TITLE: Electrochemical Synthesis of Ammonia

Summary: Development of artificial N2 fixation to ammonia via the Haber-Bosch process revolutionised our lives ~100 years ago, and it has ever since provided a solid basis for modern agriculture and food production. However, the Haber-Bosch process presents a major problem in terms of sustainability. Ammonia production is estimated to emit about 500 Mt carbon dioxide per year, which is about 1.4 % of the yearly global emission, being thus a significant contributor to the greenhouse effect. Proposed research exploits this momentum and finds motivation in lithium-mediated electrochemical reduction of nitrogen (LM-NRR) as necessary sustainable alternative for ammonia production. In order to increase platform's efficiency, a mechanistic understanding of the reaction will be achieved. The aim of proposed research is to gain a mechanistic understanding of LM-NRR to help aid in rational electrode design for these devices which could be crucial for green technologies capable of reducing carbon emissions and mitigating climate change.

Research techniques used: The candidate will target elucidation of LM-NRR electrodes by implementing multidisciplinary steps. Firstly, the candidate will develop a floating electrode configuration through which he/she will perform electrochemical characterization to pursue NH3 formation. Secondly, the candidate will complement electrochemical findings by operando spectroscopy and computational studies for in-depth understanding LM-NRR. Overall, within doctoral research the candidate will obtain expertise in heterogeneous electrochemistry and materials, operando spectroscopy and computational chemistry.

The reason why the topic is innovative: Replacing typical electrochemical investigation of NRR by floating electrode configuration**.** Due to the usage of floating electrode diagnostics, for the first time, inspection of intrinsic NRR kinetics will be possible. LM-NRR will be investigated by a versatile analytical platform based on hyphenated electrochemical techniques. This will, for the first time, provide insight into LM-NRR, the only credible, however utterly unexplained catalytic system. The experimental approach will, for the first time, enable delivery of key guiding principles for LM-NRR electrodes.

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