



November 29, 2021

Reviewer's Report on Peter Košovan's Habilitation Thesis

Acid-Base Equilibria at the Nanoscale

The habilitation thesis is based on selected author's research results conducted in the last 10 to 15 years. The results provide molecular-level insights into acid-based equilibria in model polyelectrolyte systems. The thesis starts by introducing simulation approaches – Constant-pH method and Reaction Ensemble Monte Carlo (RxMC), where the RxMC was extended by the author to include a reservoir – Grand RxMC (G-RxMC). The G-RxMC technique becomes a key result of author's research. The thesis continues with conceptually simplest case of ideal weak acid solutions and then by adding more complexity such as non-ideal solutions of weak polyacids, the thesis arrives to acid-equilibria in two-phase systems including polyelectrolytes and exchanging ions with a reservoir.

The thesis clearly demonstrates an original use of computer simulations to obtain a detail mechanistic understanding of how interactions between ionizable groups influence the acid-base properties of model weak polyelectrolytes. Such the computer modelling can bridge a gap between real but extremely complex systems and oversimplified model systems employed in theories. This can play an important role in optimisation of mechanisms affecting the acid-base equilibria in real and complex macromolecular systems.

Peter Košovan has a sustained record of high-quality research publications and he is an internationally recognized scientist in the field. This can be documented by about 45 peer-reviewed publications, h-index 18, and about 850 citations. Peter Košovan has been also rather successful in obtaining external research grants. Last but not least, Peter Košovan has a sustained record of successful teaching and supervision of students.

In summary, Peter Košovan has thus far provided an excellent example of what it means to be a scientist and university teacher in service of society. Therefore, I recommend his promotion to Reader/Associate Professor (“docent” in Czech).

Prof. Ing. Martin Lísal, DSc.