PD. Dr. Jens Smiatek

Curriculum Vitae

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Personal Information

Born April 13, 1978 in Lemgo, Germany

Nationality German

Present Work Address

Position Big Data Strategy and Handling Expert and Project Leader

Address Boehringer Ingelheim Pharma GmbH & Co. KG
Digitalization Development Biologicals CMC
Birkendorfer Strasse 65
D-88397 Biberach a. d. Riss

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Education

2017 – 2018 **Habilitation in Theoretical Physics**, *Department of Physics and Mathematics*, University of Stuttgart.

2005–2009 **Ph. D. in Theoretical Physics**, *Physics Faculty*, Bielefeld University.

1998–2005 **1st State Examination for High School Teachers in Chemistry and Physics**, Bielefeld University.

2001–2005: Studies of Physics, Social Studies and Chemistry

1999–2005: Studies of Physics and Social Studies

1998–1999: Studies of German Language and History

1997–1998 **Military Service**.

1988–1997 **Allgemeine Hochschulreife**, Städtisches Gymnasium Barntrup.

1984–1988 **Grundschule Bösingfeld**.

Habilitation Thesis

Title *Soft matter in solution: from hydrodynamics to hydrogen bonds*

Institution University of Stuttgart, Department of Physics and Mathematics

Year 2018

Ph. D. Thesis

Title	*Mesoscopic simulations of electrohydrodynamic phenomena*
Institution	Condensed Matter Theory, Physics Faculty, Bielefeld University
Date	March 16^{th}, 2009
Final mark	1.0

Work Experience

2019–Present	**Big Data Strategy and Handling Expert and Project Leader**
	Digitalization Development Biologicals CMC
	Boehringer Ingelheim Pharma GmbH & Co. KG
2017–2019	**Group Leader**
	Theory of Electrolyte Solutions
	Helmholtz Institute Münster: Ionics in Energy Storage
	Forschungszentrum Jülich GmbH
2012–Present	**Group Leader and Privatdozent (lecturer)**
	Theoretical Chemical Physics
	Institute for Computational Physics
	University of Stuttgart
2009–2012	**Scientific Associate (Post-Doc)**
	Theory of Complex Systems
	Advisor: Prof. Dr. Andreas Heuer
	Institute of Physical Chemistry
	University of Münster
2005–2009	**Scientific Associate (Ph. D. student)**
	Condensed Matter Theory
	Supervisor: Prof. Dr. Friederike Schmid
	Physics Faculty
	Bielefeld University

Research Visits Abroad

2015	Czech Academy of Sciences, Prague, Czech Republic (January 2015)
2014	University of Luxembourg, Luxembourg (December 2014)
2014	National Center of Biomolecular Research, Brno, Czech Republic (May 2014)
2010	Tsinghua University, Beijing, PR China (October – November 2010)

Research Interests

Topics	Charged soft matter in solution: polyelectrolytes and ions
	Bioprocess models
	Dynamic and structural properties of complex electrolyte solutions

Molecular theories of solutions: solvation principles and thermodynamic effects

Co-solute and specific ion effects and their influence on macromolecular folding equilibria

Hydrodynamic interactions and properties of pressure-driven or electrokinetic flows

Third-Party Funded Projects as Principal Investigator

2015 – 2018 *Molekulardynamik-Simulationen zur Untersuchung der Entfaltungspfade von DNA G-Quadruplexen*

Sonderforschungsbereich 716, Deutsche Forschungsgemeinschaft

116.400 Euro

2014 – 2017 *Atomistic and mesoscopic simulations of polyelectrolytes and ionomers*

Cluster of Excellence Simulation Technology, Deutsche Forschungsgemeinschaft

205.000 Euro

2013 – 2016 *Untersuchung über die Wechselwirkungen von gestreckten, immobilisierten Polyelektrolyten mit externen elektrischen Feldern und Flüssigkeitsströmungen in Gegenwart beschränkter Mikrogeometrien*

Single Project, Deutsche Forschungsgemeinschaft

116.400 Euro

Organization of Workshops

2014 CECAM/SFB 716 International Workshop: *Biological Molecules under Non-natural Conditions*, Stuttgart, Germany

2011 3^{rd} International TRR 61 Ph. D. Students Workshop: *Multilevel Molecular Assemblies: Structure, Dynamics and Function*, Münster, Germany

Reviewing and Editor Activities

Journals Angewandte Chemie, Journal of the American Chemical Society, Physical Review Letters, Langmuir, Journal of Physical Chemistry Letters, Soft Matter, Journal of Chemical Theory and Computation, Journal of Physical Chemistry B, Journal of Chemical Physics, ChemPhysChem, Chemistry Select, Physical Review E, Journal of Polymer Science B, Chemical Physics Letters, Physica A, Microfluidics and Nanofluidics

Organizations Department of Energy (USA), Israelian Science Foundation, Czech Science Foundation, National Science Centre Poland, Austrian Science Fund, Irish Research Council

Guest Editor Special issue *The Progresses on Polyelectrolytes and Polyelectrolyte Complexes* in *Molecules* (MDPI)

Publications

Peer-reviewed

1. Smiatek, J.; Jung, A.; Bluhmki, E.
   Towards a digital bioprocess replica: Computational approaches in biopharmaceutical development and manufacturing.
   Trends Biotechnol., DOI:10.1016/j.tibtech.2020.05.008 (2020)
2. Smiatek, J.
   Specific ion effects and the law of matching solvent affinities: A conceptual density functional theory approach.
   J. Phys. Chem. B 124, 2191 (2020)
3. Smiatek, J.
   Theoretical and computational insight into solvent and specific ion effects for polyelectrolytes: The crucial role of local molecular interactions.
   Molecules 25, 1661 (2020)
4. Solomun, T.; Hahn, M.-B.; Smiatek, J.
   Raman spectroscopic signature of ectoine conformations in bulk solution and crystalline state.
   ChemPhysChem, DOI:10.1002/cphc.202000457 (2020)
5. Sanchez, P. A.; VÃűgele, M.; Smiatek, J.; Qiao, B.; Sega, M.; Holm, C.
   PDADMAC/PSS oligoelectrolyte multilayers: internal structure and hydration properties at early growth stages from atomistic simulations.
   Molecules 25, 1848 (2020)
6. Zeman, J.; Holm, C.; Smiatek, J.
   The effect of small organic co-solutes on water structure and dynamics.
   J. Chem. Eng. Data 65, 1197 (2020)
7. Hützler, W. H.; Mossou, E.; Vollrate, R.; Kohagen, M.; El Ghrissi, I.; Grininger, M.; Zaccai, G.; Smiatek, J.; Oesterhelt, D.
   Complex transitions between dihydrate and anhydrate forms of ectoine – Unexpected behavior of a highly hygroscopic compatible solute in the solid state.
   CrystEngComm 22, 169 (2020)
8. Cekic-Laskovic, I.; von Aspern, N.; Leissing, M.; Wölke, C.; Diddens, D.; Kobayashi, T.; Börner M.; Stubbmann-Kazakova, O.; Kozel, V.; Röschenthaler, G.-V.; Smiatek, J.; Nowak, S.; Winter, M.
   Non-flammable fluorinated phosphorus(III)-based co-solvents for advanced Lithium ion battery performance.
   ChemElectroChem 7, 1499 (2020)
9. Smiatek, J.
   Enthalpic contributions to solvent–solute and solvent–ion interactions: Electronic perturbation as key to the understanding of molecular attraction.
   J. Chem. Phys. 150, 174112 (2019)
10. Kobayashi, T.; Kemna, A.; Fyta, M.; Braunschweig, B.; Smiatek, J.
    Aqueous mixtures of room-temperature ionic liquids: Entropy-driven accumulation of water molecules at interfaces.
    J. Phys. Chem. C 123, 13795 (2019)

11. Nandy, A; Smiatek, J.
    Mixtures of LiTFSI and urea: Ideal thermodynamic behavior as key to the formation of deep eutectic solvents?
    Phys. Chem. Chem. Phys. 21, 12279 (2019)
12. Oprzeska-Zingrebe, E. A.; Smiatek, J.
    Some notes on the thermodynamic accuracy of coarse-grained models.
    Front. Mol. Biosci. 6, 87 (2019)
13. Sanchez, P. A.; Vögele, M.; Qiao, B.; Smiatek, J.; Sega, M.; Holm, C.
    Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer system.
    Soft Matter 15, 9437 (2019)
14. Kohagen, M.; Uhlig, F.; Smiatek, J.
    On the nature of ion-stabilized cytosine pairs in DNA i-motifs: The importance of charge transfer processes.
    Int. J. Quant. Chem. 119, e25933 (2019)
15. Oprzeska-Zingrebe, E. A.; Smiatek, J.
    Aqueous mixtures of urea and trimethylamine-N-oxide: Evidence for kosmotropic or chaotropic behavior?
    J. Phys. Chem. B 123, 4415 (2019)
16. von Aspern, N.; Diddens, D.; Kobayashi, T.; Börner, M.; Stubbmann-Kazakova, O.; Kozel, V.; Röschenthaler, G.-V.; Smiatek, J.; Winter, M.; Cekic-Laskovic, I.
    Fluorinated cyclic phosphorus(III)-based electrolyte additives for high-voltage application in lithium ion batteries: Impact of structure-reactivity relationships on CEI formation and cell performance.
    ACS Appl. Mater. Interfaces 11, 16605 (2019)
17. Oldiges, K.; Michalowsky, J.; Grünebaum, M.; von Aspern, N.; Cekic-Laskovic, I.; Smiatek, J.; Winter, M.; Brunklaus, G.
    Tetrahydrothiophene 1-oxide as highly effective co-solvent for propylene carbonate-based electrolytes.
    J. Power Sources 437, 226881 (2019)
18. Otero-Mato, J. M.; Montes Campos, H.; Lesch, V.; Smiatek, J.; Diddens, D.; Cabeza, O.; Gallego, L. J.; Varela, L. M.
    Solvation in ionic liquid-water mixtures: A computational study.
    J. Mol. Liquids 229, 11273 (2019)
19. Jia, H.; Billmann, B.; Onishi, H.; Smiatek, J.; Roser, S.; Wiemers-Meyer, S.; Wagner, R.; Winter, M.; Cekic-Laskovic, I.
    LiPF6 stabilizer and transition metal cation scavenger: A bi-functional bipyridine-based ligand for lithium ion batteries application.
    Chem. Mater. 31, 4025 (2019)
20. Oprzeska-Zingrebe, E. A.; Kohagen, M.; Kästner, J.; Smiatek, J.
    Unfolding of DNA by co-solutes: Insights from Kirkwood-Buff integrals and transfer free energies.
    Europ. Phys. J. Spec. Top. 227, 1665 (2019)
21. Roy, T.; Szuttor, K.; Smiatek, J.; Holm, C.; Hardt, S.
    Conformation and dynamics of long-chain end-tethered polymers in micro channels.
    Polymers 11, 488 (2019)

22. Smiatek, J.; Heuer, A.; Winter, M.
    Properties of ion complexes and their impact on charge transport in organic solvent-based electrolyte solutions for lithium batteries: Insights from a theoretical perspective.
    Batteries 4, 62 (2018)
23. Oprzeska-Zingrebe, E. A.; Meyer, S.; Rohloff, A.; Kunte, H.-J.; Smiatek, J.
    Influence of compatible solute ectoine on distinct DNA structures: Thermodynamic insights into molecular binding mechanisms and destabilization effects.
    Phys. Chem. Chem. Phys. 20, 25861 (2018)
24. Krishnamoorthy, A. N.; Oldiges, K.; Winter, M.; Heuer, A.; Cekic-Laskovic, I.; Holm, C.; Smiatek, J.
    Electrolyte solvents for high voltage lithium ion batteries: Ion correlation and specific anion effects in adiponitrile.
    Phys. Chem. Chem. Phys. 20, 25701 (2018)
25. Krishnamoorthy, A. N.; Holm, C.; Smiatek, J.
    Specific ion effects for polyelectrolytes in aqueous and non-aqueous media: The importance of the ion solvation behavior.
    Soft Matter 14, 6243 (2018)
26. Hartmann, J.; Roy, T; Szuttor, K.; Smiatek, J.; Holm, C.; Hardt, S.
    Relaxation of surface-tethered polymers under moderate confinement.
    Soft Matter 14, 7926 (2018).
27. Smiatek, J.; Holm C.
    From the atomistic to the macromolecular scale: Distinct simulation approaches for polyelectrolyte solutions.
    in Handbook of Materials Modeling; pp. 1–15, edited by Andreoni W.; Yip S.; Springer (2018).
28. Michalowsky, J.; Zeman, J.; Holm, C.; Smiatek, J.
    A polarizable MARTINI model for monovalent ions in aqueous solution.
    J. Chem. Phys 149, 163319 (2018)
29. Krishnamoorthy, A. N.; Holm, C.; Smiatek, J.
    Influence of cosolutes on chemical equilibrium: A Kirkwood-Buff theory for ion pair association-dissociation processes in ternary electrolyte solutions.
    J. Phys. Chem. C 122, 10293 (2018)
30. Oprzeska-Zingrebe, E. A.; Smiatek, J.
    Aqueous ionic liquids in comparison with standard co-solutes - Differences and common principles in their interaction with protein and DNA structures.
    Biophys. Rev. 10, 809 (2018)
31. Weyman, A.: Bier, M.; Holm, C.; Smiatek, J.
    Microphase separation and the formation of ion conductivity channels in poly(ionic liquid)s: A coarse-grained molecular dynamics study.
    J. Chem. Phys. 148, 193824 (2018)
32. Oprzeska-Zingrebe, E. A.; Smiatek, J.
    Preferential binding of urea to single-stranded DNA structures: A molecular dynamics study.
    Biophys. J. 114, 1551 (2018)

33. Uhlig, F.; Zeman, J.; Smiatek, J.; Holm, C.
First-principles parameterization of polarizable coarse-grained force fields for ionic liquids.
J. Chem. Theory Comput. 14, 1471 (2018)
34. Zeman, J.; Uhlig, F.; Smiatek, J.; Holm, C.
A coarse-grained polarizable force field for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate.
J. Phys. Condens. Matter 29, 504004 (2017)
35. Smiatek, J.
Aqueous ionic liquids and their effects on protein structures: An overview on recent theoretical and experimental results.
J. Phys. Condens. Matter 29, 233001 (2017)
36. Markthaler, D.; Zeman, J.; Baz, J.; Smiatek, J.; Hansen, N.
Validation of Trimethylamine-N-Oxide (TMAO) force fields based on thermophysical properties of aqueous TMAO solutions.
J. Phys. Chem. B 121, 10674 (2017)
37. Belyanchikov, M. A.; Zhukov, E. S.; Tertia, S.; Zhugayevych, A.; Dressel, M.; Uhlig, F.; Smiatek, J.; Fyta, M.; Thomas, V. G.; Gorshunov, B. P.
Vibrational states of nano-confined water molecules in beryl based on first principles calculations and optical experiments.
Phys. Chem. Chem. Phys. 19, 30740 (2017)
38. Roy, T.; Szuttor, K.; Smiatek, J.; Holm, C.; Hardt, S.
Electric-field-induced stretching of surface-tethered polyelectrolytes in a microchannel.
Phy. Rev. E 96, 032503 (2017)
39. Roy, T.; Szuttor, K.; Smiatek, J.; Holm, C.; Hardt, S.
Stretching of surface-tethered polymers in pressure-driven flow under confinement.
Soft Matter 13, 6189 (2017)
40. Diddens, D.; Lesch, V.; Heuer, A.; Smiatek, J.
Aqueous ionic liquids and their influence on peptide conformations: Denaturation and dehydration mechanisms
Phys. Chem. Chem. Phys. 19, 20430 (2017)
41. Kobayashi, T.; Reid, J. E. S. J.; Shimizu, S.; Fyta, M.; Smiatek, J.
The properties of residual water molecules in ionic liquids: A comparison between direct and inverse Kirkwood-Buff approaches.
Phys. Chem. Chem. Phys. 19, 18924 (2017)
42. Niskanen, J.; Sahle, C. J.; Gilmore, K.; Uhlig, F.; Smiatek, J.; Föhlisch, A.
Disentangling structural information from core-level excitation spectra.
Phys. Rev. E 96, 013319 (2017)
43. Szuttor, K.; Roy, T.; Hardt, S.; Holm, C.; Smiatek, J.
The stretching force on a tethered polymer in pressure-driven flow.
J. Chem. Phys. 147, 034902 (2017)
44. Landsgesell, J.; Holm, C.; Smiatek, J.
The Wang-Landau reaction ensemble method: Simulation of weak polyelectrolytes and general acid–base reactions.
J. Chem. Theory Comput. 13, 852 (2017)

45. Michalowsky, J.; Schäfer, L. V..; Holm, C. Smiatek, J.
A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions.
J. Chem. Phys. 146, 054501 (2017)
46. Smiatek, J.; Hansen, N.; Kästner, J.
Free energy calculation methods and rare event sampling techniques for biomolecular simulations.
Chapter 6 in Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis;
pp. 185–214, edited by Tunon, I.; Moliner, V.; The Royal Society of Chemistry (2017)
47. Landsgesell, J.; Holm, C.; Smiatek, J.
Simulation of weak polyelectrolytes: A comparison between the constant pH and the reaction ensemble method.
Europ. Phys. J. Spec. Top. 226, 725 (2017)
48. Krishnamoorthy, A. N.; Zeman, J.; Holm, C.; Smiatek, J.
Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions.
Phys. Chem. Chem. Phys. 18, 31312 (2016)
49. Schroer, M. A.; Michalowsky, J.; Fischer, B.; Smiatek, J.; Grübel, G.
Stabilizing effect of TMAO on globular PNIPAM states: Preferential attraction induces preferential hydration.
Phys. Chem. Chem. Phys. 18, 31459 (2016)
50. Hahn, M. B.; Uhlig, F.; Solomun, T.; Smiatek, J.; Sturm, H.
Combined influence of ectoine and salt: Spectroscopic and numerical evidence for compensating effects on aqueous solutions.
Phys. Chem. Chem. Phys. 18, 28398 (2016)
51. Lesch, V.; Heuer, A.; Rad, B. R., Winter, M.; Smiatek, J.
Atomistic insights into deep eutectic electrolytes: The influence of urea on the electrolyte salt LiTFSI in view of electrochemical applications.
Phys. Chem. Chem. Phys. 18, 28403 (2016)
52. Micciulla, S.; Michalowsky, J.; Schroer, M. A.; Holm, C.; von Klitzing, R.; Smiatek, J.
Concentration dependent effects of urea binding to poly(N-isopropylacrylamide) brushes: a combined experimental and numerical study.
Phys. Chem. Chem. Phys. 18, 5324 (2016)
53. Lesch, V.; Heuer, A.; Holm, C.; Smiatek, J.
Properties of apolar solutes in alkyl-imidazolium based ionic liquids: The crucial importance of local interactions.
ChemPhysChem 17, 387 (2016)
54. Vögele, M.; Holm, C., Smiatek, J.
Coarse-grained simulations of polyelectrolyte complexes: MARTINI based models for poly(styrene sulfonate) and poly(diallyldimethylammonium).
J. Chem. Phys. 143, 243151 (2015)
55. Hahn, M. B.; Solomun, T., Wellhausen, R.; Hermann, S.; Seitz, H.; Meyer, S.; Kunte, H.-J.; Zeman, J.; Uhlig, F.; Smiatek, J.; Sturm, H.
Influence of the compatible solute ectoine on the local water structure: Implications for the binding of the protein G5P to DNA.
J. Phys. Chem. B 119, 15212 (2015)

56. Fahrenberger, F.; Hickey, O. A.; Smiatek, J.; Holm, C.
The influence of charge-induced variations in the local permittivity on the static and dynamic properties of polyelectrolyte solutions.
J. Chem. Phys. 143, 243140 (2015)
57. Fahrenberger, F.; Hickey, O. A.; Smiatek, J.; Holm, C.
Importance of varying permittivity on the conductivity of polyelectrolyte solutions.
Phys. Rev. Lett. 115, 118301 (2015)
58. Lesch, V.; Heuer, A.; Tatsis, V. A.; Holm, C.; Smiatek, J.
Peptides in presence of aqueous ionic liquids - Tunable co-solutes as denaturants or protectants?
Phys. Chem. Chem. Phys. 17, 26049 (2015)
59. Vögele, M.; Holm, C., Smiatek, J.
Properties of the polarizable MARTINI water model - A comparative study for aqueous electrolyte solutions.
J. Mol. Liquids 212, 103 (2015)
60. Lesch, V.; Heuer, A.; Holm, C.; Smiatek, J.
Solvent effects of 1-ethyl-3-methylimidazolium acetate: Solvation and dynamic behavior of polar and apolar solutes.
Phys. Chem. Chem. Phys. 17, 8480 (2015)
61. Wohlfarth, A.; Smiatek, J.; Kreuer, K.-D.; Takamuku, S.; Jannasch, P.; Maier, J.
Proton dissociation of sulfonated polysulfones: Influence of molecular structure and conformation.
Macromolecules 48, 1134 (2015)
62. Krishnamoorthy, A. N.; Holm, C.; Smiatek, J.
Local water dynamics around antifreeze protein residues in the presence of osmolytes: The importance of hydroxyl and disaccharide groups.
J. Phys. Chem. B 118, 11613 (2014)
63. Micciulla, S.; Sanchez, P. A.; Smiatek, J.; Qiao, B.; Sega, M.; Laschewsky, A.; Holm, C.; von Klitzing, R.
Layer-by-layer formation of oligoelectrolyte multilayers: A combined experimental and computational study.
Soft Mater. 12, S14 (2014)
64. Hickey, O. A.; Holm, C.; Smiatek, J.
Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions.
J. Chem. Phys. 140, 164904 (2014)
65. Smiatek, J.; Heuer, A.
Deprotonation mechanism of a single-stranded DNA i-motif.
RSC Adv. 4, 17110 (2014)
66. Bohner, M. U.; Zeman, J.; Smiatek, J.; Arnold, A.; Kästner, J.
Nudged-elastic band used to find reaction coordinates based on the free energy.
J. Chem. Phys. 140, 074109 (2014)
67. Smiatek, J.; Wohlfarth, A.; Holm, C.
The solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents – A computational study.
New J. Phys. 16, 025001 (2014)

68. Smiatek, J.
Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres.
J. Phys. Chem. B 118, 771 (2014)
69. Smiatek, J.; Janssen-Müller, D.; Friedrich, R.; Heuer, A.
Systematic detection of hidden complexities in the unfolding mechanism of a cytosine-rich DNA strand.
Physica A 394, 136 (2014)
70. Smiatek, J.; Harishchandra, R. K.; Galla, H.-J.; Heuer, A.
Low concentrated hydroxyectoine solutions in presence of DPPC lipid bilayers: A computer simulation study.
Biophys. Chem. 180–181, 102 (2013)
71. Smiatek, J.; Heuer, A.; Wagner, H.; Studer, A.; Hentschel, C.; Chi, L.
Coat thickness dependent adsorption of hydrophobic molecules at polymer brushes.
J. Chem. Phys. 138, 044904 (2013)
72. Hentschel, C.; Wagner, H.; Smiatek, J.; Heuer, A.; Fuchs, H.; Zhang, X.; Studer, A.; Chi, L.
AFM-based force spectroscopy on polystyrene brushes: effect of brush thickness on protein adsorption.
Langmuir 29, 1850 (2013)
73. Meinhardt, S.; Smiatek, J.; Eichhorn, R.; Schmid, F.
Separation of chiral particles in micro- or nanofluidic channels.
Phys. Rev. Lett. 108, 214504 (2012)
74. Smiatek, J.; Harishchandra, R. K.; Rubner, O.; Galla, H.-J.; Heuer, A.
Properties of compatible solutes in aqueous solution.
Biophys. Chem. 160, 62 (2012)
75. Smiatek, J.; Liu, D.; Heuer, A.
High temperature unfolding simulations of a single-stranded DNA i-motif.
Curr. Phys. Chem. 2, 115 (2012)
76. Smiatek, J.; Chen, C.; Liu, D.; Heuer, A.
Stable conformations of a single stranded deprotonated DNA i-motif.
J. Phys. Chem. B 115, 13788 (2011)
77. Smiatek, J.; Heuer, A.
Calculation of free energy landscapes: a histogram reweighted metadynamics approach.
J. Comput. Chem. 32, 2084 (2011)
78. Smiatek, J.; Schmid, F.
Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels.
Comp. Phys. Comm. 182, 1941 (2011)
79. Smiatek, J.; Schmid, F.
Polyelectrolyte electrophoresis in nanochannels: A Dissipative Particle Dynamics simulation.
J. Phys. Chem. B 114, 6266 (2010)
80. Smiatek, J.; Sega, M.; Schiller, U. D.; Holm, C.; Schmid, F.
Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study.
J. Chem. Phys. 130, 244702 (2009)
81. Smiatek, J.; Allen, M. P.; Schmid, F.
Tunable-slip boundaries for coarse-grained simulations of fluid flow.
Europ. Phys. J. E 26, 115 (2008)

Non peer-reviewed publications

82. Sanchez, P. A.; Smiatek, J.; Qiao, B.; Sega, M.; Holm, C.
Atomistic simulation of oligoelectrolyte multilayer growth.
High Performance Computing in Science and Engineering '15, Springer Publications (2016)
83. Zhou, J.; Smiatek, J.; Asmolov, E. S.; Vinogradova, O. I.; Schmid, F.
Application of tunable-slip boundary conditions in particle-based simulations.
High Performance Computing in Science and Engineering '14, Springer Publications (2015)
84. Heuer, A.; Smiatek, J.; Strauss, B.; Riedl, D.
Informationsgehalt von Fussball-Spieldaten.
Fussball in Forschung und Lehre - Beiträge und Analysen zum Fussballsport XIX in Schriften der Deutschen Vereinigung für Sportwissenschaft Band 240, Czwalina (2014)
85. Smiatek, J.; Schmid, F.
Mesoscopic simulation methods for studying flow and transport in electric fields in micro- and nanochannels.
Advances in Microfluidics, InTech Scientific Publications (2012)
86. Smiatek, J.; Schmid, F.
Mesoscopic simulations of polyelectrolyte electrophoresis in nanochannels.
High Performance Computing in Science and Engineering '10, Springer Publications (2011)

Theses

87. Smiatek, J.
    Soft matter in solution: from hydrodynamics to hydrogen bonds.
    Habilitation thesis, University of Stuttgart, Stuttgart (2018)
88. Smiatek, J.
    Mesoscopic simulations of electrohydrodynamic phenomena.
    Ph.D. thesis, Bielefeld University, Bielefeld (2009)
89. Smiatek, J.
    Untersuchung von Simulationen zur stochastischen Dynamik unter Zwangsbedingungen.
    Hausarbeit zum 1. Staatsexamen für LA Sek. I/II, Bielefeld University, Bielefeld (2005)

Summary

Peer-reviewed publications: 75

- Review articles: 5
- Publications as single author: 3
- Publications as first author: 19
- Publications as last author: 32

Citations metrics

H-index:

- ISI Web of Science: 20
- Google Scholar: 22

Sum of the times cited:

- Google Scholar: 1237

ResearcherID:

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Invited Talks

1. *Process knowledge and process robustness: Benefits of numerical methods*
   2019 ISPE Europe Biotechnology Conference, Brussels, Belgium, September 2019
2. *Aqueous ionic liquids: Consequences for biological stabilities*
   12th EBSA 10th ICBP - IUPAP Biophysics Congress 2019, Madrid, Spain, July 2019
3. *Influence of co-solutes and ions on the stability of DNA*
   Conference: Simulation of Systems with Large Particle Numbers, Heidelberg, September 2018
4. *Proteins and aqueous ionic liquids: Stabilization and destabilization mechanisms*
   RWTH Aachen, September 2018
5. *Co-solute effects: Stabilization and destabilization mechanisms in the light of molecular theories of solution*
   University of Dortmund, April 2018
6. *Biological co-solutes and their interactions with macromolecules*
   Goethe University Frankfurt a. M. , December 2017
7. *Biological co-solutes and their interactions with macromolecules*
   Institut für Mikrobiologie & Biotechnologie, Bonn, April 2017
8. *Aqueous ionic liquids and their influence on peptide conformations: Denaturation and dehydration mechanisms*
   Spring meeting Deutsche Physikalische Gesellschaft, Dresden, March 2017
9. *Aqueous ionic liquids and their influence on peptide conformations: Denaturation and dehydration mechanisms*
   DECHEMA ProcessNet Jahrestreffen MolMod, Frankfurt a. M., March 2017
10. *Solvent effects in electrolyte solutions*
    Helmholtz-Institute Ionics in Energy Storage Münster, February 2017
11. *Aqueous ionic liquids and their influence on peptide conformations: Denaturation and dehydration mechanisms*
    Lorentz Workshop: Understanding Ionic Liquids on Different Length and Time Scales, Leiden, The Netherlands, February 2017
12. *Coarse-grained simulations of soft matter in microfluidic devices*
    42^{nd} Micro and Nano Engineering, Vienna, Austria, September 2016
13. *Macromolecules in solution: The influence of physical and chemical effects*
    Bielefeld University, April 2016
14. *Molecular simulations of solution effects - Chemical and physical properties at different length scales*
    University of Münster, February 2016
15. *Macromolecules in solution - More than the sum of the parts*
    AMOLF, Amsterdam, The Netherlands, December 2015
16. *Macromolecules, solvents and co-solutes - A crucial interplay*
    Lorentz Workshop: The future of multi-scale soft matter modeling, Leiden, The Netherlands, September 2015
17. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Darmstadt, May 2015
18. *Macromolecules, solvents and co-solutes - A crucial interplay*
    Bundesanstalt für Materialforschung und -prüfung, Berlin, April 2015
19. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Würzburg, January 2015

20. *Macromolecules, solvents and co-solutes - A crucial interplay*
    Czech Academy of Sciences, Prague, Czech Republic, January 2015
21. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Luxembourg, Luxembourg, December 2014
22. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Mainz, October 2014
23. *Solvent effects and their influence on the properties of soft matter*
    Institute Charles Sadron, Strasbourg, France, June 2014
24. *Solvent effects and their influence on the properties of soft matter*
    University of Tübingen, June 2014
25. *Solvent effects and their influence on the dynamic and static properties of macromolecules*
    German Electron Synchrotron (DESY), Hamburg, May 2013
26. *Computer simulations of biological soft matter systems*
    University of Dortmund, October 2011
27. *Unfolding mechanisms and the free energy landscape of the DNA i-motif*
    Workshop: Multilevel molecular assemblies, structure and function, Beijing, PR China, October 2010
28. *Polyelectrolyte electrophoresis in microchannels: Influence of salt concentration and slippage effects*
    Workshop: Multilevel molecular assemblies, structure and function, Münster, October 2009
29. *Tunable slip boundaries and electrokinetic effects in microchannels*
    University of Münster, November 2008
30. *Tunable slip boundaries and electrokinetic effects in microchannels*
    FIAS Frankfurt, January 2008