

Lars Schäfer

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Year of birth: 1978
Place of birth: Braunschweig, Germany
Nationality: German

Education

Ph.D. in Chemistry, 10/2003 – 6/2007
Max-Planck-Institute for Biophysical Chemistry,
Göttingen, Germany
grade: *'mit Auszeichnung'* (*with distinction*)
Title of Ph.D. thesis: 'Photoactivated processes in condensed phase studied by molecular dynamics simulations', Supervisor: Prof. Helmut Grubmüller
Funding: Boehringer Ingelheim Fonds, DFG, EU Nanomot project

Diploma in Chemistry, 10/2000 – 9/2003
Technical University of Braunschweig,
Braunschweig, Germany
grade: *'mit Auszeichnung'* (*with distinction*)
Title of Diploma thesis: 'Theoretical investigation of oxidative enolate dimerisation',
Supervisor: Prof. Ullrich Jahn

Intermediate diploma in Chemistry, 10/1998 – 9/2000
Technical University of Braunschweig,
Braunschweig, Germany
grade: *'sehr gut'* (*A*)

A-levels, 6/1997
Neue Oberschule, Braunschweig, Germany
Majors: Chemistry, Biology, English, Geography
Average grade: 1.9 (B)

Professional Record

Postdoc 6/2007 –
Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany
Theoretical Biophysics group of H. Grubmüller

Ph.D. student 10/2003 – 6/2007
Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany
Theoretical Biophysics group of H. Grubmüller
Projects: Photoswitching mechanism of a fluorescent protein. Photostability of DNA. Elastic properties of photoswitchable azobenzene polymers. Implementation and testing of the 'flooding' technique in the GROMACS package.

Research student 3/2002 – 8/2002
Technical University of Braunschweig, Braunschweig, Germany
Laserchemistry group of Prof. K.-H. Gericke
Project: Photodissociation of small molecules studied by quantum chemical methods

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Professional Record (cont.)

Practical internship	2/2001 – 3/2001
BASF AG	Ludwigshafen, Germany
Projects: Kinetic analysis of thermoanalytic measurements, Modelling of auto-ignition processes	
Community service	9/1997 – 10/1998
Dachverband der Elterninitiativen Braunschweigs	Braunschweig, Germany
I worked in a kindergarten during my obligatory year of community service.	

Research Papers

1. L.V. Schäfer, G. Groenhof, M. Boggio-Pasqua, M.A. Robb, and H. Grubmüller, "Protein Environment controls Photoswitching Mechanism of the Fluoroprotein asFP595", *PLoS Comp. Biol.*, 2008, in production.
2. G. Groenhof, L.V. Schäfer, M. Boggio-Pasqua, H. Grubmüller, and M.A. Robb, "Arginine52 controls the photoisomerization process in Photoactive Yellow Protein", *J. Am. Chem. Soc.*, 2008, in production.
3. M. Boggio-Pasqua, M.A. Robb, G. Groenhof, L.V. Schäfer, and H. Grubmüller, "Ultra-fast Deactivation Channel for Thymine Dimerization", *J. Am. Chem. Soc.*, 2007, 129, 10996-10997.
4. G. Groenhof, L.V. Schäfer, M. Boggio-Pasqua, M. Goette, H. Grubmüller, and M.A. Robb, "Ultra-fast Deactivation of an Excited Cytosine-Guanine Base Pair in DNA", *J. Am. Chem. Soc.*, 2007, 129, 6812-6819.
5. L.V. Schäfer, E.M. Müller, H.E. Gaub, and H. Grubmüller, "Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations", *Angew. Chemie int. Ed.*, 2007, 46, 2232-2237.
6. L.V. Schäfer, G. Groenhof, A.R. Klingen, G.M. Ullmann, M. Boggio-Pasqua, M.A. Robb, and H. Grubmüller, "Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra", *Angew. Chemie int. Ed.*, 2007, 46, 530-536.
7. O.F. Lange, L.V. Schäfer, and H. Grubmüller, "Flooding in GROMACS: Accelerated barrier crossings in molecular dynamics", *J. Comp. Chem.*, 2006, 27, 1693-1702.
8. M. Andresen, M.C. Wahl, A.C. Stiel, F. Gräter, L.V. Schäfer, S. Trowitzsch, G. Weber, C. Eggeling, H. Grubmüller, S.W. Hell, and S. Jakobs, "Structure and mechanism of the reversible photoswitch of a fluorescent protein", *Proc. Nat. Acad. Sci. USA*, 2005, 102, 13070-13074.
9. A. Chichinin, T.S. Einfeld, K.-H. Gericke, J. Grunenberg, C. Maul, and L.V. Schäfer, "Photodissociation Dynamics of $SOCl_2$ ", *Phys. Chem. Chem. Phys.*, 2005, 7, 301-309.
10. L.V. Schäfer, N. Gödecke, O. Ott, C. Maul, K.-H. Gericke, P. S. Shternin, E. V. Orlenko, and O. S. Vasyutinskii, "Recoil velocity-dependent spin-orbit state distribution of chlorine photofragments", *Chem. Phys.*, 2004, 301, 213-224.

Selected Oral Presentations

- Uppsala University, Uppsala, Sweden, 2007
Molecular Biophysics group, invited by Prof. David van der Spoel
Photoactivated Processes in Condensed Phase studied by Molecular Dynamics Simulations
- Imperial College, London, U.K., 2006
Computational Photochemistry group, invited by Prof. M.A. Robb
Mechanism of a Fluorescent Protein

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Selected Oral Presentations (cont.)

Colloquium for Physical Chemistry, Technical University of Braunschweig, Germany, 2006, invited by Prof. K.-H. Gericke

Photoswitching Mechanism of the Fluorescent Protein asFP595: A theoretical Study

Stanford University, Palo Alto, California, 2006

Computational Structural Biology group, invited by Prof. M. Levitt

Mechanism of a Fluorescent Protein

Computer Simulation and Theory of Macromolecules, Hünfeld, Germany, 2005

Elastic Properties of Azobenzene Polymers: An AFM – Molecular Dynamics Study

Selected Poster Presentations

52nd Annual Meeting of the Biophysical Society, Long Beach, CA, USA, 2008

Reversible Photoswitching Mechanism of the Fluoroprotein asFP595 from non-adiabatic QM/MM Molecular Dynamics Simulations

Gordon Research Conference on Computational Chemistry, Les Diablerets, Switzerland, 2006

The Origin of DNA Photostability

50th Annual Meeting of the Biophysical Society, Salt Lake City, Utah, USA, 2006

Mechanism of a Fluorescent Protein – Tailoring Dyes for Subwavelength Far-Field Microscopy

Methods of Molecular Simulation, Heidelberg, Germany, 2005

Elastic Properties of Azobenzene Polymers: An AFM – Molecular Dynamics Study

49th Annual Meeting of the Biophysical Society, Long Beach, CA, USA, 2005

Accelerated Hybrid QM/MM Simulations in Condensed Phase

μ -TheoChem, Modelling and Understanding in Theoretical Chemistry, Lucca, Italy, 2004

MD Simulations accelerated by Chemical Flooding

Teaching Experience

Supervision of lab practicals to the course *Computersimulation of Biomolecular Processes*, Georg-August University, Göttingen, Germany, 2004–2006

Tutor for the EICOS (European Initiative for Communicators of Science) program at the MPI for Biophysical Chemistry, Göttingen, Germany, 2005

Supervision of lab practicals to the course *Physical Chemistry for Natural Scientists*, Technical University of Braunschweig, Germany, 2001–2003

Honors and Awards

”FIZ Chemie Berlin” award for the best dissertation 2007 from the CIC (Chemistry-Information-Computer) division of the German Chemical Society (GDCh) 09/2007

Ph.D. stipend from the Boehringer Ingelheim Fonds 08/2004 – 09/2006

Award from the “Förderverein der Freunde des Instituts für Organische Chemie an der TU Braunschweig” for the faculty’s best diploma 2003

”Braunschweiger Bürgerpreis 2002” for outstanding collegiate performance

Diploma award from the “Braunschweiger Hochschulbund”

Intermediate diploma award from the “Förderverein der Freunde des Instituts für Organische Chemie an der TU Braunschweig”

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Miscellaneous

Certificated '*Project Manager Business Chemistry*' of the German Chemical Society (GDCh), Frankfurt, Germany, 2007

Title of thesis: '*Success Strategies for Big Pharma in India*'

Participation in Seminar '*Conflict Management and Criticism Talks*', organised by the German Chemical Society (GDCh), Braunschweig, Germany, 2003

References

References are obtainable upon request