

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

Efficient and environmentally friendly energy storage technologies are required on various levels to ensure uninterrupted supply of renewable energies. Among available technologies, lithium-ion batteries (LIBs) have emerged as state-of-the-art systems for various applications despite their limited capacities and energy densities. Lithium-sulfur (LiS) batteries exceed these capacities and energy densities by far, offering also low cost and the use of abundant elemental sulfur. However, these attractive theoretical numbers are not realized in real devices due to a multitude of factors related to insufficient morphology control, low conductivity and sluggish reaction kinetics. Furthermore, Li-S batteries suffer from polysulfide dissolution and shuttle leading to ineffective sulfur utilization, capacity decay and thus finally a lower energy density as well as low cycling stability. A strategy to mitigate these irreversible processes is covalent fixation of sulfur in some form, e.g. through inverse vulcanization. The underlying structure of the resulting material is poorly understood, however.

The theoretical simulation work within the project requires a close collaboration between synthetic chemistry (M. Sommer, Chemnitz), experimental NEXAFS and x-ray emission (XES) spectroscopy (M. Müller, PTB Berlin). The project is embedded in SPP 2248 (polymer-based batteries) with extensive contacts to other groups working in the field.

Your work includes:

- Determination of Network stability and structure of novel sulfur-bridged redox-active organic networks.
- Prediction of theoretical NEXAFS and XES spectra for the materials under different conditions.
- Development of methods to calculate stabilities and barriers at given cell potentials.

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 develop novel approximations for reactivities under fixed potentials and will implement them to the state of the art DFT (and beyond) package GPAW and/or to the atomic simulation environment (ASE). Therefore experience and joy in programming are very helpful. Good communication skills in English and/or German are required. Previous experience with electronic structure calculations and 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 1.3.2024 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>