Electrochemical CO_2 and CO Reduction, A Complex and Interface Depended Reaction.

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Abstract

Electrochemical CO_2 and CO reduction holds the promise to be a cornerstone for sustainable production of fuels and chemicals. However it is indeed a complex reaction which tend to give multiple very different products[1] and consequently the product selectivity is a more complex property to understand[2]. Further, the *unique* copper catalyst, as the only metal catalyst, show a high value multiple-carbon product distribution to be both facet and electrolyte depend[3, 4].

In this talk I will discuss: (1) How we can ignore reaction pathways and solely approach the problem by grouping metals due to their product selectivity, which can be used in the search for new catalyst for a desired product[5]. (2) How explicit ab initio molecular dynamics simulations of the electrochemical interface can be used to understand how key CO reduction reaction intermediates are stabilized in solution of different electrolytes, and for different pH. (3) How results from such analysis provide insight into the electrochemical interface structure, revealing the electrochemical limitations and offer a direct comparison to experiments.

References

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