

Reaction Kinetics of Low-GWP Refrigerants from First Principles

Ass. Professorship of Sustainable Future Mobility (Prof.-Ing Agnes Jocher), Technical University of Munich

START	DURATION	LANGUAGE	LOCATION
immediately	6 months	English	Garching Campus

THE PROJECT

Refrigerants with a high global warming potential (GWP) are being phased out, and low-GWP alternatives are taking their place. How these new molecules react in the gas phase is still not well understood. In this project you will use quantum chemistry to study these reactions.

WHAT YOU WILL DO AND LEARN

- Run density functional theory (DFT) calculations in Gaussian to find the structures and energies of reactants, products and transition states, using Avogadro to build and visualise molecules.
- Performing and Interpreting ab-initio calculations for gas-phase kinetics.
- Work on a high-performance computing cluster and automate your workflow with simple scripts.
- Analyse, document and present your results as a scientific thesis.

WHO I AM LOOKING FOR

- A Master's student in chemistry or chemical engineering.
- A good understanding of physical chemistry.
- Some experience with Python, Linux and Latex is helpful but not required.
- Familiarity with chemical kinetics, transition state theory or RRKM/master equation methods is a plus
- No prior experience in quantum chemistry or statistical mechanics is needed. What matters is that you are curious, reliable and willing to learn.

SUPERVISION

I am a postdoctoral researcher and computational chemist in Prof. Jocher's group. I did my Ph.D. with Prof. C. Franklin Goldsmith at Brown University, developing detailed kinetic mechanisms.

I do not expect you to know everything from the start. Learning this field takes time, and I am looking for someone who is ready to put in that time and work through problems together. We will meet every week to keep your thesis on track, and I am available for questions in between.

You would be the first thesis student I supervise. That means close, hands-on guidance, and it also means I will be asking for your feedback on what helps you and what does not.

HOW TO APPLY

Send the following to siddha.sharma@tum.de with the subject line "Master's thesis: low-GWP refrigerants" by October 19, 2026.

- CV
- Short cover letter (one page at most) no AI, I am interested in knowing why this work interests you.

Shortlisted candidates will be invited to an interview and will receive three to four research articles beforehand. You are not expected to follow every derivation. I want to see how you read and think about new material.