List of publications, grants and teaching activities

Peter Košovan

03.05.2021

1 Peer-reviewed publications with IF, indexed by the Web of Science (WoS)

1. Roman Staňo, Peter **Košovan**, Andrea Tagliabue, and Christian Holm. Electrostatically cross-linked reversible gels – effects of pH and ionic strength. *Macromolecules*, 2021. doi: 10.1021/acs.macromol.1c00470, IF = 5.918

2. Anastasiia Murmiliuk, Sergey K. Filippov, Oleg Rud, Peter **Košovan**, Zdeněk Tošner, Aurel Radulescu, Athanasios Skandalis, Stergios Pispas, Miroslav Šlouf, and Miroslav Štěpánek. Reversible multilayered vesicle-like structures with fluid hydrophobic and interpolyelectrolyte layers. *Journal of Colloid and Interface Science*, 599:313–325, 2021. doi: 10.1016/j.jcis.2021.04.050, IF = 7.489

3. Raju Lunkad, Anastasiia Murmiliuk, Pascal Hebbeker, Milan Boublík, Zdeněk Tošner, Miroslav Štěpánek, and Peter **Košovan**. Quantitative prediction of charge regulation in oligopeptides. *Molecular Systems Design & Engineering*, 6(2):122–131, 2021. doi: 10.1039/d0me00147c, IF = 3.323

4. Raju Lunkad, Anastasiia Murmiliuk, Zdeněk Tošner, Miroslav Štěpánek, and Peter **Košovan**. Role of pka in charge regulation and conformation of various peptide sequences. *Polymers*, 13 (2):214, Jan 2021. doi: 10.3390/polym13020214, IF = 3.426

5. Oleg V. Rud, Jonas Landsgesell, Christian Holm, and Peter **Košovan**. Modeling of weak polyelectrolyte hydrogels under compression – implications for water desalination. *Desalination*, 506:114995, Jun 2021. doi: 10.1016/j.desal.2021.114995, IF = 7.098

6. Alexander D. Kazakov, Varvara M. Prokacheva, Filip Uhlík, Peter **Košovan**, and Frans A. M. Leermakers. Computer modeling of polymer stars in variable solvent conditions: a comparison of md simulations, self-consistent field (scf) modeling and novel hybrid monte carlo scf approach. *Soft Matter*, 17(3):580–591, 2021. doi: 10.1039/d0sm01080d, IF = 3.140

7. Jonas Landsgesell, Pascal Hebbeker, Oleg Rud, Raju Lunkad, Peter **Košovan**, and Christian Holm. Grand-reaction method for simulations of ionization equilibria coupled to ion partitioning. *Macromolecules*, 53(8):3007–3020, 2020. doi: 10.1021/acs.macromol.0c00260, IF = 5.918

8. Roman Staňo, Lucie Nová, Filip Uhlík, and Peter **Košovan**. Multivalent counterions accumulate in star-like polyelectrolytes and collapse the polymer in spite of increasing its ionization. *Soft Matter*, 16(4):1047–1055, 2020. doi: 10.1039/c9sm02318f, IF = 3.140

9. Roberto Fernandez-Alvarez, Lucie Nová, Filip Uhlík, Sami Kereïche, Mariusz Uchman, Peter **Košovan**, and Pavel Matějíček. Interactions of star-like polyelectrolyte micelles with hydrophobic counterions. *Journal of Colloid and Interface Science*, 546:371 – 380, 2019. doi: 10.1016/j.jcis.2019.03.054, IF = 7.489

10. Jonas Landsgesell, Lucie Nová, Oleg Rud, Filip Uhlík, David Sean, Pascal Hebbeker, Christian Holm, and Peter **Košovan**. Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. *Soft Matter*, 15(6):1155–1185, 2019. doi: 10.1039/c8sm02085j, IF = 3.140

11. Anastasiia Murmiliuk, Peter **Košovan**, Miroslav Janata, Karel Procházka, Filip Uhlík, and Miroslav Štěpánek. Local pH and effective pK of a polyelectrolyte chain: Two names for one quantity? *ACS Macro Letters*, 7(10):1243–1247, 2018. doi: 10.1021/acsmacrolett.8b00484, IF = 5.775

12. Oleg Rud, Oleg Borisov, and Peter **Košovan**. Thermodynamic model for a reversible desalination cycle using weak polyelectrolyte hydrogels. *Desalination*, 442:32 – 43, 2018. doi: 10.1016/j.desal.2018.05.002, IF = 6.035

13. Apostolos Vagias, Khulan Sergelen, Kaloian Koynov, **Košovan, Peter**, Jakub Dostálek, Ulrich Jonas, Wolfgang. Knoll, and George Fytas. Diffusion and permeation of labeled IgG in grafted hydrogels. *Macromolecules*, 50(12):4770–4779, 2017. doi: 10.1021/acs.macromol.7b00514, IF = 5.914

14. Oleg Rud, Tobias Richter, Oleg Borisov, Christian Holm, and Peter **Košovan**. A self-consistent mean-field model for polyelectrolyte gels. *Soft Matter*, 13:3264–3274, 2017. doi: 10.1039/C6SM02825J, IF = 3.709

15. Tobias Richter, Jonas Landsgesell, Peter **Košovan**, and Christian Holm. On the efficiency of a hydrogel-based desalination cycle. *Desalination*, 414:28 – 34, 2017. doi: 10.1016/j.desal.2017.03.027, IF = 6.603

16. 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

17. Peter **Košovan**, Tobias Richter, and Christian Holm. Correction to modeling of polyelectrolyte gels in equilibrium with salt solutions. *Macromolecules*, 49(6):2409–2409, 2016. doi: 10.1021/acs.macromol.6b00395, IF = 5.835

18. Filip Uhlík, Peter **Košovan**, Ekaterina B. Zhulina, and Oleg V. Borisov. Charge-controlled nano-structuring in partially collapsed star-shaped macromolecules. *Soft Matter*, 12:4846–4852, 2016. doi: 10.1039/c6sm00109b, IF = 3.889

19. Jakub Kubečka, Filip Uhlík, and Peter **Košovan**. Mean squared displacement from fluorescence correlation spectroscopy. *Soft Matter*, 12:3760–3769, 2016. doi: 10.1039/C6SM00296J, IF = 3.889

20. 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

21. Jitka Kuldová, Filip Uhlík, and Peter **Košovan**. The drag of the tails: Diffusion of sticky nanoparticles in dilute polymer solutions. *The Journal of Chemical Physics*, 143(24):243129, 2015. doi: 10.1063/1.4935389, IF = 2.894

22. Konrad Breitsprecher, Peter **Košovan**, and Christian Holm. Coarse grained simulations of an ionic liquid-based capacitor I: density, ion size, and valency effects. *Journal of Physics: Condensed Matter*, 26:284108, 2014. doi: 10.1088/0953-8984/26/28/284108, IF = 2.346

23. Konrad Breitsprecher, Peter **Košovan**, and Christian Holm. Coarse grained simulations of an ionic liquid-based capacitor II: asymmetry in ion shape and charge localization. *Journal of Physics: Condensed Matter*, 26:284114, 2014. doi: 10.1088/0953-8984/26/28/284114, IF = 2.346

24. Christine M. Papadakis, Peter **Košovan**, Walter Richtering, and Dominik Wöll. Polymers in focus: fluorescence correlation spectroscopy. *Colloid and Polymer Science*, 292(10):2399–2411, 2014. doi: 10.1007/s00396-014-3374-x, IF = 1.865

25. 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

26. Apostolos Vagias, Peter **Košovan**, Kaloian Koynov, Christian Holm, Hans-Jürgen Butt, and George Fytas. Dynamics in stimuli-responsive poly(n-isopropylacrylamide) hydrogel layers as revealed by fluorescence correlation spectroscopy. *Macromolecules*, 47(15):5303–5312, 2014. doi: 10.1021/ma500928p, IF = 5.800

27. Apostolos Vagias, Riccardo Raccis, Kaloian Koynov, Ulrich Jonas, Hans-Jürgen Butt, George Fytas, Peter **Košovan**, Olaf Lenz, and Christian Holm. Complex tracer diffusion dynamics in polymer solutions. *Physical Review Letters*, 111(8):088301, 2013. doi: 10.1103/PhysRevLett.111.088301, IF = 7.728

28. Rajarshi Chakrabarti, Stefan Kesselheim, Peter **Košovan**, and Christian Holm. Tracer diffusion in a crowded cylindrical channel. *Phys. Rev. E*, 87:062709, 2013. doi: 10.1103/PhysRevE.87.062709, IF = 2.326

29. Jitka Kuldová, Peter **Košovan**, Zuzana Limpouchová, and Karel Procházka. Computer study of the association behavior of gradient copolymers: Analysis of simulation results based on a new algorithm for recognition and classification of aggregates. *Macromolecular Theory and Simulations*, 22(1):61–70, 2013. doi: 10.1002/mats.201200055, IF = 1.793

30. Petra Bačová, Peter **Košovan**, Filip Uhlík, Jitka Kuldová, Zuzana Limpouchová, and Karel Procházka. Double-exponential decay of orientational correlations in semiflexible polyelectrolytes. *Eur. Phys. J. E Soft Matter*, 35:1–10, 2012. doi: 10.1140/epje/i2012-12053-6, IF = 1.824

31. Karel Procházka, Zuzana Limpouchová, Filip Uhlík, Peter **Košovan**, Pavel Matejíček, Miroslav Štěpánek, Mariusz Uchman, Jitka Kuldová, Radek Šachl, Jana Humpolíčková, and Martin Hof. Fluorescence spectroscopy as a tool for investigating the self-organized polyelectrolyte systems. In AHE Muller and O Borisov, editors, *Self Organized Nanostructures of Amphiphilic Block Copolymers I*, volume 241 of *Advances in Polymer Science*, pages 187–249. Springer Berlin Heidelberg, 2011. ISBN 978-3-642-22486-7; 978-3-642-22485-0. doi: 10.1007/12_2010_56, IF = 3.890

32. Zdeněk Preisler, Peter **Košovan**, Jitka Kuldová, Filip Uhlík, Zuzana Limpouchová, Karel Procházka, and Frans A. M. Leermakers. Depletion profiles for dilute solutions of linear chains, stars and h-branched molecules by self-consistent field calculations and monte carlo simulations. *Soft Matter*, 7:10258–10265, 2011. doi: 10.1039/C1SM05651D, IF = 4.390

33. Peter **Košovan**, F Uhlík, J Kuldová, M Štěpánek, Z Limpouchová, K Procházka, A Benda, J Humpolíčková, and M Hof. Monte carlo simulation of fluorescence correlation spectroscopy data. *Collection of Czechoslovak Chemical Communications*, 76(3):207–222, 2011, IF = 1.283

34. Miroslav Štěpánek, Peter **Košovan**, and Karel Procházka. Self-assembly of poly(4-methylstyrene)-g-poly(methacrylic acid) graft copolymer in selective solvents for grafts: Scattering and molecular dynamics simulation study. *Langmuir*, 26(12):9289–9296, 2010, IF = 4.269

35. Jitka Kuldová, Peter **Košovan**, Zuzana Limpouchová, Karel Procházka, and Oleg V. Borisov. Self-association of copolymers with various composition profiles. *Collection of Czechoslovak Chemical Communications*, 75(4):493–505, 2010. doi: 10.1135/cccc2009539, IF = 0.853

36. Peter **Košovan**, Jitka Kuldová, Zuzana Limpouchová, Karel Procházka, Ekaterina B. Zhulina, and Oleg V. Borisov. Molecular dynamics simulations of a polyelectrolyte star in poor solvent. *Soft Matter*, 6:1872–1874, 2010. doi: 10.1039/B925067K, IF = 4.457

37. Peter **Košovan**, J Kuldová, Z Limpouchová, K Procházka, EB Zhulina, and OV Borisov. Amphiphilic graft copolymers in selective solvents: Molecular dynamics simulations and scaling theory. *Macromolecules*, 42(17):6748–6760, 2009, IF = 4.539

38. M Charlaganov, **Košovan, P**, and FAM Leermakers. New ends to the tale of tails: adsorption of comb polymers and the effect on colloidal stability. *Soft Matter*, 5(7):1448–1459, 2009, IF = 4.869

39. Peter **Košovan**, Z Limpouchová, and K Procházka. Charge distribution and conformations of weak polyelectrolyte chains in poor solvents. *Coll. Czech. Chem. Commun.*, 73(4):439–458, 2008, IF = 0.784

40. Peter **Košovan**, Z Limpouchová, and K Procházka. Conformational behavior of comb-like polyelectrolytes in selective solvent: Computer simulation study. *Journal of Physical Chemistry B*, 111:8605–8611, 2007, IF = 4.086

41. Peter **Košovan**, Z Limpouchová, and K Procházka. Molecular dynamics simulation of time-resolved fluorescence anisotropy decays from labeled polyelectrolyte chains. *Macromolecules*, 39(9):3458–3465, 2006, IF = 4.277

42. Josef Buršík, Peter **Košovan**, and Jan Šubrt. Thick fe2o3, fe3o4 films prepared by the chemical solution deposition method. *Journal of Sol-gel Science and Technology*, 39(2):85–94, 2006, IF = 1.009

2 Peer-reviewed publications indexed by Scopus but not by the Web of Science

1. Peter **Košovan**, Tobias Richter, and Christian Holm. Molecular simulations of hydrogels. In Gabriele Sadowski and Walter Richtering, editors, *Intelligent Hydrogels*, volume 140 of *Progress in Colloid and Polymer Science*, pages 205–221. Springer International Publishing, 2013. ISBN 978-3-319-01682-5, SJR = 10.43

2. Apostolos Vagias, Peter **Košovan**, Christian Holm, Hans-Jürgen Butt, Kaloian Koynov, and George Fytas. Tracer mobility in aqueous poly(n-isopropylacrylamide) grafted networks: Effect of interactions and permanent crosslinks. In Gabriele Sadowski and Walter Richtering, editors, *Intelligent Hydrogels*, volume 140 of *Progress in Colloid and Polymer Science*, pages 53–62. Springer International Publishing, 2013. ISBN 978-3-319-01682-5. doi: 10.1007/978-3-319-01683-2_5, SJR = 10.43

3. Johannes Höpfner, Tobias Richter, Peter **Košovan**, Christian Holm, and Manfred Wilhelm. Seawater desalination via hydrogels: Practical realisation and first coarse grained simulations. In Gabriele Sadowski and Walter Richtering, editors, *Intelligent Hydrogels*, volume 140 of *Progress in Colloid and Polymer Science*, pages 247–263. Springer International Publishing, 2013, SJR = 10.43

4. Axeld Arnold, Olaf Lenz, Stefan Kesselheim, Rudolf Weeber, Florian Fahrenberger, Dominic Röhm, Peter **Košovan**, and Christian Holm. ESPResSo 3.1 — molecular dynamics software for coarse-grained models. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VI*, volume 89 of *Lecture Notes in Computational Science and Engineering*, pages 1–23. Springer, 2013. doi: 10.1007/978-3-642-32979-1_1, SJR = 0.610

3 Textbooks and lecture scripts

1. Jan Sedláček, Pavel Matějka, David Havlíček, Michal Bláha, Peter **Košovan**, and Iva Zusková. *Příklady z obecné chemie*. Karolinum, Praha, 3. vydání edition, 2009. ISBN 978-80-246-1646-9

4 Selected conference contributions

Main organizer	(bio)Macromolecular Ionic Systems 2017 and 2015 (www.bmis.cz)
Invited speaker	Fluorescence correlation spectcroscopy in Polymer Science 2013 `https://www.softmatter.ph.tum.de/en/fcs-workshop-2013`
Local organizing committee member	ECIS 2010, Prague, cca 600 participants `http://www.ecis-web.eu/prague2010.htm`

5 Research grants

2021 – 2023	Simulations of reaction equilibria in polymer systems - method development and applications, Czech Science Foundation, project No. 21-31978J
2019 – 2021	Controlling encapsulation and release by charge regulation and multivalent interactions with supramolecular polymer carriers, Czech Science Foundation, project No. 19-10429S
2017 – 2019	Multiscale modeling of responsive polymer gels, Czech Science Foundation, project No. 17-02411Y
2013 – 2015	Interactions and dynamics in polymeric nanostructures, Ministry of education, youth and sports of the Czech Republic, project No. LK21302
2006 – 2009	Molecular Dynamics Simulations of Annealed Polyelectrolytes, Grant Agency of the Czech Academy of Sciences of the Czech Republic, project No. KJB401110701
2006 – 2009	Persistence length of polyelectrolytes, Grant Agency of the Charles University, project No. 43-257-269

6 Popular science

1. Peter **Košovan**. Nebezpečné bublinky. *Přírodovědci – Magazím přírodovědecká fakulty Univerzity Karlovy*, (01):12–13, 2021