Jens Smiatek

Curriculum Vitae

✉ *smiatek@icp.uni-stuttgart.de*

Present Work Adress

Position Research group leader (Habilitand)

Address Institute for Computational Physics
University of Stuttgart
Allmandring 3
70569 Stuttgart (Germany)

Education

2005–2009 **Ph. D. in Physics**, *Physics Faculty*, Bielefeld University.
Supervisor: Prof. Dr. Friederike Schmid

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

1997–1998 **Military Service**.
6. Panzergrenadierbataillon 212 (General-Feldmarschall-Kaserne Augustdorf)

1988–1997 **Städt. Gymnasium Barntrup**.

1984–1988 **Grundschule Bösingfeld**.

State Examination Thesis

Title *Untersuchung von Simulationen zur stochastischen Dynamik unter Zwangsbedingungen*

Year 2005

Supervisor Prof. Dr. Friederike Schmid

Ph. D. Thesis

Title *Mesoscopic simulations of electrohydrodynamic phenomena*

Year 2009

Supervisor Prof. Dr. Friederike Schmid

Work Experience

2012–Present **Research Group Leader (Habilitand)**, Institute for Computational Physics, University of Stuttgart.

2009–2012 **Scientific Associate (Post-Doc)**, Institute of Physical Chemistry, University of Münster, Advisor: Prof. Dr. Andreas Heuer.

2005–2009 **Scientific Associate (Ph. D. student)**, Faculty of Physics, Bielefeld University, Advisor: Prof. Dr. Friederike Schmid.

Research Visits

January 2015 Group of Prof. Dr. Pavel Jungwirth at Czech Academy of Sciences, Prague (CZ)

December 2014 Group of Prof. Dr. Tanja Schilling at University of Luxembourg, Luxembourg (L)

May 2015 Group of Prof. Dr. Jiri Sponer at Masaryk University, Brno (CZ)

October – November 2010 Group of Prof. Dr. Dongsheng Liu at Tsinghua University, Beijing (PR China)

Languages

German **Mothertongue**

English **Fluent**

French **Intermediate**

Research Interests

- Soft condensed matter theory
- Solvation science
- Static and dynamic properties of proteins, DNA, RNA and polyelectrolytes
- Electrohydrodynamic phenomena
- Free energy landscapes
- Method- and algorithm development
- Evaluation of sport statics (soccer and handball)

Third-Party Funding

- *Molekulardynamik-Simulationen zur Untersuchung der Entfaltungspfade von DNA G-Quadruplexen*, Sonderforschungsbereich 716, 116.400 Euro (2015–2018)
- *Atomistic and mesoscopic simulations of polyelectrolytes and ionomers*, Cluster of Excellence *Simulation Technology*, 205.000 Euro (2014–2017)
- *Untersuchung über die Wechselwirkungen von gestreckten, immobilisierten Polyelektrolyten mit externen elektrischen Feldern und Flüssigkeitsströmungen in Gegenwart beschränkter Mikrogeometrien*, Deutsche Forschungsgemeinschaft, 116.400 Euro (2013 – 2016)

Organization of Scientific Conferences

May 2011 *3rd International TRR 61 Workshop on Multilevel Molecular Assemblies: Structure, Dynamics and Function*, Stuttgart, Germany

March 2014 CECAM/SFB 716 International Workshop *Biological Molecules under non-natural conditions*, Stuttgart, Germany

Reviewing Activities

Journals Physical Review Letters, Macromolecules, Journal of the American Chemical Society, Journal of Chemical Theory and Computation, Langmuir, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, ChemPhysChem, Journal of Physical Chemistry B, Journal of Chemical Physics, Computer Physics Communications, Computational Science & Discovery, Physical Review E, Physica A, Chemical Physics Letters, Zeitschrift für Physikalische Chemie, Colloids and Surfaces A, Microfluidics and Nanofluidics, European Physical Journal E, Journal of Molecular Liquids

Publications

Peer-Reviewed Articles

- 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., DOI:0.1039/C5CP07544K (2016)
- 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)
- 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 (2015)
- 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)
- 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)
- 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)
- Lesch, V.; Heuer, A.; Tatsis, V. A.; Holm, C.; and Smiatek, J.
  Peptides in presence of aqueous ionic liquids - Tunable so-solutes as denaturants or protectants?
  Phys. Chem. Chem. Phys. 17, 26049 (2015)
- 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)
- Lesch, V.; Heuer, A.; Holm, C.; and 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)
- Wohlfarth, A.; Smiatek, J.; Kreuer, K.-D.; Takamuku, S.; Jannasch, P.; and Maier, J.
  Proton dissociation of sulfonated polysulfones: Influence of molecular structure and conformation.
  Macromolecules 48, 1134 (2015)

- 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)
- Micciulla, S.; Sanchez, P. A.; Smiatek, J.; Qiao, B.; Sega, M.; Laschewsky, A.; Holm, C.; avon Klitzing, R.
  Layer-by-layer formation of oligoelectrolyte multilayers: a combined experimental and computational study.
  Soft Mater. 12, S14 (2014)
- 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)
- Smiatek, J.; Heuer, A.
  Deprotonation mechanism of a single-stranded DNA i-motif.
  RSC Adv. 4, 17110 (2014)
- 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)
- 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)
- Smiatek, J. Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres.
  J. Phys. Chem. B 118, 771 (2014)
- 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)
- 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)
- 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)
- 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)
- Meinhardt, S.; Smiatek, J.; Eichhorn, R.; Schmid, F.
  Separation of Chiral Particles in Micro- or Nanofluidic Channels.
  Phys. Rev. Lett. 108, 214504 (2012)

- Smiatek, J.; Harishchandra, R. K.; Rubner, O.; Galla, H.-J.; Heuer, A.
  Properties of compatible solutes in aqueous solution
  Biophys. Chem. 160, 62 (2012)
- Smiatek, J.; Liu, D.; Heuer, A.
  High temperature unfolding simulations of a single-stranded DNA i-motif.
  Curr. Phys. Chem. 2, 115 (2012)
- 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)
- Smiatek, J.; Heuer, A.
  Calculation of free energy landscapes: A histogram reweighted metadynamics approach.
  J. Comput. Chem. 32, 2084 (2011)
- Smiatek, J.; Schmid, F.
  Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels.
  Comp. Phys. Comm. 182, 1941 (2011)
- Smiatek, J.; Schmid, F.
  Polyelectrolyte Electrophoresis in Nanochannels: A Dissipative Particle Dynamics Simulation.
  J. Phys. Chem. B 114, 6266 (2010)
- Smiatek, J.; Sega, M.; Holm, C.; Schiller, U. D.; Schmid, F.
  Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study.
  J. Chem. Phys. 130, 244702 (2009)
- Smiatek, J.; Allen, M. P.; Schmid, F.
  Tunable-slip boundaries for coarse-grained simulations of fluid flow.
  Europ. Phys. J. E 26, 115 (2008)

Invited Chapters

- Sanchez, P. A.; Smiatek, J.; Qiao, B.; Sega, M.; Holm, C.
  Atomistic simulation of oligoelectrolyte multilayer growth.
  High Performance Computing in Science and Engineering '14, Springer Publications (2015)
- 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 (2014)
- 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)
- Smiatek, J.; Liu, D.; Heuer, A.
  Unfolding pathways and the free energy landscape of a single-stranded DNA i-motif.
  From Computational Biophysics to Systems Biology (CBSB11), IAS Series, NIC-Publishing (2012)
- 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)
- Smiatek, J.; Schmid, F.
  Mesoscopic simulations of polyelectrolyte electrophoresis in nanochannels.
  High Performance Computing in Science and Engineering '10, Springer Publications (2011)

Theses

- Smiatek, J.
  Mesoscopic simulations of electrohydrodynamic phenomena.
  PhD thesis, Bielefeld University, Germany (2009)
- Smiatek, J.
  Untersuchung von Simulationen zur stochastischen Dynamik unter Zwangsbedingungen
  State Examination Thesis, Bielefeld University, Germany (2005)

Submitted Manuscripts

- Tzaras, E. R.; Weik, F.; Holm, C.; Smiatek, J.
  Polymer translocation through thin nanopores: An unbiased perspective on free energy lanscapes and essential dynamics.
  submitted (2016)
- Smiatek, J.; Riedl, D.; Heuer, A.
  Statistical properties of soccer, basketball and handball - A quantitative comparison.
  submitted (2016)

Five Most Important Articles

- Lesch, V.; Heuer, A.; Tatsis, V. A.; Holm, C.; and Smiatek, J.
  Peptides in the presence of aqueous ionic liquids: tunable co-solutes as denaturants or protectants?
  Phys. Chem. Chem. Phys. 17, 26049 (2015)
- Smiatek, J. Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres.
  J. Phys. Chem. B 118, 771 (2014)
- Meinhardt, S.; Smiatek, J.; Eichhorn, R.; Schmid, F.
  Separation of Chiral Particles in Micro- or Nanofluidic Channels.
  Phys. Rev. Lett. 108, 214504 (2012)
- Smiatek, J.; Heuer, A.
  Calculation of free energy landscapes: A histogram reweighted metadynamics approach.
  J. Comput. Chem. 32, 2084 (2011)
- Smiatek, J.; Schmid, F.
  Polyelectrolyte Electrophoresis in Nanochannels: A Dissipative Particle Dynamics Simulation.
  J. Phys. Chem. B 114, 6266 (2010)

Invited and Contributed Talks

- *Macromolecules in solution - More than the sum of the parts*
  AMOLF, Amsterdam, The Netherlands, December 2015
- *Macromolecules in solution - The importance of the local environment*
  University of Münster, Münster, Germany, October 2015
- *Solvent effects of ionic liquids: implications for the solvation properties and the dynamic behavior of solutes*
  EMLG Meeting 2015: Ionic liquids meet molecular liquids: From fundamentals to applications, Rostock, Germany, September 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  Workshop: The future of multi-scale soft matter modeling, Leiden, The Netherlands, September 2015
- *Osmolyte effects: Impact on the qqueous solution around macromolecules*
  Bunsentagung 2015, Bochum, Germany, May 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  Technical University of Darmstadt, Darmstadt, Germany, May 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany, April 2015
- *Osmolyte effects: Impact on the aqueous solution around macromolecules*
  Spring Meeting Deutsche Physikalische Gesellschaft 2015, Berlin, Germany, March 2015
- *Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions*
  Spring Meeting Deutsche Physikalische Gesellschaft 2015, Berlin, Germany, March 2015
- *A conceptual statistical framework to compare different sports and its application in basketball, handball and soccer*
  Spring Meeting Deutsche Physikalische Gesellschaft 2015, Berlin, Germany, March 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  University of Würzburg, Würzburg, Germany, January 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  Czech Academy of Sciences, Prague, Czech Republic, January 2015
- *Macromolecules, solvents and co-solutes - A crucial interplay*
  University of Luxembourg, Luxembourg, December 2014
- *Solvent effects and their influence on the properties of soft matter*
  Institute Charles Sadron, Strasbourg, France, June 2014
- *Solvent effects and their influence on the properties of soft matter*
  University of Tübingen, Tübingen, Germany, June 2014
- *Solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents*
  Spring Meeting Deutsche Physikalische Gesellschaft 2014, Berlin, Germany, March 2014
- *Atomistic simulation of the layer-by-layer deposition of a polyelectrolyte multilayer: the four layers system*
  SPP 1369 Meeting, Frankfurt a. M., Germany, June 2013

- *Solvent effects and their influence on the dynamic and static properties of macromolecules*
  DESY Hamburg, Hamburg, Germany, May 2013
- *DPPC lipid bilayers in presence of hydroxyectoine*
  Spring Meeting Deutsche Physikalische Gesellschaft 2013, Regensburg, Germany, March 2013
- *Deprotonation mechanism and the unfolding free energy landscape of the DNA i-motif*
  Spring Meeting Deutsche Physikalische Gesellschaft 2013, Regensburg, Germany, March 2013
- *A statistical view on team handball results*
  Spring Meeting Deutsche Physikalische Gesellschaft 2013, Regensburg, Germany, March 2013
- *Solvent effects and their influence on the dynamic and static properties of macromolecules*
  37th Colloquium of the SFB 716, Stuttgart, Germany, November 2012
- *Dissipative Particle Dynamics âĂŞ An introduction*
  ESPResSo-Summer School, Stuttgart, Germany, October 2012
- *Protein adsorption at hydrophobic polymer brushes*
  Spring Meeting Deutsche Physikalische Gesellschaft 2012, Berlin, Germany, March 2012
- *From atomistic to coarse-grained: Influence of solvent effects on biological and charged matter*
  University of Stuttgart, Stuttgart, Germany, October 2011
- *Computer simulations of biological soft matter systems*
  Technical University of Dortmund, Dortmund, Germany, October 2011
- *Unfolding pathways and the free energy landscape of a single-stranded DNA i-motif*
  Mainz Materials Simulation Days, Mainz, Germany, May 2011
- *Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels*
  Spring Meeting Deutsche Physikalische Gesellschaft 2011, Dresden, Germany, March 2011
- *Unfolding mechanisms and the free energy landscape of the DNA i-motif*
  Spring Meeting Deutsche Physikalische Gesellschaft 2011, Dresden, Germany, March 2011
- *Impact of compatible solutes on the local water structure and the structural organization of lipid monolayers*
  Spring Meeting Deutsche Physikalische Gesellschaft 2011, Dresden, Germany, March 2011
- *Unfolding mechanisms and the free energy landscape of the DNA i-motif*
  2^{nd} Workshop on Multilevel molecular assemblies, structure and function, Tsinghua University, Peking, PR China, October 2010
- *Polyelectrolyte electrophoresis in microchannels: Influence of salt concentration and slippage effects*
  Workshop on Multilevel molecular assemblies, structure and function, Münster, Germany, October 2009

- *Tunable slip boundaries and electrokinetic effects in microchannels* University of Münster, Münster, Germany, November 2008
- *Tunable slip boundaries and electrokinetic effects in microchannels* FIAS Frankfurt, Frankfurt a. M., Germany, January 2008
- *A new way of implementing partial slip boundary interactions*
  Workshop on computer simulations of soft matter and biosystems, Heidelberg, Germany, March 2007
- *A new way of implementing partial slip boundary interactions*
  Max Planck-Institute for Polymer Research, Mainz, Germany, March 2007