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“Fertilizer from air and water: From theory to experiments”

Artificial nitrogen fixation is essential to provide food security. Today ammonia is produced through the Haber-Bosch process from nitrogen and hydrogen gases whereas nitrates are produced through the Ostwald process from ammonia and oxygen. From these, various nitrogen containing fertilizers are produced depending on the application of use. The Haber-Bosch process is, however, not sustainable since it relies on natural gas resources for hydrogen generation, and at the same time highly polluting of CO₂ emission. It is therefore necessary to develop alternative routes for ammonia and nitrate synthesis. One of the most attractive solution would be to have a heterogenous electrolytic cell with an aqueous electrolyte that works at ambient conditions, where a nitrogen fertilizer can be produced on-site. There are, however, several factors that make it difficult to accomplish this, mainly because the N₂ molecule is inert and difficult to reduce or oxidize and because of the side reactions, the hydrogen evolution reaction (HER) or the oxygen evolution reactions (OER), which usually take place more easily than the nitrogen reduction reaction (NRR) or the nitrogen oxidation reaction (NOR), respectively. It has been predicted that all the transition metals will much more easily catalyze HER than NRR but the direct electrochemical NOR has been much less explored.

Over the last few years we have been searching, using density functional theory (DFT) calculations, for alternative materials that can catalyze NRR while suppressing HER. The class of materials we have investigated are transition metal nitrides, transition metal oxides and transition metal sulfides. I will, in particular, present our newest contribution to the NRR field where we have joined forces with Fujitsu Limited in Japan to continue our search for NRR catalysts (1). Several promising candidates are predicted within each class of materials and we have tested several of them experimentally. There, we grow the catalysts in thin-films using magnetron sputtering, which are then tested in a micro reactor for electrocatalytic performance. The electrochemical micro reactor is connected in-line with the ammonia detection unit, preventing any possible contamination which makes the results reliable and robust. Experiments are done both in N₂ saturated electrolyte and in Ar saturated electrolyte and isotope labelled ¹⁵N₂ is used to proof catalysis. In this presentation, I will discuss both the theoretical predictions and the experimental performance of several candidates for NRR. Finally, our initial calculations on NOR will be presented.

1. “High-throughput computational screening of doped transition metal oxides as catalysts for nitrogen reduction”
Á.B. Höskuldsson, T. Dang, Y. Sakai, A. Ishikawa & E. Skúlason.
Cell Reports Physical Science **4** (2023) 101595.
2. “Perspectives on the Competition between the Electrochemical Water and N₂ Oxidation on a TiO₂(110) Electrode”
E. Tayyebi, Á.B. Höskuldsson, A. Wark, N. Atrak, B.M. Comer, A.J. Medford & E. Skúlason
The Journal of Physical Chemistry Letters **13**, (2022) 6123