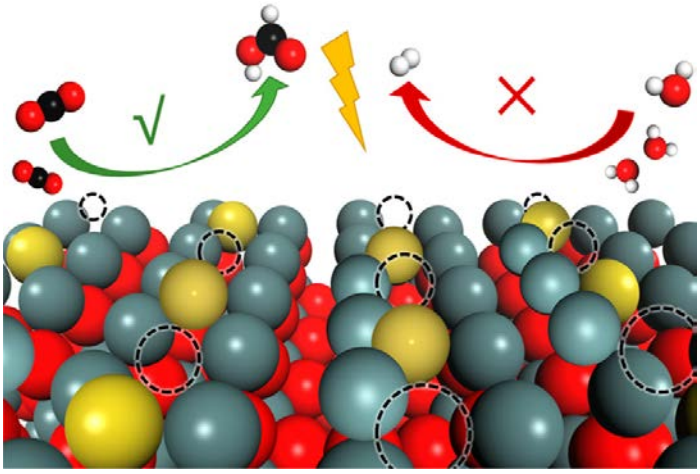
Inorganic Materials & catalysis

Research Project – Emiel Hensen / Ivo Filot / Zhaochun Liu

INORGANIC MATERIALS & CATALYSIS

CO_2 Electrochemical reduction to Formate on SnO_x catalysts

Background



A large amount of carbon dioxide (CO_2) produced by fossil fuels has caused a series of global climate and environmental problems. [1] Using electrochemical conversion of CO_2 into liquid fuels and value-added chemicals is considered to be one of the most promising ways to address these issues simultaneously. [2] Liquid products of CO_2 reduction, such as HCOOH, have gained considerable attention for their numerous advantages. Tin oxide (SnO_x) has emerged as a promising metal oxide catalyst for the CO_2 reduction reaction (CO_2RR) into value-added chemicals such as formic acid/formate. Formic acid is one such molecule that is widely used as feedstock in chemical industry and is promising as a hydrogen carrier for on demand energy storage and production. Formic acid can be produced using renewable energy and CO_2 from air. Formate is an economically more valuable chemical than CO. In addition, formate is much more convenient for storage and transport than gaseous products.

In this project, we aim at investigating the mechanism of adsorption, surface reaction and the influence of the electrochemical potential on the activation barriers for CO_2 Electrochemical reduction to Formate on an SnO_x surface. By incorporation of various transition metals (e.g. Cu, Ni, and Co) into the SnO_x lattice, we will also investigate the promotional effect of those materials on the formation of oxygen vacancies as they are considered to be the active sites for the CO_2 activation. Furthermore, we also wish to investigate the activity for CO_2 Electrochemical reduction to Formate at the interface between transition metal nanoparticles and SnO_x

Techniques used:

- DFT calculations will combine with Genetic Algorithm (GA) to locate the global minimum structure for a TM cluster supported on a certain support.
- Perform DFT calculations to explore stable structures and elementary reaction steps.
- Develop microkinetic modelling simulations to investigate the reaction mechanisms.
- PH affect, current densities as a function of potential (i-V curves), Faradaic efficiency, and surface coverage can be used and computed for understanding the whole reaction mechanisms.

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References:

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[2]Gao, S.; Lin, Y.; Jiao, X.; Sun, Y.; Luo, Q.; Zhang, W.; Li, D.; Yang, J.; Xie, Y. Partially Oxidized Atomic Cobalt Layers for Carbon Dioxide Electroreduction to Liquid Fuel. *Nature* 2016, *529*, 68– 71.