PhD Position in Computer Simulations of Ion and Electron Transport in Redox-Active Polymers: Münster, Germany

A PhD position (salary level TV-L E13, 50%) on the topic "Computer simulations of ion and electron transport in redox-active polymers" is open in the group of Prof. Andreas Heuer at the Institute of Physical Chemistry of the University of Münster (Germany) for a 3-year period. The position is available immediately and intended to be filled by the earliest convenient date.

JOB DESCRIPTION

Our group has a strong background in studying the microscopic properties of complex systems such as electrolytes, polymers, glasses, and (biological) soft matter from a theoretical perspective using computer simulations. In this project, the successful candidate will perform both classical molecular dynamics simulations and quantum chemistry calculations to study the ion and electron transport in redox-active polymers, which are promising electrode materials for next-generation batteries. In particular, a hybrid scheme, in which classical molecular dynamics simulations are augmented by quantum chemical information about the electron hopping dynamics, will be implemented. These activities will be carried out in close collaboration with experimental groups working on the synthesis and characterization of these materials within the priority programme "Polymer-based Batteries" (SPP 2248), which is funded by the German Research Foundation (DFG). In this way, the insights gained in this project can directly be transferred to the optimization of novel organic electrode materials. The work will be supervised by Dr. Diddens (Helmholtz-Institute Münster).

We are looking for a highly motivated person with a completed diploma or master's degree (or equivalent) in physics, chemistry, materials science, or a related field of study. Applicants should have an excellent background in atomistic simulations of complex systems and theoretical chemistry. Programming experience in at least one programming language and basic knowledge of Unix-like operating systems are mandatory. Furthermore, excellent cooperation and communication skills in written and spoken English are required for frequent exchange with internal and external collaborators.

We offer excellent research conditions and a vibrant working atmosphere. At the University of Münster, the Institute of Physical Chemistry has a long-term expertise in the research on polymeric ion conductors, whereas the neighboring institutions Münster Electrochemical Energy Technology (MEET) and the Helmholtz-Institute Münster (HI MS) are internationally renown for their research on batteries, making Münster a key location for research on electrolytes.

ABOUT THE EMPLOYER

The University of Münster is an equal opportunity employer and is committed to increasing the proportion of women academics. Consequently, we actively encourage applications by women. Female candidates with equivalent qualifications and academic achievements will be preferentially considered within the framework of the legal possibilities. The University of

Münster is committed to employing more staff with disabilities. Candidates with recognized severe disabilities who have equivalent qualifications are given preference in hiring decisions.

YOUR APPLICATION

Applicants are requested to send a statement of interest, a full CV including certificates as well as names and addresses of at least two references to Ms. Andrea Staubermann via Andrea.Staubermann@uni-muenster.de. The position will remain open until filled.

Further information about the group can be found here: https://www.uni-muenster.de/Chemie.pc/en/forschung/heuer/forschung/index.html