Lehrstuhl für Technische Thermodynamik
RWTH AACHEN UNIVERSITY
Apl.-Prof. Dr. rer. nat. Kai Leonhard

Type of thesis: Master thesis

March 2022

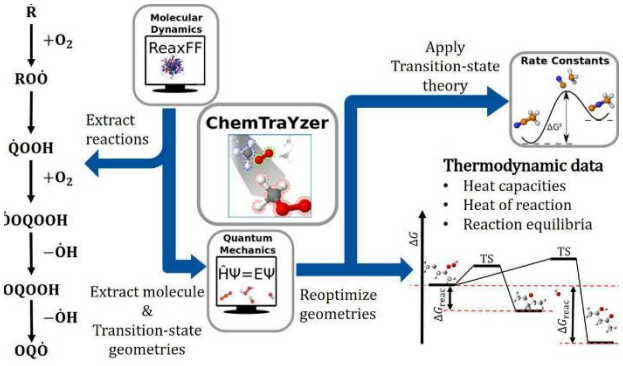
A Computational Catalytic Polycarbonates Synthesis Study Using ChemTraYzer

Our profile:

The research group Molecular Systems Engineering of the Institute of Technical Thermodynamics (LTT) headed by Prof. Leonhard focuses on the design of molecular systems in energy and chemical engineering. To understand the reaction mechanisms that are important in various fields of organic chemistry at the molecular level, we perform state-of-the-art quantum chemical and molecular dynamics simulations

Background:

The project Carbon2Chem featuring industry partners Thyssen-Krupp and COVESTRO aims at cross-linking steel, chemical and energy industries. On the one hand, the purpose is to absorb power peaks which arise in renewable power generation by electrolytic hydrogen production. Thereby, the project contributes to the grid stability and the integration of renewable energy sources into the energy supply. On the other hand, the project aims at the utilization of carbon-rich flue gases from steel industries. Previously, these gases were mainly used for heat generation. In contrast, the goal of Carbon2Chem is the chemical utilization of these flue gases for the production, e.g. of fuels and polymers. In the sub-project Carbon2Polymers, we aim at the utilization of carbon-rich flue gases from steel industries in the production of polycarbonates. For this purpose, we explore new catalytic synthesis routes with our in-house chemistry software tool ChemTraYzer.



Your task:

- Automatize a 5-steps chain of process steps necessary to produce state-of-the-art liquid phase reaction rate constants with ChemTraYzer using Python programming
- Apply your automatized workflow to uncover hundreds of reactions and create a reaction model
- Validate your reaction model with experimental kinetic data from our partner COVESTRO

Your profile:

- Above-average studies in Chemistry / Physics / Mechanical Engineering / CES Energietechnik / Verfahrenstechnik or similar
- Good knowledge of / interest in quantum mechanic methods and chemical reactions
- Experience with quantum chemical software tools is desirable
- Programming skills, especially with Python, are highly desirable
- Open and innovative thinking, as well as a careful and independent way of working

What you can get from the project:

You will work on an innovative topic and will get a good insight into the field of kinetic modeling. You will also learn skills and knowledge in the field of quantum chemical simulations. Work in a motivated team with multidisciplinary and multicultural backgrounds. If you are interested, please write to Lukas Krep via e-mail (Lukas.krep@ltt.rwth-aachen.de) with CV and grading.

Start: As soon as possible

Lukas Krep
Lukas.krep@ltt.rwth-aachen.de