Modeling of branched weak polyelectrolytes in solution
(postdoc project proposal)

Weak polyelectrolytes are charged polymers with a variable ionization which can be controlled by pH, external electric potential, or by other stimuli. Exploiting the stimuli-responsive ionization in applications requires understanding how the ionization is related to the macromolecular architecture and to polymer-solute interactions. The postdoc project entails the use of coarse-grained molecular simulations to obtain molecular-level understanding of ionization of branched weak polyelectrolytes. We taget two specific problems connected by the star-branched architecture of the weak polyelectrolytes: (i) their application in redox-flow batteries, and (ii) their interaction with hydrophobic and ampholytic solutes, such as drugs, peptides or proteins.

Redox-flow batteries (RFB) present a promising alternative for a large-scale energy storage which is desired for efficient exploitation of renewable energy sources such as solar or wind. Solutions of branched weak polyelectrolytes have been proposed as an affordable, safe, non-toxic and scalable solution for RFBs [Nature 78, 527 (2015)]. Our team has recently joined an international collaboration aimed at development of polymer systems for RFB applications. The goal of this project is to employ coarse-grained simulations to study changes in the solution properties which occur upon charging of polymers due to the electric potential applied at the electrode. The results will help understanding the relation between the polymer architecture and its energy storage capacity, solubility, and solution viscosity. In collaboration with experimentalists doing synthesis, characterization, and commercial implementation of the studied materials, the simulation results will be used to guide the selection of materials for improved performance.

Interactions of synthetic star-like weak polyelectrolytes with hydrophobic solutes and ampholytes exhibit counter-intuitive behavior. For instance, the BSA protein adsorbs inside PE brushes of PAA on the “wrong side of the isoelectric point” i.e. when the charge of both protein and the brush have the same sign. This effect has been interpreted in terms of patchy distribution of charges on the protein, while the variable ionization of weak acid and base groups has been neglected. Our preliminary simulations and experiments indicate that charged hydrophobic solutes induce ionization of the inner part of weak polyelectrolyte micelles. This allows for loading of bigger amounts of such solute inside the micelles, than what could be expected if the ionization was fixed.

The candidate's task will be to contribute to the design the simulation models, to carry out the simulations and to analyze the simulation data. To simulate the ionization of weak polyelectrolytes, we will use the reaction ensemble method [J. Chem. Phys. 100, 3019–3027 (1994)] and the Espresso simulation software [www.espressomd.org]. The simulation results will be used for fundamental understanding of the physical process, as well as for interpretation of experimental results from collaborating teams.

Salary: equivalent of 2000 EUR / month.

Profile of an ideal candidate:

- Completed PhD or a fixed date of PhD defense
- Good knowledge of English (FCE equivalent or better)
- Strong background in soft matter and statistical mechanics
- Experience with molecular simulation, programming and Linux OS

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