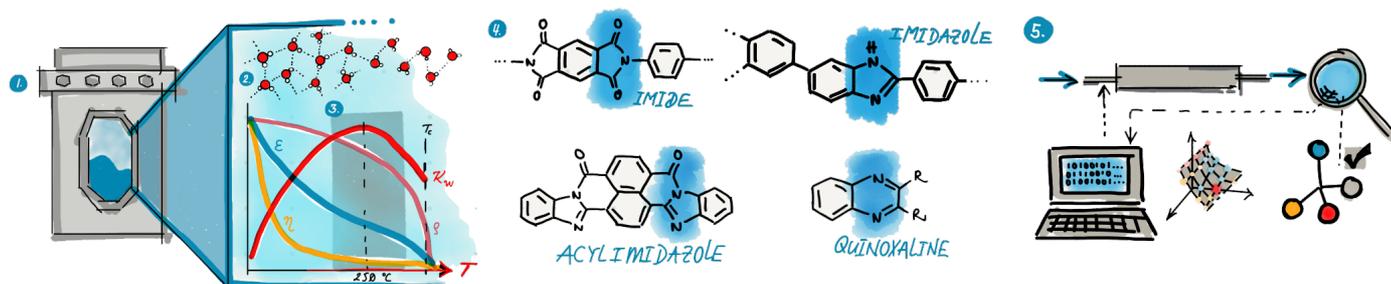


PhD position in automation of chemical synthesis

What we offer: One PhD position in an interdisciplinary and vibrant research group at the wonderful University of Konstanz. We provide cutting-edge scientific training including chemical synthesis, handling of reactors, advanced characterization techniques, and presentation and discussion of data. We furthermore provide ample soft skills training and support all team members in reaching their full potential.

The project: Hydrothermal synthesis (HTS) relies on using high-temperature liquid water as reaction medium. Mimicking the natural formation of various minerals (e.g. zeolites), HTS has been explored for decades in inorganic chemistry.^[1] HTS is conventionally performed in batch, for instance in autoclaves (1), where H₂O and the starting compounds are heated to ~180-250 °C. With increasing *T*, H₂O's hydrogen-bonding breaks down successively (2), which results in favorable changes in H₂O's physicochemical properties. For instance (3), polarity (ϵ), viscosity (η), and density (ρ) decrease, while H₂O's autoprotolysis (K_w) increases (maximum at 250 °C). Recently HTS has been shown to also be amenable to the synthesis of organic compounds. Our group provided several examples including e.g. aromatic polyimides, rylene dyes, perinone, polybenzimidazoles, and quinoxalines (4).^[2-6] We believe that HTS bears the potential to be suitable for synthesizing many more organic scaffolds. To explore this potential efficiently and bringing HTS to the next level, we aim to maximally automate HTS in flow (5). This effort will include the artificial intelligence (AI)-supported prediction of organic HTS, carrying these out in flow, in-line/on-line analysis of the reaction outcome, and data-collection plus feedback into the prediction algorithms. The ultimate goal of this project is to profit from the unique features of high-temperature water for efficiently and rapidly accessing untapped areas of the chemical space in a sustainable manner.



References: [1] M. M. Unterlass, *Biomimetics* **2017**, *2*(2), 8-27. [2] B. Baumgartner, M. J. Bojdys, & M. M. Unterlass, *Polym. Chem.* **2014**, *5*, 3771-3776. [3] B. Baumgartner, A. Svirikova, J. Bintinger, C. Hametner, M. Marchetti-Deschmann, & M. M. Unterlass, *Chem. Commun.* **2017**, *53*, 1229-1232. [4] M. J. Taublaender, F. Glöckhofer, M. Marchetti-Deschmann, & M. M. Unterlass, *Angew. Chem. Int. Ed.* **2018**, *57*, 12270-12274. [5] M. J. Taublaender, S. Mezzavilla, S. Thiele, F. Glöckhofer, & M. M. Unterlass, *Angew. Chem. Int. Ed.* **2020**, *59*, 15050-15060. [6] F. A. Amaya-García, M. Caldera, A. Koren, S. Kubicek, J. Menche, & M. M. Unterlass, *ChemSusChem* **2021**, *14*, 1-12.

What we are looking for: Candidates are required to hold a Masters/Diploma/Magister university degree in chemical engineering, process engineering, chemistry, or a related discipline. Experience in working with reactors, reactor design and optimization, design of experiments, and programming is desired, but not strictly necessary. Basic skills in organic chemistry (ideally of aromatics and heterocyclics) and related characterization techniques are a plus. The ideal candidate is passionate about next-generation synthesis and chemical production, automation of synthesis and analysis, and automated discovery of compounds and syntheses. Full working proficiency in English as well as the ability to work in an interdisciplinary team is a must.

How to apply: Applications are to be submitted in English via email to miriam.unterlass@uni-konstanz.de as a single pdf named "surname_givenname.pdf". Applications may be submitted from now on until August 25th, 2021. The submitted application pdf must include: (i) motivation letter, (ii) curriculum vitae including a list of publications, conference contributions, and other scientific activities (if applicable), (iii) transcript of records of the Bachelor and Master studies, (iv) title and a short summary of the diploma/master thesis, (v) contact details of two referees.

Basic data: The deadline of application is August 25th, 2021. The intended starting date is December 2021/January 2022. Other starting dates can be arranged. The project will be situated at our laboratories at the University of Konstanz in Germany. Short stays at our second branch at the CeMM Research Centre for Molecular Medicine of the Austrian Academy of Sciences in Vienna, Austria, are part of this project.

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