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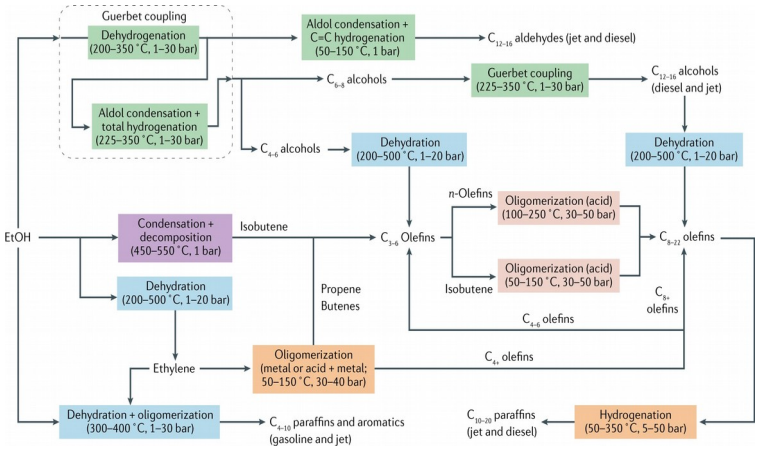
Computational Investigation of Acid Catalyzed Aldol Condensation for the Production of Sustainable Aviation Fuels from Biomass

Aim

The aim of the study is to obtain mechanistic insights into to the aldol condensation of aldehydes to longer chain alcohols. We will investigate the reaction kinetics on acid catalysts 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 for the production of 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 CO2 emissions. Therefore, there are several global efforts to design novel chemical pathways to synthesize SAF from different sources. Among these, there are several process 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 catalytic processes. However, the mechanism of the thermo-catalytic pathway is complicated and has to be understood in more detail to optimize the overall process. Therefore, in this project we will work on the computational investigation of acid catalyzed aldol condensation to guide the optimization of the thermo-catalytic process. The computational insights will be complimented by experimental testing and further incorporated into process models to deliver optimal process efficiency.



Different pathways that are available for the production of SAF from biomass[1]

Program

1. Conduct a literature review on acid catalyzed aldol condensation.
2. Perform DFT calculations to identify a computational model to represent acidic catalysts.
3. Calculate the kinetics for the elementary reactions of aldol condensation based on model biomass compounds.
4. Identify the rate limiting steps and use the mechanistic understanding to optimize the acid catalysts.

References

1) Eagan et al., Nat. Rev. Chem., 2019, 3, 223-249.

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