

Three year DFG funded PhD position for simulation of mechanoresponsive (mechanochromic) polymers open at the University of Freiburg Germany

Smart materials that are able to respond to external stimuli are under extensive investigation because of their vast range of applications in biology, information technology, self-healing, sensing, energy-related topics, and others. Mechanically responsive polymers are specifically designed to direct mechanical energy towards a reaction center in order to favor a certain process over unselective bond scission, which is the usual response of polymer materials to large deformation. Mechano-responsive polymers change properties drastically upon exposure to mechanical stress, which can be used to switch reactivity or to bias distinct reaction pathways otherwise difficult to access. The term *mechanochromism* entails a change of the visible absorption spectrum upon mechanical deformation. Typical mechanophores are spiropyrans (SP), which we have successfully addressed in the past [1-3]. The new PhD project is devoted to the exploration of flexible mechanochromophors that do not only offer coloration when a threshold is reached, but could be able to flexibly indicate forces at the molecular level as soon as these are present.

In order to be accepted as a PhD student at the Institute of Physics at University of Freiburg sufficiently high marks in the master degree are needed. The PhD work will require substantial programming work, mainly in Python. Therefore experience and joy in programming are pre-conditions. Experience with electronic structure calculations and is a plus. In close collaboration with experiment, we will develop descriptions of macroscopic forces acting directly on molecules embedded in polymers. This work might involve extensions to the state of the art DFT (and beyond) package GPAW and/or to the atomic simulation environment (ASE). Good communication skills in English and/or German are required.

We offer the work on a topic that is directly connected to the experimental work performed in the group of Prof. Michael Sommer, Chemnitz, Germany. The University of Freiburg provides a lively research environment in a large variety of research topics. The PhD work is well funded (67% TV-L E13) for the period of three years. Last, but not least, Freiburg is a town of high living quality. Possible starting date is 1.3.2019 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] Temperature and loading rate dependent rupture forces from universal paths in mechanochemistry

Oliver Brüchner and Michael Walter *Phys. Rev. Materials* **2** (2018) 113603

[2] A Simply Synthesized, Tough Polyarylene with Transient Mechanochromic Response

Fabian Kempe, Oliver Brüchner, Hannah Buchheit, Sarah N. Momm, Felix Riehle, Sophie Hameury, Michael Walter and Michael Sommer *Angew. Chemie Int. Ed.* **57** (2018) 997-1000

[3] Alkyl-substituted spiropyran: Electronic effects, model compounds and synthesis of aliphatic main-chain copolymers

Simon Schmidt, Fabian Kempe, Oliver Brüchner, Michael Walter, and Michael Sommer *Polymer Chemistry* **8** (2017) 5407-5414