

Three year DFG funded PhD position open at the University of Freiburg Germany

The development of functional materials and for fundamental investigations, mechanochromic systems with tunable force range and that change the spectroscopic properties with acting force are highly desirable. The force response of single polymer chain experiments can be predicted with remarkable accuracy [1], but the force distribution within real macroscopic samples is unknown, and furthermore changes with time through relaxation processes ("ageing"). The theoretical description by time-dependent optical properties of mechanophores has so far been elusive.

The theoretical simulation work within the project requires a close collaboration between synthetic chemistry (M. Sommer, Chemnitz) and experimental polymer physics (G. Reiter, Freiburg).

Your work includes:

- Theoretical design of mechanochromic molecules in close collaboration with synthetic chemistry.
- Model building to include effects of the complex environment on initial strain distributions and on the mechanochromic response.
- Analysis and model building to understand time dependent experimental signal distributions.

The PhD will be located in Physics and in order to be accepted at the Institute of Physics at University of Freiburg sufficiently high marks in the master degree in Physics, Chemistry or related fields are needed. We will extensively use the state of the art DFT (and beyond) package GPAW and the atomic simulation environment (ASE). Therefore experience and joy in programming are very helpful. Good communication skills in English are required. Previous experience with electronic structure calculations or effective model building (e.g. kinetic theory) is a clear plus.

The University of Freiburg provides a lively research environment in a large variety of research topics. The PhD work is well funded (75% TV-L E13) for the period of three years. Last, but not least, Freiburg is a town of high living quality. The town is located in the south-west corner of Germany with pleasant living conditions. Possible starting date is 1.3.2025 or as soon as possible after this date.

Please, send your application to Michael.Walter@mf.uni-freiburg.de

<http://www.functional-nanosystems.uni-freiburg.de/People/PDWalter/group>

[1] Mechanistically Different Mechanochromophores Enable Calibration and Validation of Molecular Forces in Glassy Polymers and Elastomeric Networks Raphael Hertel, Maximilian Raisch, Michael Walter, Günter Reiter and Michael Sommer *Ang. Chem. Int. Ed* (2024) DOI : 10.1002/anie.202409369