Fully funded PhD and postdoc position in the Soft Matter group

Faculty of Science, Charles University, Prague, Czechia

Project title: Controlling encapsulation and release by charge regulation in macromolecules - *Combining simulations with experiments*

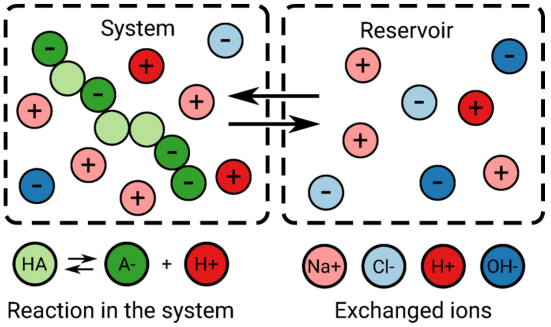
Contact person and project supervisor: Dr. Peter Košovan, peter.kosovan@natur.cuni.cz

Research group: Soft Matter www.physchem.cz/research/soft-matter

Department: Physical and Macromolecular Chemistry www.physchem.cz

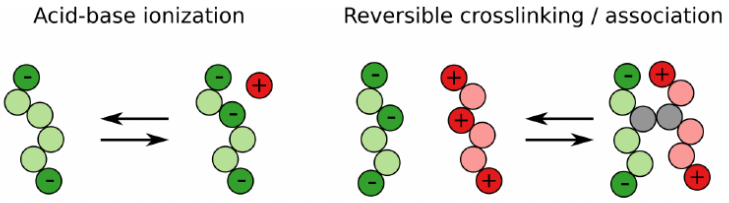
Area of research:
The Soft Matter group combines a variety of experimental methods and simulations/theory to investigate self-assembling polymer systems, such as polyelectrolyte solutions, micelles, interpolyelectrolyte complexes or polymer gels. We focus on fundamental understanding of thermodynamic and kinetic aspects of the behaviour of these systems.

Project summary:
Two-phase systems based on polyelectrolyte gels or coacervates are potential candidates for charge-based protein sequestration, while polymers modified by boronic acids are capable of sugar sensing. Their common feature is a chemical reaction inside the system, coupled to partitioning of solutes between the system and the bulk solution [1,2]. Experimental studies of such systems have long shown a deficit in theoretical support, partly due to the lack of suitable simulation methods.



We have recently introduced the Grand-reaction ensemble method which enables simulating reactive polymer systems in equilibrium with a reservoir [2]. Within the proposed project we further develop this method and apply it to simulations of two-phase systems, addressing specific questions arising from experiments performed by our collaborators within the project, or by our external partners. We will use the computer simulations to predict the properties of both phases: supernatant solution and the coacervate of polyelectrolyte gel. Furthermore, We will use this method to predict the partitioning of small ionic solutes between both phases.

The main job of the candidate will be performing the simulations, analyzing the data, refining the models and implementing new simulation algorithms or new simulation protocols. Optionally, the job may also include experimental investigation of these systems.



[1] J. Landsgesell, L. Nová, O. Rud, F. Uhlík, D. Sean, Pascal Hebbeker, C. Holm, P. Košovan: Simulations of ionization equilibria in weak polyelectrolyte solutions and gels, *Soft Matter* (2019) DOI: 10.1039/c8sm02085j
[2] J. Landsgesell, P. Hebbeker, O. Rud, R. Lunkad, P. Košovan, C. Holm: Grand-reaction method for simulations of ionization equilibria coupled to ion partitioning. Macromolecules, 53(8):30073020, 2020

Features of an ideal candidate:
Required: MSc. or equivalent in Chemistry, Physics or a related field, good knowledge of English
Beneficial: Solid background in Physical Chemistry, Soft Matter or Polymer Science. Experience with molecular simulations, programming or Linux.

Our Offer:

- *Interdisciplinary work environment, where theoretical and experimental research is conducted hand-in-hand.*
- *Work in an international group in the beautiful city of Prague.*
- *Participation at international conferences and workshops.*
- *Collaborations and further scientific training through international partners.*
- *Flexible salary or scholarship to ensure a comfortable living standard in Prague (to be negotiated with selected candidates).*