**University of Stuttgart**
Germany

**Institute for Computational Physics**

**Director**
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**Call for postdoctoral research associate on simulations of reaction equilibria in polymer systems**

The Institute for Computational Physics at the University of Stuttgart is seeking a highly motivated postdoctoral research associate to work on coarse-grained simulations of reacting polyelectrolyte systems. The research should be carried out under the supervision of Prof. Dr. Christian Holm in close collaboration with the group of Dr. Peter Košovan from the Department of Physical and Macromolecular Chemistry of the Charles University in Prague, Czech Republic.

**Background**

Reacting (pH sensitive) systems in contact with a reservoir are ubiquitous in chemical research, especially in colloid and polymer science, and widely used to separate or purify substances. pH-sensitive polyelectrolytes affect the partitioning of exchangeable ions between the system and the reservoir, thereby strongly affecting the pH. The acid-base equilibrium combined with ion partitioning results in a complicated feedback loop. Representing such a system in molecular simulations is a challenging task, and the recent development of the Grand-Reaction Ensemble Method (GREM) has allowed for a correct simulation of this scenario. The aim of the current project is to further develop, implement and apply the GREM for simulating coacervates, reversible polymer gels and partitioning of solutes; use computer simulations to predict their structure, stability and ability to sequestrate ions at various pH; and compare the predictions to experiments and theory.

**What we are looking for**

Applicants should possess a PhD in Physics, Physical Chemistry or related areas. A solid background on theoretical and statistical mechanics as well as willingness for collaborations and team work is expected. A strong background in simulations and software design are important. Experience on programming in Python and C/C++ is advantageous. The main task consists on designing the models, implementing them into the simulation package ESPREesSo (www.espressomd.org), carrying out the simulations, analysing the data and writing the publications.

**What we are offering**

- Full-time position in TVL-E13 remuneration of the German State Employees for 1-3 years, depending on agreement and performance. The opportunity to get to know a broad variety of simulation approaches and techniques.
- Close interaction with other groups on theoretical modelling and experiments.
- An interdisciplinary and flexible research environment where we also encourage the contribution of new research ideas and directions.

The position is available immediately, and will be open until the position is filled. Please send your applications as PDF file to application@icp.uni-stuttgart.de, including CV, 2 letters of reference, and a motivation letter.

In an effort to strengthen the presence of female workers in scientific areas, the University of Stuttgart invites women to apply for this job opening. Disabled people will have priority as long as equally qualified.

With kind regards

Christian Holm