Advancing Green Catalysis with Molecularly Engineered Electrodes

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While molecular electrocatalysts allow for structural optimization and detailed investigation of reaction mechanisms, their susceptibility to decomposition under harsh operating conditions, along with low catalytic current density, limits their commercial viability.

We design and synthesize electrocatalysts for carbon capture and utilization,[1,2] green hydrogen production,[3-5] and PFAS remediation (Figure 1)[6,7]. Based on key performance metrics—including overpotential, product selectivity, turnover numbers (TONs), and Faradaic efficiency—we identify the most promising candidates for the next stage, i.e., electrode fabrication.

To optimize charge and electron transfer from the catalytic center to the conducting electrode surface, we explore various covalent linkers (e.g., $–CH_2–$, $–CH_2CH_2–$, $–C_6H_4–$). Additionally, we investigate different conducting materials (e.g., graphene, MXene) to achieve the improved catalytic current and overall efficiency without compromising the product selectivity from these molecularly engineered electrodes.

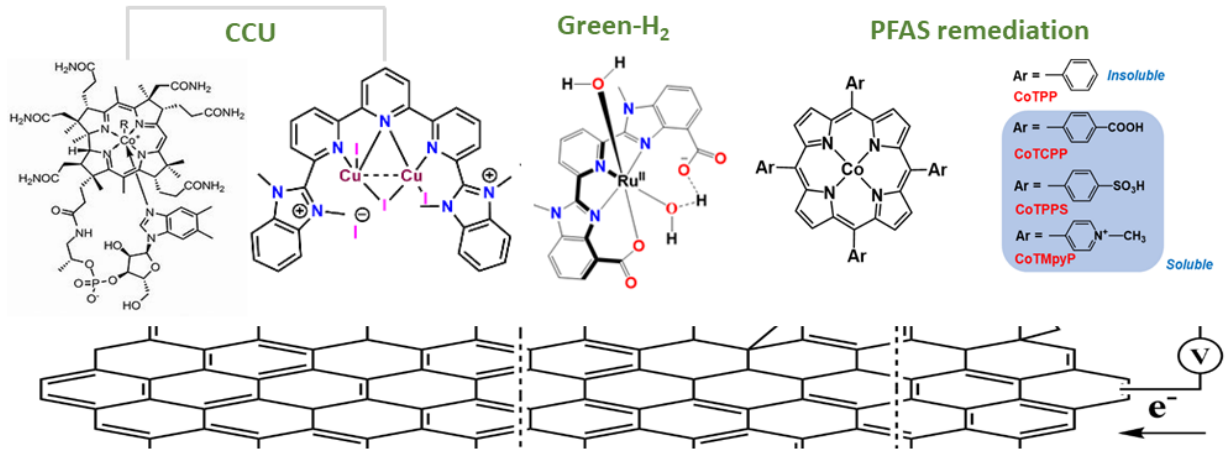

Figure 1. Pictorial representation of the investigated electrocatalysts and electrodes

References:

(1) Chen Jia, (…), and Biswanath Das, ACS *Applied Materials & Interfaces*, **2020**, 12, 41288-41293; **(2)** Pamela Bengtsson, (...), Belén Martín-Matute, and Biswanath Das **2025**, *Submitted manuscript*; **(3)** Biswanath Das, Esteban A Toledo-Carrillo, (…), Björn Åkermark, *Journal of Materials Chemistry A*, **2023**, 11, 13331-13340; **(4)** Jamal El-Abid, (…), Anders Thapper, Biswanath Das, *Scientific Reports*, **2025**, 15, 5882: **(5)** Biswanath Das, (…) Björn Åkermark, *Accounts of Chemical Research*, **2021**, 54, 3326–3337; **(6)** Jun Sun, (…), Biswanath Das, Naresh Kumar, *Water Research*, **2024**, 258, 121803; **(7)** Maryam Mirabediny, (…), Biswanath Das, Naresh Kumar, *Chemosphere*, **2023**, 321, 138109.