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Topic of a Master thesis

Experimental Investigation and Multi-Phase Product Analysis of Nitrate Electroreduction to Ammonia Using an RDE Batch Half Cell.
Experimental / theoretical

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Motivation:
The planetary nitrogen cycle relies on nitrogen fixation, currently dominated by the energy-intensive Haber-Bosch process to synthesize ammonia. The primary difficulty in traversing the multi-step reaction landscape from N_2 to NH_3 stems from the extreme inertness of the N≡N triple bond, requiring severe operating temperatures and pressures to overcome high activation barriers [1].

Simultaneously, industrial manufacturing—such as nuclear processing and explosives production—discharges highly concentrated nitrate waste streams, threatening aquatic ecosystems. While biological denitrification is mature, it remains unsuitable for harsh, toxic industrial effluents [2]. Electrocatalytic nitrate (NO^-_3) reduction under ambient conditions offers an attractive sustainable alternative by transforming concentrated reactive nitrogen into ammonia. However, real-world industrial wastewaters present complex matrix interferences, including dissolved organic matter, salts, and suspended solids, which impede desired reduction pathways towards ammonia [2]. Gaining fundamental mechanistic insights into reaction selectivity, suppressing parasitic side products, and maintaining catalytic stability under ambient conditions are critical milestones for realizing competitive, electrochemical nitrogen recovery.

Problem definition:
This thesis focuses on experimental activities utilizing a Rotating Disk Electrode (RDE) batch half-cell. You will perform multi-phase product detection during electrocatalytic nitrate reduction over Cu and CuNi electrodes. Dissolved liquid (by-)products will be tracked via ion chromatography (IC), while volatile gaseous N-species by gas chromatography (GC). The generated experimental data will be used to validate a computational microkinetic model, establishing a baseline for catalytic activity and selectivity before introducing targeted electrolyte impurities.

Task list:
· Conduct basic experiments using the Rotating Disk Electrode (RDE) batch half-cell setup.
· Vary parameters (concentration, pH) as well as operating conditions to study the effect on reaction kinetics.
· Analyze data to find functional dependencies on experimental parameters.

Start: immediately
Duration: 6 months

Prior knowledge:
· Basics of (electro)chemistry, engineering, lab work and measurement analysis

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References:
[1] Lehnert N., Musselman B.W. and Seefeldt L.C. (2021) Grand challenges in the nitrogen cycle. Chem Soc Rev 50:3640-3646.
[2] Duca M. and Koper M.T.M. (2012) Powering denitrification: the perspectives of electrocatalytic nitrate reduction. Energy Environ Sci 5:9726-9742.