Samir Darouich

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EDUCATION

Massachusetts Institute of Technology (MIT) Cambridge, USA
Visiting PhD student in Chemical Engineering. 09.2025 – 11.2025
Topic: *Machine Learning for Reactivity Elucidation in Computational Chemistry* with Prof. H. J. Kulik.

University of Stuttgart Stuttgart, Germany
PhD in Theoretical Chemistry and Machine Learning. 06.2024 –
Topic: *Machine Learning for Reactivity Elucidation in Computational Chemistry* with Profs. J. Kästner (theoretical chemistry) and M. Niepert (artificial intelligence).

University of Stuttgart Stuttgart, Germany
Master of Science in Chemical and Biological Engineering: **Grade: 1.0** 10.2021 – 09.2023
MS Thesis: *Vapor-liquid equilibria of binary mixtures estimated from molecular dynamics free energy simulations in the liquid phase* with Profs. N. Hansen and J. Gross.

University of Stuttgart Stuttgart, Germany
Bachelor of Science in Chemical and Biological Engineering: **Grade: 1.7** 10.2018 – 09.2021
BS Thesis: *Investigation of the transferability of the TAMie force field for primary alcohols to secondary alcohols and diols* with Profs. N. Hansen and J. Gross.

PUBLICATIONS

- **Darouich, S.;** Tong, V.; Bien, T.; Kästner, J., Niepert, M. „Adaptive Transition State Refinement with Learned Equilibrium Flows" Preprint at https://arxiv.org/abs/2507.16521 (2025).
- Fleck, M; **Darouich, S**.; Pleiss, J.; Hansen, N; Spera, M. "Physics-Informed Multifidelity Gaussian Process: Modeling the Effect of Water and Temperature on the Viscosity of a Deep Eutectic Solvent" *J. Chem. Inf. Model.* **65**, 3999–4009 (2025)
- Spera, M.; **Darouich, S.**; Pleiss, J.; Hansen, N. "Influence of water content on thermophysical properties of aqueous glyceline solutions predicted by molecular dynamics simulations" *Fluid Phase Equilibria* **592**, 114324 (2025).
- Mishra, R.; **Darouich, S.**; In 't Veld, P.J.; Flatt, R.; Heinz, H. "Understanding Phase Equilibria, Mechanical Properties, Thermal Expansion, and Organic Interfacial Interactions of Calcium Sulfate Hydrates from the Atomic Scale" *Cement and Concrete Research* **189**, 107740 (2025).
- Fleck, M.; **Darouich, S**.; Hansen, N.; Gross, J. "TAMie Force Field for Alkanethiols: Multifidelity Gaussian Processes for Dealing with Scarce Experimental Data" *J. Phys. Chem. B* **128**, 9544–9552 (2024).
- Fleck, M.; **Darouich, S**.; Hansen, N.; Gross, J. "Transferable Anisotropic Mie Potential Force Field for Alkanediols" *J. Phys. Chem. B* **128**, 4792–480 (2024).
- Deng, Q.; Jeschke, S.; Mishra, R.; Spicher, S.; **Darouich, S.**; Schreiner, E.; Eiden, P.; Deglmann, P.; Gorges, J. Chen, X.; Keil, P.; Cole, I. "Design of alkyl-substituted aminothiazoles to optimise corrosion inhibition for galvanised steel: A combined experimental and molecular modelling approach" *Corrosion Science* **227**, 111733 (2024).

HONORS & ACHIEVEMENTS

- Pro3 Research Fellowship 2022
- Participation in the Annual Program of the School for Talents 2021
- Teaching assistant qualification 2021

EXPERIENCE

University of Stuttgart Stuttgart, Germany
Data Steward, Collaborative Research Center 1333 10.2023 - 05.2024

- Establishing FAIR (findable, accessible, interoperable, and reusable) data management in chemistry by developing data models and workflows to acquire, analyze and upload data to a chosen Dataverse.
- Developed a Python module to setup and analyze molecular dynamics simulations.

BASF SE Ludwigshafen, Germany
Working student, Molecular Modeling & Drug Discovery 04.2023 – 09.2023

- Studied the interfacial tension between tricalcium aluminate and water, as well as the effect of salt additives. Led to the prediction of the best salt additives for inhibiting the reaction of tricalcium aluminate with water.
- Explored and refined workflows for all-atom force field development and validation steps (Reproduction of lattice constants, density, vibrational spectra, surface energy, mechanical properties, thermal properties, and free solvation energy).

BASF SE Ludwigshafen, Germany
Internship, Molecular Modeling & Drug Discovery 10.2022 – 03.2023

- Introduced a novel method to scan adsorption free energies of organic molecules on inorganic mineral surfaces using all-atom force field models. Organized training session for BASF modeling researchers. Included this work in BASF modeling workflows.
- Investigated the adsorption behavior of organic additives on various inorganic mineral surfaces (metal oxides, cement minerals, etc.) using molecular dynamics simulations. Results guided the understanding of binding mechanisms and selection of the best adsorbent.

University of Stuttgart Stuttgart, Germany
Pro3 Research Fellowship, Institute of Technical Thermodynamics 04.2022 – 10.2022

- Examined conformers for various diols using quantum mechanical methods resulting in development of new TAMie force field parameters.
- Introduced a ML (machine learning) algorithm to force field parameterization schemes to deal with insufficient experimental data.

Dürr Systems AG Bietigheim-Bissingen, Germany
Working student, Process Technology 09.2021 – 03.2022

- Worked on separation of CO_2 from exhaust gas streams and the regeneration of the scrubbing solutions by using bipolar membrane technology.
- Developed and produced a prototype for the measurement and evaluation of CO_2 mass transfer from gas to liquid phases.

University of Stuttgart Stuttgart, Germany
Teaching Assistant, Institute of Technical Thermodynamics 10.2020 – 03.2022

- Provided instruction and theoretical as well as technical guidance to a group of 20 undergraduate students in technical thermodynamics on a weekly basis, including grading.
- Mentored two groups of 25 undergraduate students each in advanced engineering mathematics, reviewing and correcting their homework and exams.

Robert Bosch GmbH Stuttgart, Germany
Working student, Exhaust aftertreatment systems 11.2019 – 10.2020

- Prepared diesel exhaust catalysts samples for laboratory bench testing.
- Developed, executed, and evaluated test procedures to characterize greenhouse gas emission reduction.

SKILLS & INTERESTS

Software:

- Python, C/C++, MATLAB, Aspen Plus, LabVIEW, Microsoft Office (Word, Excel, PP)

Scientific skills:

- Developing methods for flow matching, diffusion models, and deep geometric learning.
- Gaussian process regression and multi-fidelity modeling.
- Molecular dynamics / Monte Carlo simulations, DFT and force field development.

Certificates:

- Deep learning (by IBM, 2024)

Languages:

- German, English, French, Spanish

Hobbies:

- Working out, Padel-Tennis, Calisthenics