Steffen Wedig

Academic Education

2024–2025 **MPhil Scientific Computing**, *Churchill College, University of Cambridge*
Focus on atomistic simulation. Lectures on high-performance computing, electronic structure calculation, and atomistic modelling of materials.

2022–2024 **MSc. Materials Science & Engineering**, *Technical University Munich*, *Grade 1.3*
Elective focus "Uncertainty Quantification and Mathematical Modeling". Lectures included probability theory, multiscale modeling, and molecular dynamics.

2019–2022 **BSc. Chemical Engineering**, *Technical University Munich*, *Grade 1.8*
Focus on heterogeneous catalysis and industrial process engineering.

2013–2019 **Abitur**, *Privates Internatsgymnaisum Schloss Torgelow*, *Grade 1.0*
German high-school diploma, top of class.

2016–2017 **Indian Springs School, Birmingham, Alabama, USA**
Junior year at a US high-school

Research Projects

Apr 2024 – Sep 2024 **Prior Potentials for Stable Molecular Dynamics Simulations with Machine Learning Force Fields**, *Master's Thesis at the Chair for Multiscale Modeling of Fluid Materials*, *Grade 1.0*
Developed Δ-Learning methods to use stable empirical force fields for top-down training of ML potentials on experimental observables. Extended functionality of in-house library for training ML-potentials. Supervised by Prof. Julija Zavadlav.

Feb 2024 – Apr 2024 **Active Learning of Equivariant Graph Neural Network Potentials for Metal-Organic Frameworks**, *Research Internship at the Chair for Simulation of Nanosystems for Energy Conversion*
Implemented active learning workflow, including metadynamics in PLUMED, DFT calculations in CP2K, and ML training to obtain NequIP potentials for simulation of metal-organic frameworks. Supervised by Prof. Alessio Gagliardi.

Aug 2023 – Jan 2024 **Internship at Spaceship EAC**, *European Space Agency (ESA)*, Cologne
Initiated project developing experimental 3D-printer for lunar additive manufacturing. Responsible for mechanical design, simulation of the sintering process, development of printer control software, and manufacturing/assembly. Supervised by Dr. Aidan Cowley.

Apr 2022 – Sep 2022 **Application of Nickel-containing Inks in the Binder Jet 3D-Printing of Ni/Al_2O_3 Catalysts for CO_2 Methanation"**, *Bachelor's Thesis at the Chair of Technical Chemistry*, *Grade 1.0*
Developed 3D-printing manufacturing process of alumina supported nickel catalysts for CO_2-reduction. Laboratory work contained a wide range of mechanical, physical, and chemical characterization. Supervised by Prof. Kai-Olaf Hinrichsen.

Scholarships and Prizes

2019-2025 **German Academic Scholarship Foundation**
Supported Bachelor's, Master's Studies at Technical University of Munich, Supported MPhil at University of Cambridge with additional "Study-Abroad" program.

2013-2019 **Foundation Begabt**
Supported high school education at boarding school.

2016-2017 **Foundation ASSIST**
Scholarship for attending Indian Springs School, Alabama, US.

2011 **History Competition of the German Federal President**
Research report on the Contergan scandal, 1st prize nationwide, 2000€ award.
Titled "Contergan - Tragedy? Catastrophe? Scandal?"

Extracurricular Activity

2021 – 2023 **Scientific Workgroup for Rocketry and Spaceflight (WARR)**
Project REBELS. Student group working on moon rover for additive manufacturing.
Team Lead Experimental: Planning and conducting test campaign.
Payload Software: Developing embedded software for sensors/actuators on payload.

2022 – 2023 **TUM: Junge Akademie**
Team CheckMate: 20-month research project to investigate Fake News consumption and recognition in high-school students.

2018 – 2023 **Climate-Initiative One for the Climate e.V**
Project for alleviation of poverty and mitigation of climate change impacts for families in Rwanda through the use of renewable energy systems.
Member Digital Workgroup, developing a platform connecting cooperative members globally.

Skills

Software Development	Python, C++, Matlab. Git, SLURM. Shell-scripting. Application Areas: Scientific Computing, Embedded+ Robotics, Numerical Methods, Data Analysis
Machine Learning	ML projects in PyTorch and JAX. Mostly focused on methods for Geometric Deep Learning.
Simulation	Molecular Dynamics in GROMACS, LAMMPS, JAX MD. Metadynamics Simulations with PLUMED. Machine Learning Force Fields (NequIP). DFT calculations in CP2K.
Laboratory	Solid-State Synthesis, Catalyst Preparation and Characterization, Analytical Chemistry Methods.

Languages

German	Mother tongue
English	C2

Publications

[1] Hanh My Bui, Tim Kratky, Insu Lee, Rachit Khare, Max Hiller, Steffen Wedig, Sebastian Günther, and Olaf Hinrichsen. In situ impregnated Ni/Al_2O_3 catalysts prepared by binder jet 3d printing using nickel nitrate-containing ink. *Catalysis Communications*, 182:106738, 2023.