Dr. Jens Smiatek

Curriculum Vitae

Work Address

Position Group leader: Theoretical Physical Chemistry

Address Institute for Computational Physics
University of Stuttgart
Allmandring 3
D-70569 Stuttgart

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Academic Education

2005–2009 **Ph.D. student in theoretical physics**.
Physics Faculty, Bielefeld University
Thesis: Mesoscopic simulations of electrohydrodynamic phenomena
Supervisor: Prof. Dr. Friederike Schmid

2001–2005 **Student of physics, social studies and chemistry (LA Sek. I/II)**.
Bielefeld University
1st state examination thesis in theoretical physics:
Untersuchung von Simulationen zur stochastischen Dynamik unter Zwangsbedingungen
Supervisor: Prof. Dr. Friederike Schmid

Academic Career

2012–Present **Group leader: Theoretical Physical Chemistry**
Institute for Computational Physics
University of Stuttgart

2009–2012 **Scientific associate (Post-Doc)**
Theory of Complex Systems
Prof. Dr. Andreas Heuer
Institute of Physical Chemistry
University of Münster

Research Visits

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

I am in particular interested in the theory of solutions in terms of statistical mechanical descriptions like the Kirkwood-Buff theory. I aim to further develop and to apply these theories for a molecular description of soft matter properties in solution. Therefore, my research mainly focuses on structural and dynamic effects of solvents and co-solutes and their influence on macromolecules. Typical systems of interest include polyelectrolytes, DNA and proteins in conjunction with ions, ionic liquids and low weight organic co-solutes in different solvents and under external influences. Over the last years, I mainly studied the molecular mechanisms behind polyelectrolyte and counterion properties, solvent effects, transport and solvation in electrolyte and ionic liquid solution and the influence of aqueous ionic liquids and co-solutes on macromolecular confomations. Moreover, I am also interested in electrokinetic phenomena, which are mostly represented by electroosmosis and electrophoresis in presence of slippage effects. Due to these reasons, I worked on the coupling between electrostatic, hydrodynamic and friction effects and the corresponding implications for transport properties and macromolecular separation techniques. Finally, I developed and applied free energy and rare event methods to study transition pathways and the influence of enthalpic and entropic contributions on free energy minima. The theoretical understanding of hidden complexities and the corresponding implications like hysteresis effects in low-dimensional free energy landscapes further attracted my interest.

Third-Party Funds

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

Project TP C.8, Co-PI with Prof. Kästner

Sonderforschungsbereich 716, Deutsche Forschungsgemeinschaft

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

Project PN 1.2, Co-PI with Prof. Holm

Cluster of Excellence 'Simulation Technology', Deutsche Forschungsgemeinschaft

Advised Theses

Ph.D. theses

2014–Present Anand Narayanan Krishnamoorthy (University of Stuttgart)

2014–Present Ewa Anna Oprzeska-Zingrebe (University of Stuttgart)

2016–Present Julian Michalowsky (University of Stuttgart)

Master theses

2016 Alexander Weyman (University of Stuttgart)

2016 Kai Szuttor (University of Stuttgart)

2016 Julian Michalowsky (University of Stuttgart)

2015 Jonas Landsgesell (University of Stuttgart)

2014 Martin Vögele (University of Stuttgart)

2013 Katharina Wenzel (University of Münster)

2008 Sebastian Meinhardt (Bielefeld University)

Bachelor theses

2017 Julian Zeller (University of Stuttgart)

2015 Ingo Tischler (University of Stuttgart)

2015 Felix Gross (University of Stuttgart)

2015 Patrick Küssner (University of Stuttgart)

2015 Evangelos Ribeiro Tzaras (University of Stuttgart)

2013 Jonas Landsgesell (University of Stuttgart)

2013 Julian Michalowsky (University of Stuttgart)

2013 Patrick Kreissl (University of Stuttgart)

2011 Daniel Janssen-Müller (University of Münster)

Reviewing Activities

Journals 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, Physical Review E, Chemical Physics Letters, Physica A, Microfluidics and Nanofluidics, Computer Physics Communications, Computational Science & Discovery, Physica A, Zeitschrift für Physikalische Chemie and Colloids and Surfaces A

Organizations Department of Energy (USA)

Publications

Peer-reviewed

1. Landsgesell, J.; Holm, C.; Smiatek, J.
   Simulation of weak polyelectrolytes: a comparison between the constant pH and the reaction ensemble method.
   accepted for publication in *Europ. Phys. J. Spec. Top.* (2016)
2. 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)
3. 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)
4. 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)
5. 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)
6. 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; edited by Tunon, I.; Moliner, V.; RSC Publishing (2016)
7. 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)
8. 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)
9. 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)
10. 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)
11. 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)

12. 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)
13. 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)
14. 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)
15. 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)
16. 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)
17. 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)
18. 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)
19. 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)
20. Smiatek, J.; Heuer, A.
    Deprotonation mechanism of a single-stranded DNA i-motif.
    RSC Adv. 4, 17110 (2014)
21. 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)
22. 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)
23. Smiatek, J.
    Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres.
    J. Phys. Chem. B 118, 771 (2014)

24. 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)
25. 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)
26. 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)
27. 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)
28. Meinhardt, S.; Smiatek, J.; Eichhorn, R.; Schmid, F.
    Separation of chiral particles in micro- or nanofluidic channels.
    Phys. Rev. Lett. 108, 214504 (2012)
29. Smiatek, J.; Harishchandra, R. K.; Rubner, O.; Galla, H.-J.; Heuer, A.
    Properties of compatible solutes in aqueous solution.
    Biophys. Chem. 160, 62 (2012)
30. Smiatek, J.; Liu, D.; Heuer, A.
    High temperature unfolding simulations of a single-stranded DNA i-motif.
    Curr. Phys. Chem. 2, 115 (2012)
31. 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)
32. Smiatek, J.; Heuer, A.
    Calculation of free energy landscapes: A histogram reweighted metadynamics approach.
    J. Comput. Chem. 32, 2084 (2011)
33. Smiatek, J.; Schmid, F.
    Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels.
    Comp. Phys. Comm. 182, 1941 (2011)
34. Smiatek, J.; Schmid, F.
    Polyelectrolyte electrophoresis in nanochannels: A Dissipative Particle Dynamics simulation.
    J. Phys. Chem. B 114, 6266 (2010)
35. 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)
36. 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

37. 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)
38. 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)
39. 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)
40. 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)
41. Smiatek, J.; Schmid, F.
Mesoscopic simulations of polyelectrolyte electrophoresis in nanochannels.
High Performance Computing in Science and Engineering '10, Springer Publications (2011)

Theses

42. Smiatek, J.
Mesoscopic simulations of electrohydrodynamic phenomena.
Ph.D. thesis, Bielefeld University, Bielefeld (2009)
43. Smiatek, J.
Untersuchung von Simulationen zur stochastischen Dynamik unter Zwangsbedingungen.
Hausarbeit zum 1. Staatsexamen für LA Sek. I/II, Bielefeld University, Bielefeld (2005)

Submitted articles

44. Landsgesell, J.; Holm, C.; Smiatek, J.
The Wang-Landau Reaction Ensemble Method: Simulation of weak polyelectrolytes and general acid-base reactions.
in Revision, J. Chem. Theory Comput. (2016)
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.
in Revision, J. Chem. Phys. (2016)

Invited Talks

1. *Aqueous ionic liquids and their influence on peptide conformations: denaturation and dehydration mechanisms*
   Spring meeting Deutsche Physikalische Gesellschaft, Dresden, March 2017
2. *Coarse-grained simulations of soft matter in microfluidic devices*
   42^{nd} Micro and Nano Engineering, Vienna, Austria, September 2016
3. *Macromolecules in solution: The influence of physical and chemical effects*
   Bielefeld University, April 2016
4. *Molecular simulations of solution effects - chemical and physical properties at different length scales*
   University of Münster, February 2016
5. *Macromolecules in solution - More than the sum of the parts*
   AMOLF, Amsterdam, The Netherlands, December 2015
6. *Macromolecules, solvents and co-solutes - A crucial interplay*
   Lorentz Workshop: The future of multi-scale soft matter modeling, Leiden, The Netherlands, September 2015
7. *Macromolecules, solvents and co-solutes - A crucial interplay*
   University of Darmstadt, May 2015
8. *Macromolecules, solvents and co-solutes - A crucial interplay*
   Bundesanstalt für Materialforschung und -prüfung, Berlin, April 2015
9. *Macromolecules, solvents and co-solutes - A crucial interplay*
   University of Würzburg, January 2015
10. *Macromolecules, solvents and co-solutes - A crucial interplay*
    Czech Academy of Sciences, Prague, Czech Republic, January 2015
11. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Luxembourg, Luxembourg, December 2014
12. *Macromolecules, solvents and co-solutes - A crucial interplay*
    University of Mainz, October 2014
13. *Solvent effects and their influence on the properties of soft matter*
    Institute Charles Sadron, Strasbourg, France, June 2014
14. *Solvent effects and their influence on the properties of soft matter*
    University of Tübingen, June 2014
15. *Solvent effects and their influence on the dynamic and static properties of macromolecules*
    German Electron Synchrotron (DESY), Hamburg, May 2013
16. *Computer simulations of biological soft matter systems*
    University of Dortmund, October 2011
17. *Unfolding mechanisms and the free energy landscape of the DNA i-motif*
    Workshop: Multilevel molecular assemblies, structure and function, Beijing, PR China, October 2010
18. *Polyelectrolyte electrophoresis in microchannels: Influence of salt concentration and slippage effects*
    Workshop: Multilevel molecular assemblies, structure and function, Münster, October 2009
19. *Tunable slip boundaries and electrokinetic effects in microchannels*
    University of Münster, November 2008
20. *Tunable slip boundaries and electrokinetic effects in microchannels*
    FIAS Frankfurt, January 2008