**Topic: "Exploring the Gas-Phase Reaction Kinetics of Regenerative Fuel"**

Decarbonization in road transportation requires innovation in fuel systems such as the application of synthetic fuels that are produced via captured carbon dioxide and renewable power. As one promising fuel additive, Solketal which is a gloycerol-based fuel can strongly reduce the pollutant formation i.e., $CO_2$, $NO_x$, and soot in current internal combustion engines. Combination of analytical and theoretical methods is one best way to understand the conversion chemistry of a new fuel system and will accelerate its technical application. At PTB Braunschweig state-of-the-art analytical and modeling methods, namely the molecular beam mass spectrometer (MBMS) and the Reaction Mechanism Generator (RMG) will be applied to deeply investigate the thermochemical conversion of Solketal at application relevant conditions. The obtained experimental data and developed chemical kinetics mechanism will be used further for high fidelity simulations, e.g., 3D computational fluid dynamic (CFD) simulation. Moreover, the methodology developed in this project will be adapted for learning other promising fuel systems.

Planned task in the project:

*Develop a comprehensive reaction mechanism for the thermochemical conversion of Solketal by employing ab initio calculations and the RMG software. The specific tasks include:*

- Literature Review on the oxidation of Solketal, including experimental studies and computational investigations. Identify the current knowledge gaps and challenges in understanding the reaction mechanism.
- Perform quantum chemical calculations using ab initio methods to determine the energetics and thermodynamics of key reaction steps involved in the Solketal oxidation process.
- Utilize the RMG software, a powerful tool for automatic reaction mechanism generation, to propose a detailed reaction network for the Solketal oxidation. Use the output from

the ab initio calculations to guide the selection and validation of reaction families and parameters within RMG.

- Develop a kinetic model based on the proposed reaction mechanism using the rate constants obtained from the ab initio calculations and RMG.
- Validate the developed reaction mechanism and kinetic model by comparing the simulated results with available experimental data from task 1. Assess the accuracy and reliability of the model in capturing the key features of the Solketal oxidation.

**Professional and personal requirements for employment:**

- Completed university studies (bachelor's degree) in physical chemistry, physics, mechanical engineering or comparable, with at least a good degree.
- Knowledge and/or practical experience in one or more of the following fields: Mass spectrometry, reaction kinetics, combustion chemistry, high vacuum, quantum chemistry.
- Interest in experimental work and computer simulations; software knowledge in Labview, Matlab/Python, or Cantera/Chemkin/Gaussian
- Prior knowledge in the field of theoretical and computational chemistry, with experience in ab initio calculations and reaction mechanism development is a plus
- High level of commitment, initiative, creativity, interest in independent scientific work, ability to work in a team, strong sense of responsibility and very good communication skills
- Good scientific and technical English skills, both written and spoken. Fluency in German is an advantage.

The proposed task is open for a HiWi (Werkstudent) for at least 10 months, which can be taken up as a Masters' thesis work subsequently. The job is entitled to 80 working hours per month.

We are looking for someone from the background of either Chemistry (preferably Physical Chemist), Chemical Engineering or Mechanical Engineering. The interested candidate can reach us in the below-mentioned details with a brief resume.

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