

Selectivity in Electrochemical Reduction Reactions

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Electrochemistry holds the promise to be a cornerstone for the sustainable production of fuels and chemicals. The electrochemical reduction of NO_x , CO_2 , N_2 , and the combinations is particularly interesting. 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 reactions can be understood by ignoring the reaction pathways and grouping the catalysts by simulated DFT binding energies.

- i) Electrochemical CO_2 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_x reduction, also multiple products are formed; N_2O , N_2 and NH_3 [4]. Uniquely again the copper catalyst stands out as a catalyst which enables reduction to produce ammonia [5]. However recent experiment show interesting performance from Co and Fe based catalysts close to their reduction potential [6].
- iii) Electrochemical N_2 reduction to ammonia (NH_3) at ambient conditions is burgeoning [7-8]. Most interesting for the direct electrochemical N_2 reduction in aqueous there is not a “copper” catalyst [9]. While in non-aqueous, the univocally working system is a Li-mediate system [10]. In general, it is a challenge from a computational point of view how we address non-aqueous electrocatalytic systems [11]. For this system, I will show that varying multiple experimental parameters display similar performance characteristics [12].

Finally, I will discuss how one can use these insights to form products beyond the typical reduction reaction products [13].

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