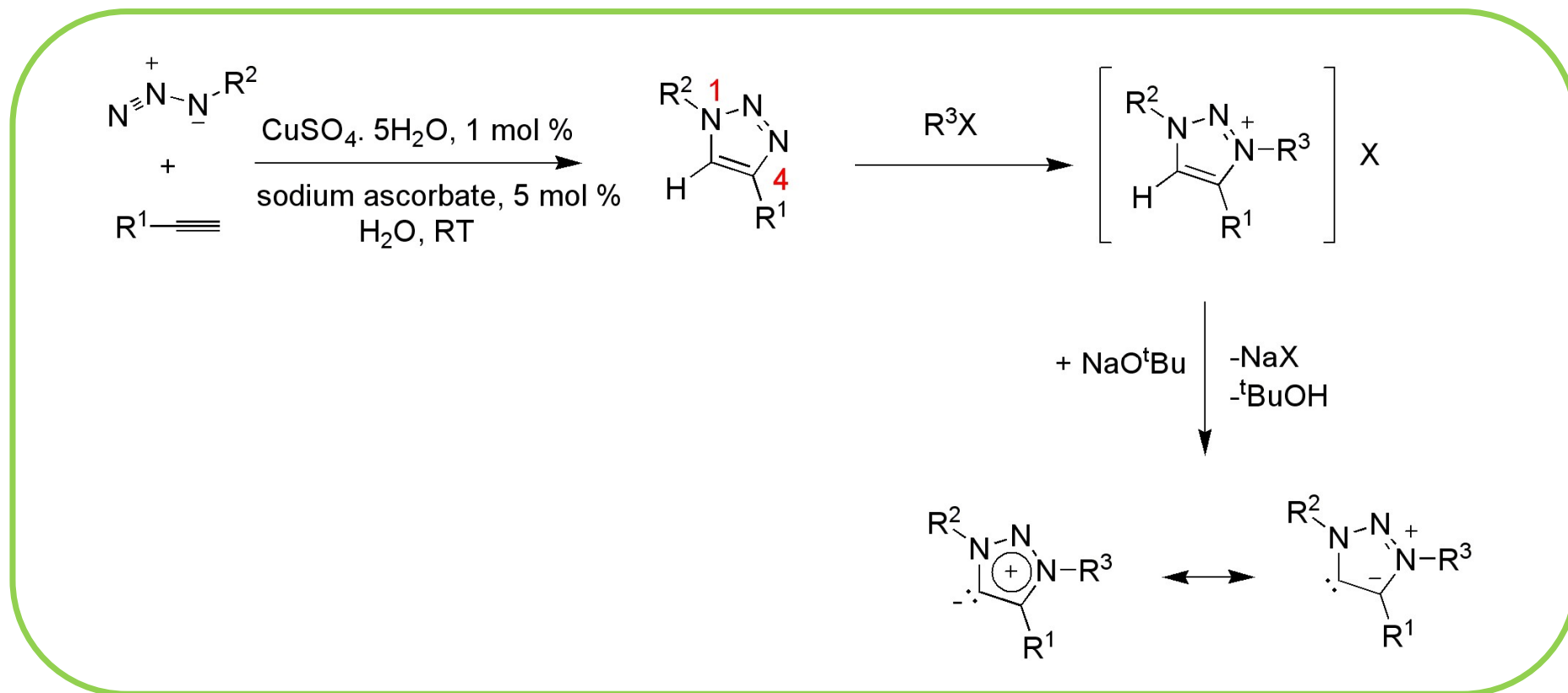
Our Chemical Tools: Redox-Active Ligands (Porphyrins, Corroles, Quinones, Azo)



ChemSusChem, (2023), **16**, e202201146
Chem. Eur. J. (2022), **28**, e202104550
Angew. Chem. Int. Ed. (2015), **54**, 13769

Nature Commun., (2024), **in press**
Chem. Sci. (2022), **13**, 10532
Angew. Chem. Int. Ed. (2019), **58**, 9802

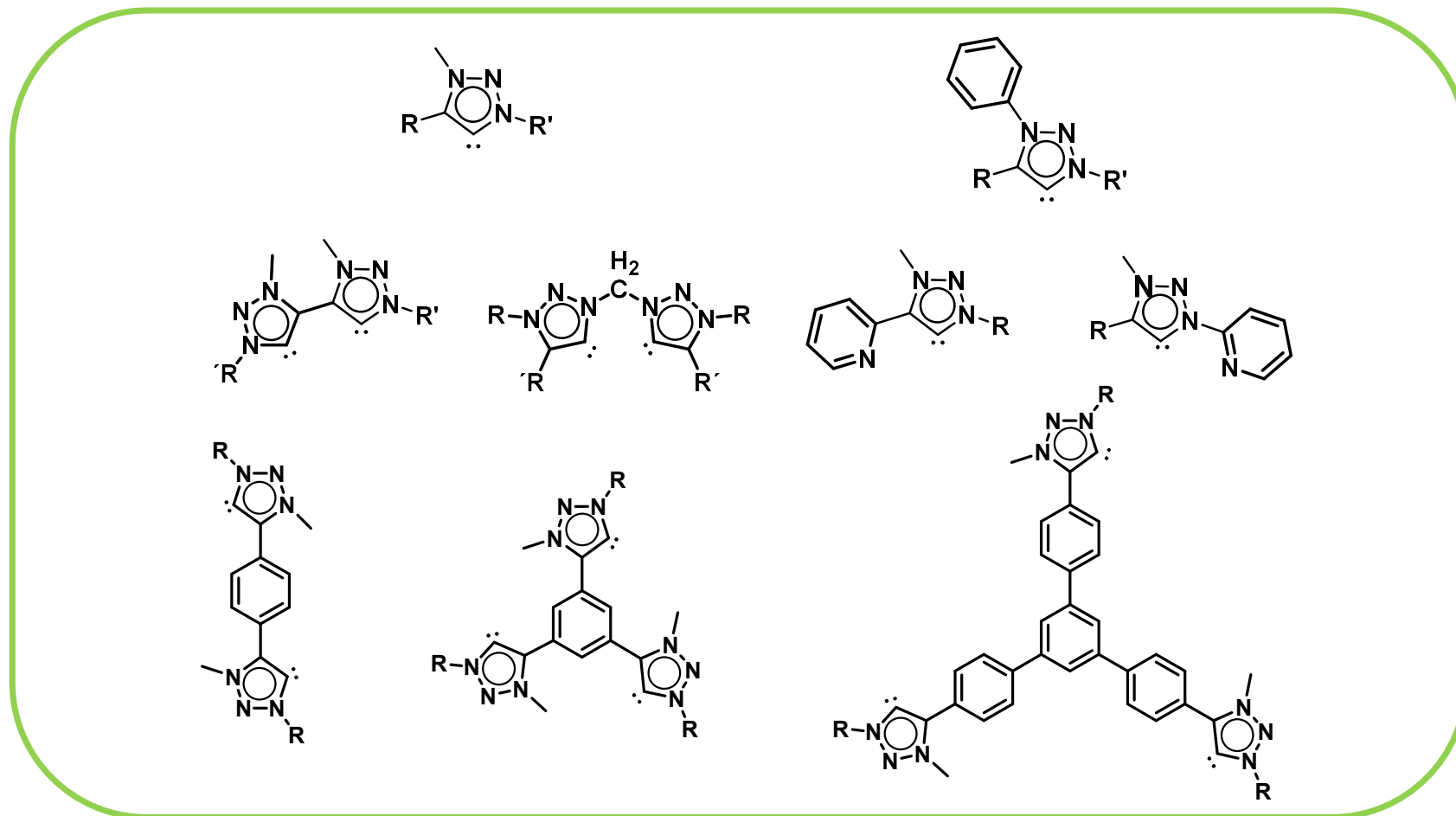
Our Chemical Tools: Mesoionic Carbenes (MIC)



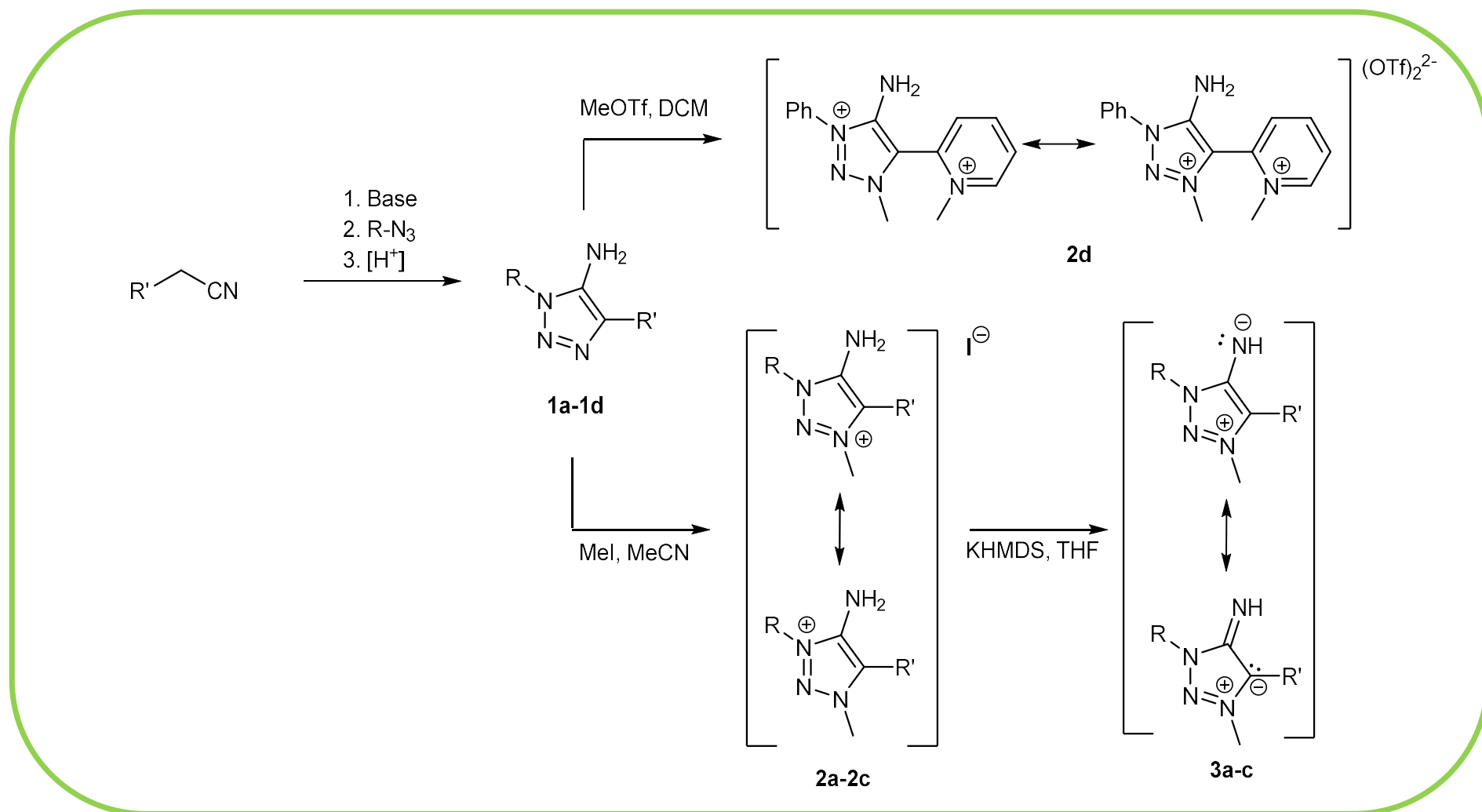
Adaptable Ligands: Carbenes or Carbanions??

JACS Au (2022), **2**, 22

Our Chemical Tools: Mesoionic Carbenes (MICs)



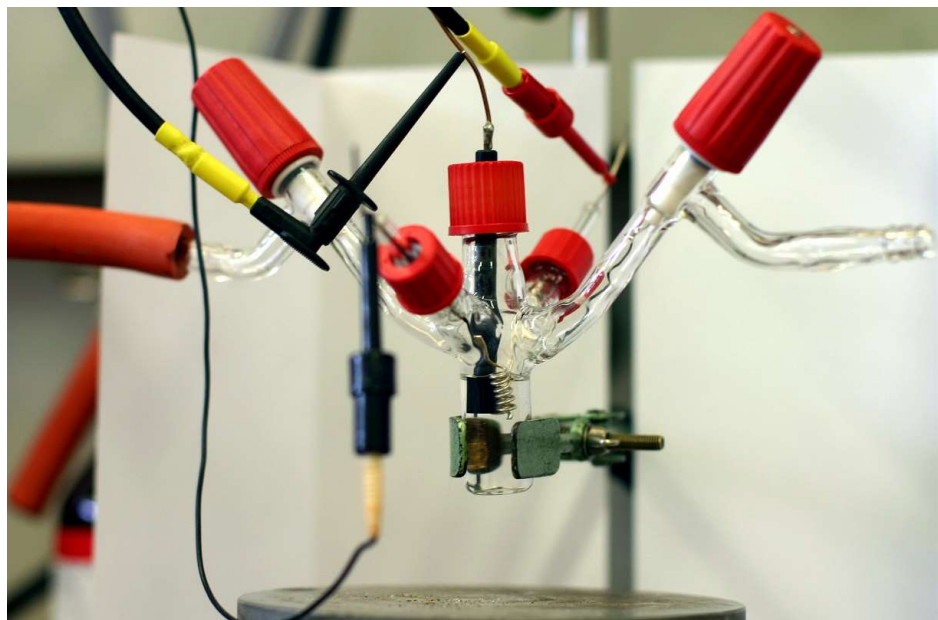
Our Chemical Tools: Mesoionic Imines (MIIs)



Adaptable Ligands: Imines or Amides??

Angew. Chem. Int. Ed. (2022), **61**, e202200653
Chem. Eur. J. (2024), **30**, e202400730

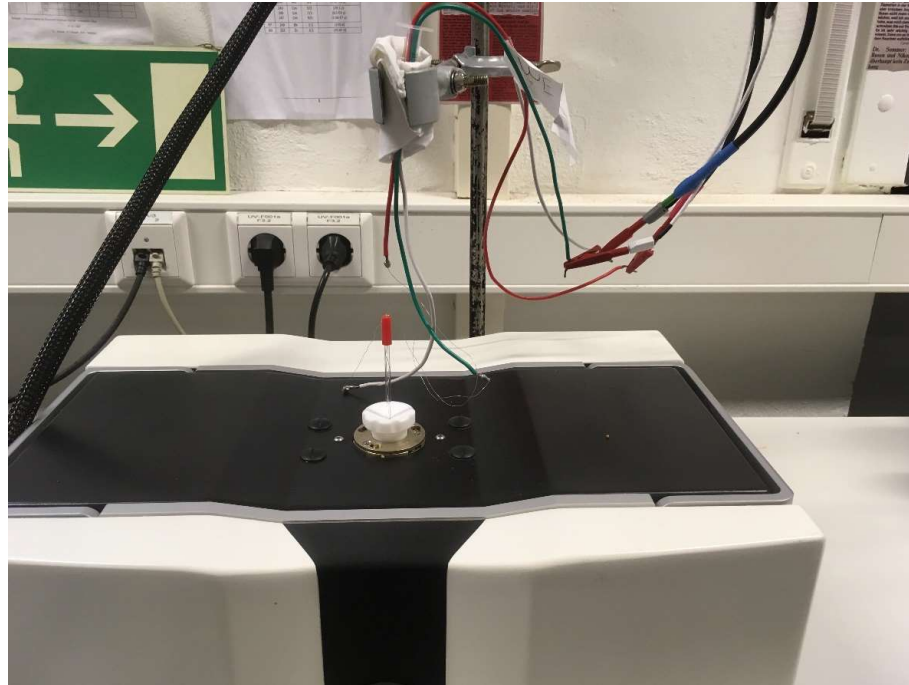
Method Development: Electrochemistry



Home-made cyclic voltammetry and bulk-electrolysis cells

Advantages: Modular set-up, measurements with only 1 ml (for CV) solvent possible

Method Development: EPR Spectroelectrochemistry

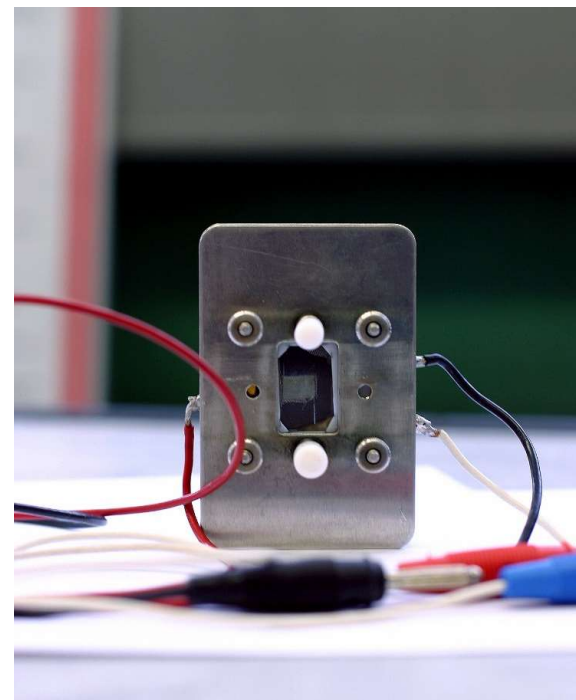
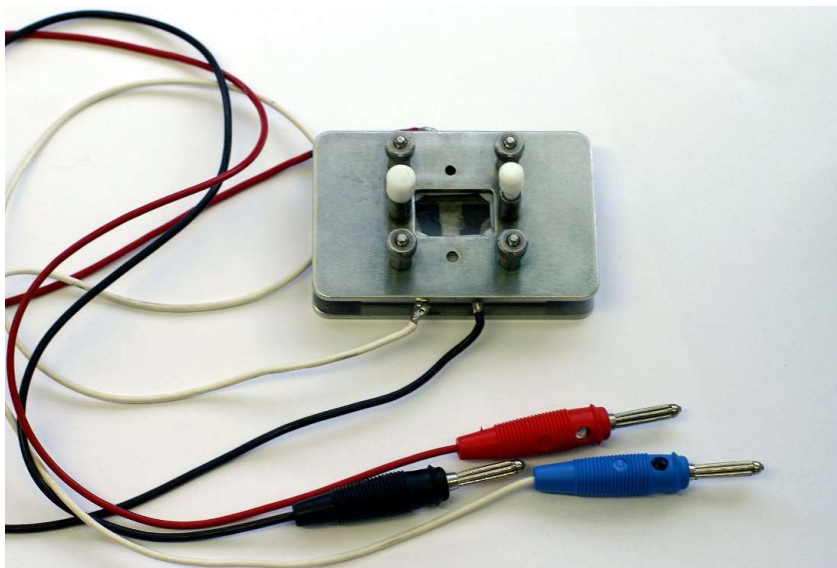


Home-made three-electrode EPR spectroelectrochemistry cell

Advantages:

- **Detection of one/two/three....electron oxidized/reduced paramagnetic species**
- **Mechanistic investigations of electrocatalytic reactions**

Method Development: UV-vis-NIR and IR Spectroelectrochemistry

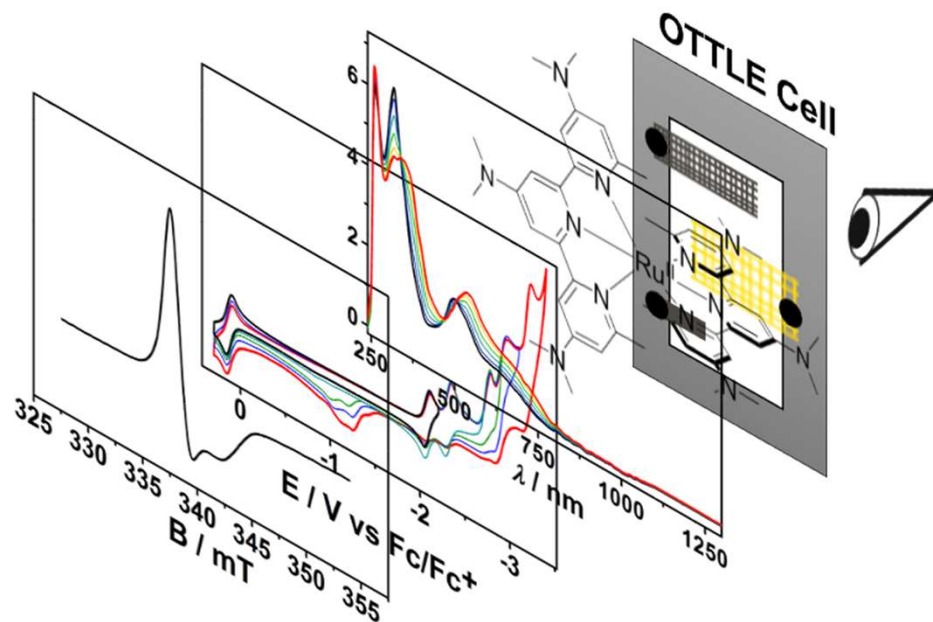


Home-made three-electrode UV-vis-NIR and IR spectroelectrochemistry cell

Advantages:

- Structural information on all accessible redox states
- Mechanistic investigations of electrocatalytic reactions
- Spectroscopic signatures of catalytic intermediates

Method Development: UV-vis-NIR and IR Spectroelectrochemistry

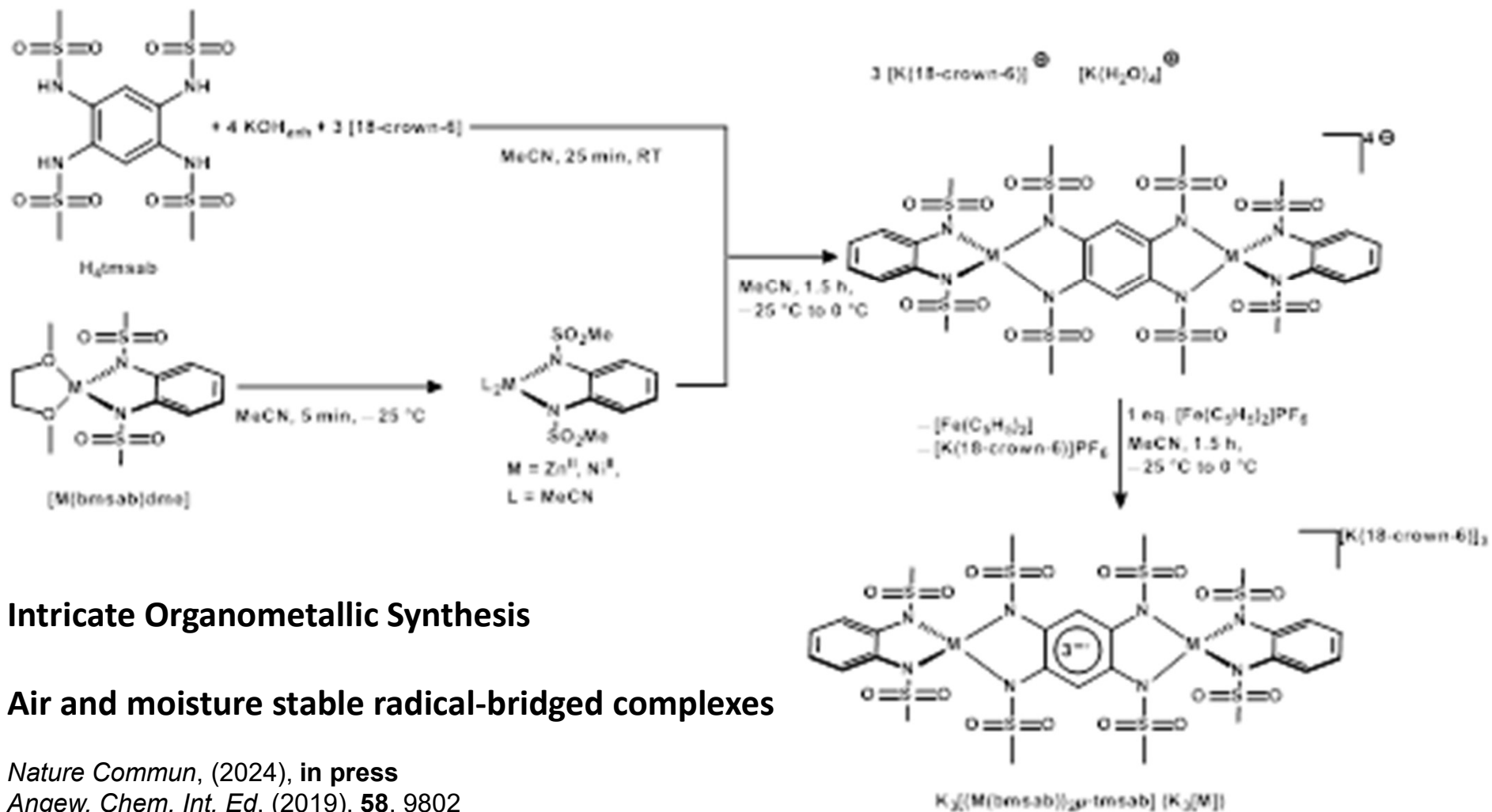


Modular change of the working electrode in the spectroelectrochemical cell

Platinum, glassy carbon, gold..... as working electrodes

Important while investigating electrocatalytic reactions

State of the Art Single Ion Magnets



Intricate Organometallic Synthesis

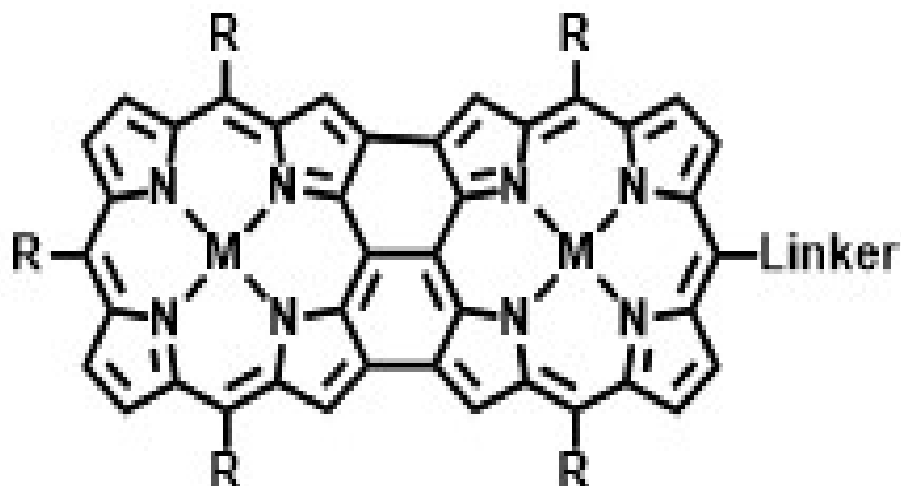
Air and moisture stable radical-bridged complexes

Nature Commun., (2024), in press

Angew. Chem. Int. Ed. (2019), **58**, 9802

Nature Commun. (2016), **7**, 10467

Most Efficient Molecular Electrocatalysts for Dihydrogen Production

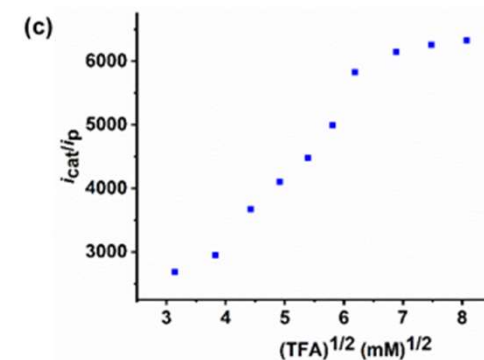
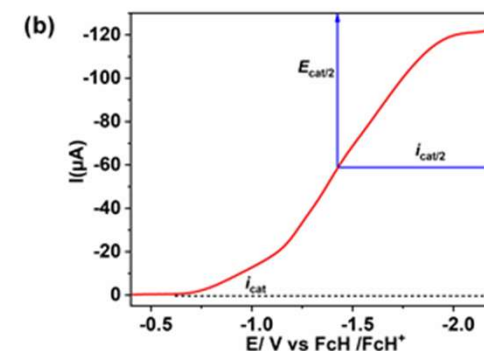
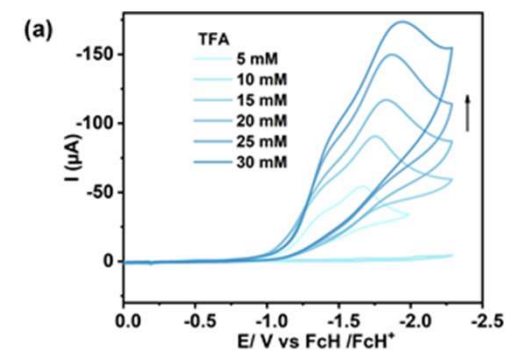


Fused Porphyrins as Privileged Ligands in Electrocatalysis

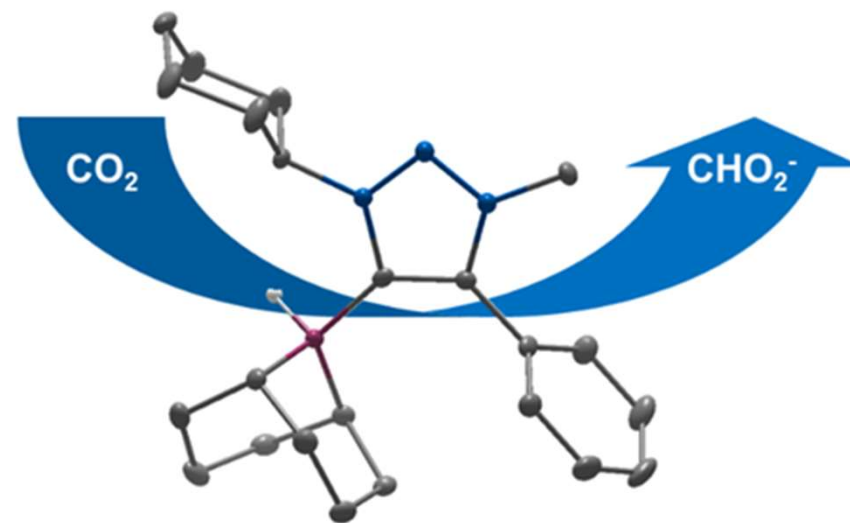
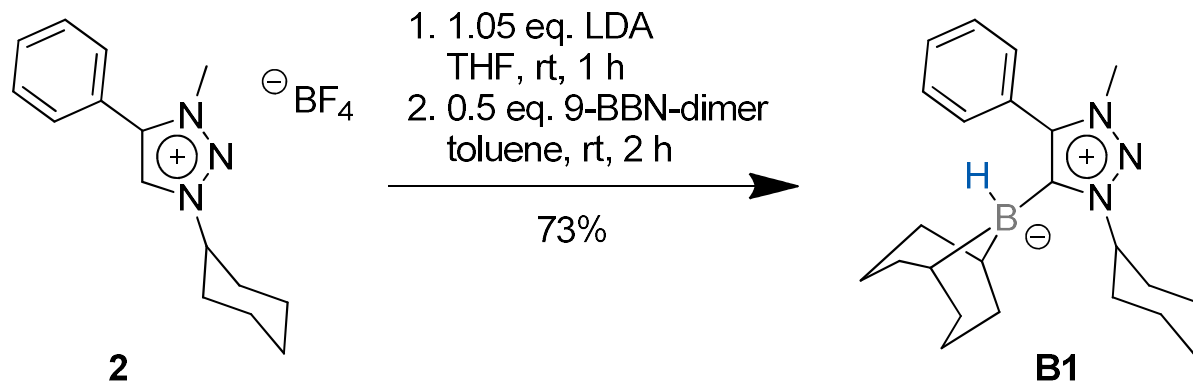
Mechanistic Investigations Through (Spectro)Electrochemistry

ChemSusChem, (2023), **16**, e202201146

Chem. Eur. J. (2022), **28**, e202104550



Atmospheric CO₂ Capture and Fixation



Mesoionic Carbenes for CO₂ Capture and Reduction

Simple Metal-free Systems

[10.26434/chemrxiv-2024-5w7nc](https://doi.org/10.26434/chemrxiv-2024-5w7nc)



Possible Projects in the Group

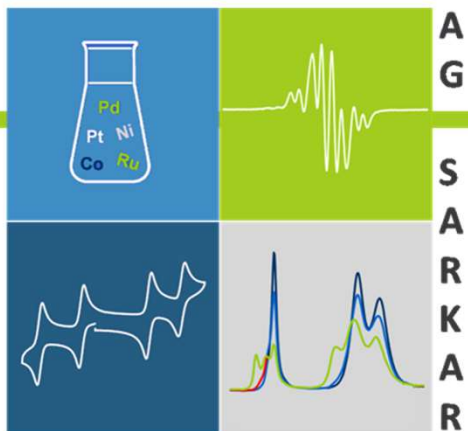
We are a group that is involved in the synthesis of electronically adaptable ligand systems (carbenes, imines, non-innocent ligands and so on), and their classical coordination complexes as well as organometallic compounds.

Additionally, we are heavily involved in the use of methods such as:

Multinuclear NMR spectroscopy, single crystal X-ray diffraction, electrochemistry, UV-Vis-NIR- IR- and EPR-spectroelectrochemistry and electrocatalysis.

Possible Topics:

- 1) **Molecular systems for CO₂ capture and conversion.**
- 2) **Molecular catalysts for the electrocatalytic conversion of CO₂ and O₂ and for H₂ production.**
- 3) **Electrocatalysis for organic synthesis.**
- 4) **Adaptive catalysts for performing redox switchable catalysis.**
- 5) **Synthesis and characterization of molecules for applications as single molecule magnets and molecular qubits.**
- 6) **Molecular electrochromic materials.**
- 7) **Metal complexes as luminescent probes for bio-orthogonal chemistry.**
- 8) **Synthesis of electronically ambiguous mesoionic compounds.**
- 9) **Mechanistic investigations of electrocatalytic reactions with the help of electrochemical and spectroelectrochemical methods.**



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**Large Number of National
and International
Collaborations**

Freie Universität



Berlin



Group Trip: July 2024

First Co-Workers in Berlin: February 2025