

PROF. DR. LARS SCHÄFER

*1978, German

Center for Theoretical Chemistry, Molecular Simulation Group
Ruhr University Bochum, D-44780 Bochum, Germany

POSITIONS

- Since 2014 Professor (W2) for Molecular Simulation, Ruhr University Bochum, Germany
2012 – 2014 Emmy Noether Research Group Leader, Johann Wolfgang Goethe University Frankfurt, Germany
2008 – 2012 Postdoctoral Research Fellow, Molecular Dynamics Group, University of Groningen, The Netherlands
2007 – 2008 Postdoc, Theoretical Biophysics Department, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

EDUCATION

- 2007 Dr. rer. nat., Max Planck Institute for Biophysical Chemistry, Göttingen, Germany (with distinction)
2003 Diploma in Chemistry, Technical University Braunschweig, Germany (with distinction)

SCIENTIFIC HONOURS/AWARDS

- 2012 – 2018 Emmy Noether Fellowship of the German Research Foundation (DFG)
2008 – 2011 Veni Postdoc Fellowship of the Netherlands Organisation for Scientific Research (NWO)
2007 FIZ Chemie Berlin PhD Award from the CIC (Chemistry-Information-Computer) division of the German Chemical Society (GDCh)
2004 – 2006 PhD scholarship from the Boehringer Ingelheim Fonds (BIF)
2003 Braunschweiger Hochschulbund Award for the best Diploma in chemistry
2002 Braunschweiger Bürgerpreis for outstanding student achievements

RESEARCH FIELD AND EXPERTISE

Theoretical chemistry and biophysics, biomolecular simulation, computational structural biology

SELECTED PUBLICATIONS

complete list: <https://scholar.google.com/citations?user=1zKTZAMAAAAJ>

- H. Göddeke, L. V. Schäfer. Capturing Substrate Translocation in an ABC Exporter at the Atomic Level. *J. Am. Chem. Soc.* **142**, 12791 (2020).
- O. Fiset, G. F. Schröder, L. V. Schäfer. Atomistic Structure and Dynamics of the Human MHC-I Peptide-Loading Complex. *Proc. Natl. Acad. Sci. U.S.A.* **117**, 20597 (2020).
- S. Wingbermühle, L. V. Schäfer. On Obtaining Boltzmann-Distributed Configurational Ensembles from Expanded Ensemble Simulations with Fast State Mixing. *J. Chem. Theory Comput.* **15**, 2774 (2019).
- M. Prieß, H. Göddeke, G. Groenhof, L. V. Schäfer. Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. *ACS Cent. Sci.* **4**, 1334 (2018).
- O. Fiset, C. Päslock, R. Barnes, J. M. Isas, R. Langen, M. Heyden, S. Han, L. V. Schäfer. Hydration Dynamics of a Peripheral Membrane Protein. *J. Am. Chem. Soc.* **138**, 11526 (2016).