

## Selectivity in Electrochemical Reduction Reactions

Alexander Bagger

Department of Chemistry, University of Copenhagen

Universitetsparken 5, 2100 Copenhagen

Alexander@chem.ku.dk

Electrochemistry holds the promise to be a cornerstone for sustainable production of fuels and chemicals. Electrochemical reduction of NO<sub>x</sub>, CO<sub>2</sub>, N<sub>2</sub> and the combinations is of particular interest. Importantly, all these reactions share a direct competition with hydrogen, and furthermore several products are formed from each reactant of these reactants.

In this talk I will give a unified approach to these reduction reactions, by showing how the product distributions from these types of reactions can be understood by ignoring the reaction pathways and instead grouping the catalysts by simulated DFT binding energies.

- i) Electrochemical CO<sub>2</sub> reduction is a complex reaction that has been shown to give multiple different products depending on metal catalyst [1]. I will show why copper is unique as catalyst, which results in a high value multiple-carbon product distribution [2]. Following I will show what insights can be gained from copper facets to steer the product distribution [3].
- ii) Electrochemical NO<sub>x</sub> reduction, also multiple products are formed; N<sub>2</sub>O, N<sub>2</sub> and NH<sub>3</sub>[4]. Uniquely again the copper catalyst stands out as a catalyst which enables reduction to produce ammonia [5].
- iii) Electrochemical N<sub>2</sub> reduction to ammonia (NH<sub>3</sub>) at ambient conditions is burgeoning [6-7]. Most interesting for the direct electrochemical N<sub>2</sub> reduction in aqueous there is not a “copper” catalyst [8].

I end my talk discussing how one can use these insights to form products beyond the typical reduction reaction products [9].

- [1] Y. Hori et. al., *Journal of the Chemical Society, Faraday Transactions*, **1989**, 85, 2309-2326.
- [2] A. Bagger, W. Ju, ..., P. Strasser, J. Rossmeisl, *ChemPhysChem*, **2017**, 18, 3266–3273.
- [3] A. Bagger, W. Ju, ..., P. Strasser, J. Rossmeisl, *ACS Catalysis*, **2019**, 9, 7894–7899
- [4] V. Rosca, M. Duca, M. T. de Groot, M. T. M. Koper, *Chem. Rev.* **2009**, 109, 2209–2244
- [5] H. Wan, A. Bagger, J. Rossmeisl, *Angewandte Chemie*, **2021**, 133 (40), 22137-22143
- [6] S. Z. Andersen et al. *Nature*, **2019**, 570, 504-508.
- [7] N. Lazouski et al, *Nature Catalysis*, **2020**, 3, 2520-1158.
- [8] A. Bagger, H. Wan, I.E.L. Stephens, J. Rossmeisl, *ACS Catalysis*, **2021**, 11 (11), 6596-6601
- [9] H. Wan, ... A. Bagger, J. Rossmeisl., draft.