Bachelorthesis/Masterthesis

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# Design of Sustainable Refrigerants and Working Fluids

### Keywords

Energy technology and molecular thermodynamics

### Our Profile

The Chair of Technical Thermodynamics (LTT) at RWTH Aachen investigates challenges of energy and chemical engineering along the entire “thermodynamic elevator“: This ranges from the structure and properties of individual molecules, over the analasys of a single process towards the evaluation of entire energy systems. The group molecular systems engineering at the LTT explores the behaviour and properties of fluid and solid substances depending on their molecular structure and interactions.

The „Sector Coupling“ group at the Institute of Energy and Process Systems Engineering of the ETH-Zürich develops Power-to-Heat technologies. One focus of the research are the interactions between refrigerants and vapour compression heat pumps.

The advertised student thesis is the product of a cooperation of the two institutes and will be jointlycollectively supervised.

### Background

Due to the Montreal protocol, refrigerants no longer have an Ozone Depletion Potential (ODP). However, most modern refrigerants exhibit a high Global Warming Potential (GWP) and need to be replaced in the future. The search for alternatives produced a new generation of refrigerants with a low GDP, however most of them are highly flammable and therefore pose new risks in case of malfunction.

Our group developed a framework for the automated computer-aided design of molecules. The framework uses a genetic algorithm in order to create, evaluate and optimize new molecules in silico. Previous works integrated models for the prediction of ODP, GDP and adiabatic flame temperature, as a first indicator of the flammability, of a molecule into the framework and have used them for the design of molecules.

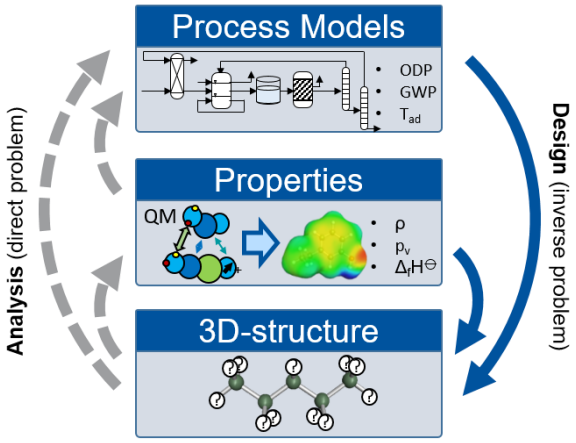


Abbildung 1: Schematic depiction of the CAMPD Framework

### Problem Statement

In a Bachelor- or Master thesis you will extend the existing model for flammability of substances with Machine Learning (ML) approaches developed by yourself or given in the literature. Subsequently, you integrate your model into our design framework and use it to optimize molecules towards a low flammability and at the same time a low ODP and GDP. The goal is the execution and validation of a design for promising molecules and the simulation of cooling processes with these molecules.

### Your Profile

You study Maschinenbau/Wirt.-Ing. MB/CES with specialization in chemical or energy engineering or something comparable. You are interested in current research topics concerning thermodynamics and chemical engineering, you are proficient in thermodynamics of mixtures or molecular thermodynamics. Previous experience in Python, Matlab or a comparable


Arbeitsbeginn: ab sofort / nach Absprache

Bei Interesse wende dich bitte an:

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programming language are of advantage but not absolutely necessary. You can work on complex assignments individually and target oriented.

**Our offer**

You work in a young and motivated team in a current research topic and have a frequent exchange with your supervisors. The thesis is supervised in cooperation with EPSE@ETH, therefore you have the possibility to gain insights into two different workgroups and universities. In addition, you can extend your knowledge in the fields of thermodynamics and programming. As this is a theoretical thesis it is possible to conduct in entirely out of the home office with a close supervision via online meetings. However the thesis can also be supervised in person and you have the opportunity to carry out the work at the university. If you are interested please notify us via E-Mail (Please append your current Grades and CV)

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