LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	Supervisor(s)	Funding
Dr. Ali Can Kizilkaya	Prof. Mark Saeys	SAFARI

Computational investigation of ethanol oxidation to acetaldehyde via electrocatalysis to produce sustainable aviation fuels from biomass

Aim

The aim of the study is to obtain mechanistic insights into the electrocatalytic oxidation of ethanol to acetaldehyde. We will investigate the reaction kinetics based on based on Density Functional Theory (DFT) calculations. The results will be ultimately used to optimize the novel catalytic process currently developed in LCT to produce Sustainable aviation Fuels (SAF) from biomass.

Justification

Fossil fuel derived kerosene is the sole fuel of choice in the aviation industry. The use of this jet fuel results in 2.5% of the global CO_2 emissions. Therefore, there are several global efforts to design novel chemical pathways to synthesize SAF from different sources. Among these, there are several processes that can convert biomass to jet fuel. However, these processes are still energy intensive. At LCT, we currently work on the development of a novel synthesis method that combines electrocatalysis and thermocatalysis, which has the potential to significantly reduce the energy cost of SAF production from biomass. One of the critical factors that contributes to the process efficiency is the performance of the initial electrocatalytic pathway, which converts ethanol to acetaldehyde. This can be done via electrocatalysis[1] as well as the thermocatalytic pathway[2]. Therefore, in this project we will first compare the advantages/disadvantages associated with different catalytic methods via a literature survey and then work on the computational investigation of ethanol oxidation via electrocatalysis.

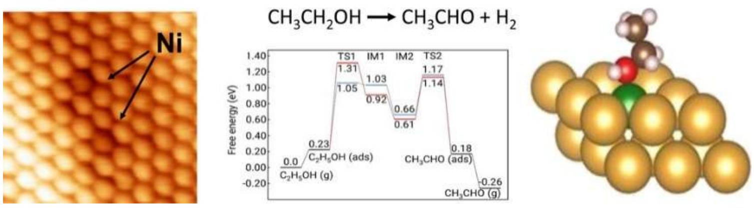

Image showing the reaction mechanism for ethanol oxidation to acetaldehyde on a thermal catalyst[2]

Program

1. Conduct a critical literature review that compares the different options for ethanol oxidation to acetaldehyde, including thermocatalytic and electrocatalytic pathways.
2. Perform DFT calculations to identify a computational model to represent the electrocatalyst.
3. Calculate the kinetics for the elementary reactions of ethanol oxidation.
4. Identify the rate limiting steps and use the mechanistic understanding to optimize the catalysts.

<u>References</u>

1) Wang and Stahl, Acc. Chem. Res. 2020, 53, 561−574.
2) Giannakis and Sykes et al., J. Am. Chem. Soc., 2021, 143, 21567−21579.