
 <p>FACULTY OF SCIENCE Charles University</p> <p>Dr. Zdeněk Tošner NMR laboratory Faculty of Science Charles University Prague https://natur.cuni.cz/eng</p>	 <p>TECHNISCHE UNIVERSITÄT MÜNCHEN</p> <p>Prof. Dr. Bernd Reif Biological solid-state NMR TUM School of Natural Sciences Technische Universität München https://www.bio.nat.tum.de/ocb/home/</p>
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Postdoc and PhD positions in the Development of advanced NMR methods using optimal control and artificial intelligence

We are an international research group focusing on the development of advanced solid-state NMR experiments through computer optimizations. In solid-state NMR, structural information is obtained from correlations between atoms established via intriguing interplay of radiofrequency pulses and fast sample rotation, which modulates orientation dependent anisotropic interactions. By application of optimal control theory, we have demonstrated a significant enhancement in the sensitivity of each magnetization transfer step within high dimensional experiments essential for resonance assignment in protein applications, with gains on the order of x2-3 per transfer (Tošner et al., 2018; Blahut et al., 2022, 2023).

We are looking for postdoctoral fellows and PhD candidates to carry on the quest to improve the sensitivity and ease of use of magnetic resonance spectroscopy.

The proposed projects aim to mitigate the adverse effects of hardware properties of (ultra)fast-spinning MAS probes, including spatial rf field distributions, pulse transients, and MAS frequency fluctuations. Computer optimizations will use adaptive algorithms accounting for multi-spin effects in proton dipolar networks. Innovative techniques will exploit the concept of sensitivity enhancement via coherence order transfers in multidimensional correlation experiments. Implementing non-traditional transfers will require new data processing techniques, supported by artificial intelligence and machine learning algorithms, to streamline the interpretation of spectroscopic data.

The research will be carried out in close collaboration between the groups of Zdeněk Tošner, Charles University, Prague, and Bernd Reif, Technical University of Munich. Interested candidates should have a solid background in either physical chemistry, quantum mechanics, or math, according to their career stage. Theoretical and practical experience with NMR will be an advantage. Competitive remunerations are offered. Applications to MSCA fellowships will be supported.

Selected references

- Tošner Z, Sarkar R, Becker-Baldus J, Glaubitz C, Wegner S, Engelke F, Glaser SJ, Reif B (2018) Overcoming volume selectivity of dipolar recoupling in biological solid-state NMR. *Angew Chem Int Ed Engl.* 57: 14514-14518; doi: [10.1002/anie.201805002](https://doi.org/10.1002/anie.201805002).
- Blahut J, Brandl MJ, Pradhan T, Reif B, Tosner Z (2022) Sensitivity-Enhanced Multidimensional Solid-State NMR Spectroscopy by Optimal-Control-Based Transverse Mixing Sequences. *J. Am. Chem. Soc.* 144: 17336-17340; doi: [10.1021/jacs.2c06568](https://doi.org/10.1021/jacs.2c06568).
- Blahut J, Brandl MJ, Sarkar R, Reif B, Tošner Z (2023) Optimal Control Derived Sensitivity-enhanced CA-CO Mixing Sequences for MAS Solid-state NMR – Applications in Sequential Protein Backbone Assignments. *JMRO* 16-17: e100122; doi: [10.1016/j.jmro.2023.100122](https://doi.org/10.1016/j.jmro.2023.100122).

General Information

The **Tošner group** is located at the Faculty of Science, **Charles University** (www.natur.cuni.cz/eng/), which belongs to the leading research institutions in the Czech Republic. The campus, located in the center of Prague, is home to prominent groups in physical and organic chemistry, among others. Our on-campus facilities are complemented by powerful supercomputing systems (e.g., 15.7 PFlop/s on the Karolina supercomputer) operated by IT4Innovations (www.it4i.cz/en), and top-level NMR spectrometers installed at the Josef Dadok National NMR Centre in Brno (nmr.ceitec.cz/).

The **Reif group** is integrated into the **Bavarian NMR Center** (www.bnmrz.org) and is associated with the **Institute of Structural Biology** (www.helmholtz-munich.de/en/stb) at the Helmholtz-Zentrum München (HMGU). Labs are located in the Bavarian NMR Center at Campus Garching, together with the Groups of Prof. Sattler, Prof. Hagn and Prof. Glaser. In addition to a high-end NMR facility, our group has direct access on campus to a [X-ray crystallography facility](#), as well as to a [cryo-EM platform](#) equipped with a Selectrix X imaging filter and a modern Falcon 4i direct electron detector enabling cutting-edge single-particle analysis and in situ cryo-electron tomography. While working at BNMRZ, you participate in the scientific seminars organized by the [BNMRZ](#), the [STB](#) and the cooperate research center [SFB1035](#).

If you are interested, please send an email with a copy of your CV to tosner@natur.cuni.cz or reif@tum.de.

Department of Chemistry at the Charles University in Prague



Bavarian NMR Center at the Technical University Munich in Garching

