

Three most important publications

Peter Košovan

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1. Filip Uhlík, Peter **Košovan**, Zuzana Limpouchová, Karel Procházka, Oleg V. Borisov, and Frans A. M. Leermakers. Modeling of ionization and conformations of starlike weak polyelectrolytes. *Macromolecules*, 47(12):4004–4016, 2014. doi: 10.1021/ma500377y, IF = 5.800, 41 citations, 5.13 citations/year

This article was our first contribution to coarse-grained simulations of acid-base equilibria in weak polyelectrolytes in solution. In this publication we showed how the reaction ensemble Monte Carlo method can be used for simulations of acid-base equilibria. We also showed a first direct comparison of a very good agreement between our simulation results and experiments. This success has triggered further work in this direction, that has become the core of the presented habilitation.

2. Lucie Nová, Filip Uhlík, and Peter **Košovan**. Local pH and effective pK_A of weak polyelectrolytes - insights from computer simulations. *Phys. Chem. Chem. Phys.*, 19:14376–14387, 2017. doi: 10.1039/C7CP00265C, IF = 3.906, 30 citations, 6.00 citations/year

This publication is our third contribution to computer simulations of acid-based equilibria in polyelectrolytes. It describes the analogy between the "effective pK_A " and "local pH" – two terms, that are being used by different groups to describe the same phenomenon. We have shown how the deviations from Henderson-Hasselbalch equation depend on the polymer chain length, its concentration, and on the permittivity of the solvent.

3. Peter **Košovan**, Tobias Richter, and Christian Holm. Modelling of polyelectrolyte gels in equilibrium with salt solutions. *Macromolecules*, 48:7698–7708, 2015. doi: 10.1021/acs.macromol.5b01428, IF = 5.554, 43 citations, 6.14 citations/year

In this publication, we investigated the swelling of polyelectrolyte gels in salt solutions, and partitioning of salt ions in these systems. These results are being used by various experimental teams to interpret and predict the swelling properties and ion partitioning in such gels. This work has become a starting point of a series of publications related to the use of such gels for desalination applications, finally leading to introduction of the grand-reaction ensemble method.

The author would like to add a note that the selection above is based on the evidence from the Web of Science, determined by the total number of citations and average number of citations per year. The author anticipates that some of his works published in 2020 and 2021 may soon become more influential than those listed above.