

Open doctoral student position in solid-state NMR spectroscopy

The research group of Prof. Dr. Thomas Wiegand at the MPI CEC and the Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen is looking for an enthusiastic

Doctoral student (m/f/d) for studying ATP-hydrolysis in ATPases by solid-state Nuclear Magnetic Resonance spectroscopy.

Available topic. Protein-nucleotide interactions play a central role in biology and control a variety of processes, such as ATP hydrolysis and DNA replication, both relying on very specific molecular interactions for adequate functionality. This project aims at expanding and applying our solid-state NMR toolbox to probe protein-nucleotide interactions using the example of the ATPase SmsC belonging to the Sms-system responsible for the formation of Fe-S clusters. From a methodological perspective, we aim among others at introducing ^{19}F -detected solid-state NMR at fast MAS frequencies (>100 kHz) into our toolbox allowing us to derive distance restraints between ^{19}F -labelled nucleotides and the protein. Such studies will be complemented by proton-detected experiments enabling the positioning of the nucleotide phosphate backbone in the nucleotide-binding domain, as well as by ^{31}P - ^{31}P distance measurements to probe the phosphate geometry. We aim at deriving a detailed understanding of the mechanism of ATP-hydrolysis in the ATPase SmsC, e.g. by performing real-time solid-state NMR studies employing suitable ATP-mimics. For some selected publications see Wu, Zehnder, Schröder, et al. *J. Am. Chem. Soc.* **2024**, *146*, 9583–9596; Malär et al. *Nat. Commun.* **2021**, *12*, 5293; Wiegand, Schledorn, et al. *ChemBioChem.* **2020**, *21*, 324-330.

Prerequisites. Successful candidates should have a science education in chemistry, physics or biology and a strong interest in spectroscopic techniques. The candidate should be interested in biochemical laboratory work.

How to apply. Your complete application should contain a curriculum vitae (CV) and the names of two professional references whom we may contact, which should also be sent by e-mail to Prof. Dr. Wiegand. We are looking forward to getting to know you! The starting date is flexible, the position is open from June 2025. Deadline for application is May 31st.

About us. We study molecular-recognition events in biology and chemistry by magnetic-resonance spectroscopy. This is achieved by developing and applying a set of dedicated solid-state Nuclear Magnetic Resonance (NMR) experiments enabling the detection and quantification of noncovalent interactions that are guiding such processes at the molecular level. In that vein, the group currently focuses on four selected molecular recognition processes, namely cellular organization by phase separation events, ATP-hydrolysis in ATPases, solid-state molecular recognition processes in organic mechanochemistry and recognition of substrate molecules on immobilized catalyst surfaces. The lab located at the Institute of Technical and Macromolecular Chemistry at RWTH Aachen University is equipped with NMR spectrometers up to 700 MHz enabling magic-angle spinning (MAS) experiments up to 111 kHz.

Questions. For further information regarding the available positions, please contact Prof. Dr. Wiegand directly by e-mail wiegand@itmc.rwth-aachen.de.