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Publications

Peer-reviewed

31. *Pressure confinement effects on water collective density fluctuations*
D. Russo, A. Filabozzi, A. Laloni, M. Heyden
***Proc Natl Acad Sci USA**, in press* (doi:10.1073/pnas.1705279114)

30. *Solvent entropy contributions to catalytic activity in designed and optimized Kemp eliminases*
S. Belsare, V. Pattni, M. Heyden and T. Head-Gordon
***J Phys Chem B**, in press* (DOI**:** 10.1021/acs.jpcb.7b07526)

29. *Signatures of solvation thermodynamics in spectra of intermolecular vibrations*
R. A. X. Persson, V. Pattni, A. Singh, S. M. Kast and M. Heyden
J Chem Theory Comput 13, 4467-4481 (2017).

28. *Distinct protein hydration water species defined by spatially resolved spectra of intermolecular vibrations*
V. Pattni, T. Vasilevskaya, W. Thiel and M. Heyden,
J Phys Chem B 121, 7431-7442 (2017, cover article).

27. *Hydration dynamics of a peripheral membrane protein*
O. Fisette, C. Päslack, R. Barnes, J. Isas, R. Langen, M. Heyden, S. Han and L. Schäfer
J Am Chem Soc 138, 11526-11535 (2016).

26. *Multi-conformation Monte Carlo: A method for introducing flexibility in efficient simulations of many-protein systems*
V. Prytkova*, M. Heyden*, D. Khago, J. A. Freites, C. T. Butts, R. W. Martin, and D. J. Tobias
J Phys Chem B 120, 8115-8126 (2016). *contributed equally

25. *"Bind and Crawl" Association mechanism of Leishmania major peroxidase and cytochrome c revealed by Brownian and molecular dynamics simulations*
J. B. Fields, S. A. Hollingsworth, G. Chreifi, M. Heyden, A. P. Arce, H. I. Magaña-Garcia, T. L. Poulos, and D J. Tobias
Biochemistry 54, 7272-7282 (2015).

24. *Molecular dynamics simulations of a powder model of the intrinsically disordered protein tau*
Y. Fichou, M. Heyden, G. Zachaï, M. Weik and D. J. Tobias
J Phys Chem B 119, 12580-12589 (2015).

23. *Anomalous behaviour of water inside the SecY translocon*
S. Capponi, M. Heyden, A.-N. Bondar, D. J. Tobias and S. H. White
Proc Natl Acad Sci USA 112, 9016-9021 (2015).

22. *Curvature dependence of hydrophobic hydration dynamics*
R. G. Weiss, M. Heyden and J. Dzubiella
Phys Rev Lett 114, 187802 (2015).

21. *Translational diffusion of hydration water correlates with functional motions in folded and intrinsically disordered proteins*
G. Schiro, Y. Fichou, F.-X. Gallat, K. Wood, F. Gabel, M. Moulin, M. Härtlein, M. Heyden, J.-P. Colletier, A. Orecchini, A. Paciaroni, J. Wuttke, D. J. Tobias and M. Weik
Nat Commun 6, 6490 (2015).

20. *Excluded volume effects in living cells*
D. Gnutt, M. Gao, O. Brylski, M. Heyden and S. Ebbinghaus
Angew Chem Int Ed 54, 2548-2551 (2015, *inside back cover*).

19. *Resolving anisotropic distributions of correlated vibrations in protein hydration water*
M. Heyden
J Chem Phys 141, 22D509 (2014).
Invited article: Chemical Physics of Biological Water (special issue)

18. Comment on *'Hydration and mobility of trehalose in aqueous solution'*
M. Heyden, G. Schwaab and M. Havenith
J Phys Chem B 118, 10802-10805 (2014).

17. *Spatial dependence of protein-water collective hydrogen-bond dynamics*
M. Heyden and D. J. Tobias
Phys Rev Lett 111, 218101 (2013).

16. *Allosteric mechanism of water channel gating by Ca^{2+}/calmodulin*
S. L. Reichow, D. M. Clemens, J. A. Freites, K. L. Németh-Cahalan, M. Heyden, D. J. Tobias, J. E. Hall and T. Gonen
Nat Struct Mol Biol 20, 1085-1092 (2013).

15. *Terahertz absorption of dilute aqueous solutions*
M. Heyden, D. J. Tobias and D. V. Matyushov
J Chem Phys 137, 235103 (2012).

14. *Understanding the origins of dipolar couplings and correlated motion in the vibrational spectrum of water*
M. Heyden, J. Sun, H. Forbert, G. Mathias, M. Havenith and D. Marx
J Phys Chem Lett 3, 2135–2140 (2012).

13. *Assembly and stability of α-helical membrane proteins*
M. Heyden, J. A. Freites, M. B. Ulmschneider, S. H. White and D. J. Tobias
Soft Matter 8, 7742-7752 (2012).

12. *Hot and crowded:*
New insights into the dynamics of thermophilic enzymes from multiscale modeling
M. Heyden and D. J. Tobias
Biophys J 101, 2553-2553 (2011).

11. *Watching the low-frequency motions in aqueous salt solutions:*
The terahertz vibrational signatures of hydrated ions
S. Funkner, G. Niehues, D. A. Schmidt, M. Heyden, G. Schwaab, K. M. Callahan, D. J. Tobias and M. Havenith
J Am Chem Soc 134, 1030-1035 (2011).

10. *Exploring hydrophobicity by THz absorption spectroscopy of solvated amino acids*
G. Niehues, M. Heyden, D. A. Schmidt and M. Havenith
Faraday Disc 150, 193-207 (2011).

9. *Correlated structural kinetics and retarded solvent dynamics at the metalloprotease active site*
M. Grossman*, B. Born*, M. Heyden*, D. Tworowski, G.B. Fields, I. Sagi and M. Havenith
Nat Struct Mol Biol 18, 1102-1108 (2011). *contributed equally

8. *Combining THz spectroscopy and MD simulations to study protein-hydration coupling*
M. Heyden and M. Havenith
Methods 52, 74-83 (2010).

7. *Dissecting the THz spectrum of liquid water from first principles via correlations in time and space*
M. Heyden, J. Sun, S. Funkner, H. Forbert, G. Mathias, M. Havenith and D. Marx
Proc Natl Acad Sci USA 107, 12068-12073 (2010).

6. *Characterization of interfacial water in MOF-5 ($Zn_4(O)(BDC)_3$)*
—A combined spectroscopic and theoretical study
K. Schröck, F. Schröder, M. Heyden, R. A. Fischer and M. Havenith
Phys Chem Chem Phys 10, 4732-4739 (2008).

5. *Long-range influence of carbohydrates on the solvation dynamics of water*
—Answers from terahertz absorption measurements and molecular modeling simulations
M. Heyden, E. Bründermann, U. Heugen, G. Niehues, D. M. Leitner and M. Havenith
J Am Chem Soc 130, 5773-5779 (2008).

4. *Protein sequence- and pH-dependent hydration probed by terahertz spectroscopy*
S. Ebbinghaus, S. J. Kim, M. Heyden, X. Yu, M. Gruebele, D. M. Leitner and M. Havenith
J Am Chem Soc 130, 2374-2375 (2008).

3. *An extended dynamical hydration shell around proteins*
S. Ebbinghaus, S. J. Kim, M. Heyden, X. Yu, U. Heugen, M. Gruebele, D. M. Leitner and M. Havenith
Proc Natl Acad Sci USA 104, 20749-20752 (2007).

2. *Solute-induced retardation of water dynamics probed directly by terahertz spectroscopy*
U. Heugen, G. Schwaab, E. Bründermann, M. Heyden, X. Yu, D. M. Leitner and M. Havenith
Proc Natl Acad Sci USA 103, 12301-12306 (2006).

1. *Terahertz time-domain spectroscopy as a new tool for the characterization of dust forming plasmas*
S. Ebbinghaus, K. Schröck, J. C. Schauer, E. Bründermann, M. Heyden, G. Schwaab, M. Böke, J. Winter, M. Tani and M. Havenith
Plasma Sources Sci Technol 15, 72-77 (2006).

Conference Proceedings

2. Protein-*water network dynamics during metalloenzyme hydrolysis observed by kinetic THz absorption (KITA)*
B. Born, M. Heyden, M. Grossman, I. Sagi and M. Havenith
Proc. of SPIE Vol. 8585 – Terahertz and Ultrashort Electromagnetic Pulses for Biomedical Applications
23rd of February 2013, San Francisco, CA, USA

1. *Statistically converged properties of water from ab initio molecular dynamics simulations*
M. Heyden and M. Havenith
High Performance Computing in Science and Engineering 2009 – Transactions of the Fourth Joint HLRB and KONWIHR Result and Reviewing Workshop, Springer (2010), 687-698
8th – 9th of December 2009, Leibniz-Rechenzentrum, Garching, Germany

Book Chapters

2. *Biomolecular Solvation*
M. Heyden
in ***Lecture Notes Jülich – CECAM School***
Computational Trends in Solvation and Transport in Liquids, pp. 129-147
edited by G. Sutmann, J. Grotendorst, G. Gompper, D. Marx

1. *THz spectroscopy as a tool to study hydration dynamics*
M. Heyden, S. Ebbinghaus and M. Havenith
in ***Encyclopedia of Analytical Chemistry,***
edited by R. A. Meyers, Wiley & Sons: DOI: 10.1002/9780470027318.a9162

Other Publications

5. *Das Innere einer Zelle – Ein komplexes Lösungsmittel*
M. Heyden, S. Ebbinghaus, R. Winter
Chemie in unserer Zeit 51, 26-33 (2017, german)

4. *Vom Reagenzglas in die Zelle*
D. Gnutt, S. Ebbinghaus, M. Heyden
Nachrichten aus der Chemie 64, 310-313 (2016, german).

3. *Resolving correlated motion in biomolecular solutions*
M. Heyden
Bunsenmagazin 01/2015, 10-15

2. *Biomoleküle im Kontext ihrer molekularen Umgebung*
M. Heyden
Jahrbuch der Max-Planck-Gesellschaft 2014/2015, 1/1-7/7 (german)

1. *Ist Wasser immer gleich Wasser? – Einflüsse von Biomolekülen auf das Wasser ihrer Hydrathülle*
M. Heyden
GIT Labor-Fachzeitschrift 9/2014, 48-51 (german)

Media

1. *Planets instead of atoms – Chemist simulates solarsystem /*
   Planeten statt Atome – Chemiker simuliert Sonnensystem
   Dr. J. Weiler
   RUBIN **Wissenschaftsmagazin** 2/2015
   http://rubin.rub.de/en/editors-desk-planets-instead-atoms (english)
   http://rubin.rub.de/de/aus-der-redaktion-planeten-statt-atome (german)

Scientific Communication

40 invited talks (summary)

14 invited Lectures at International Conferences

Gordon Research Conference (GRC): Water & Aqueous Solutions; American Chemical Society (ACS) National Meeting; American Physical Society (APS) March Meeting; Telluride Science Research Center (TSRC) Workshops; CECAM Workshops; ICTP workshop; KIAS Conference on Protein Structure and Function; Pacifichem; Congress of the World Association of Theoretical and Computational Chemists (WATOC)

26 Seminars

International
Stanford University; University of California: Santa Barbara, San Diego, Irvine; Ecole Normale Supérieure Paris; Université Henri Poincaré Nancy; Insitute de Biologie Structurale; Sookmyung Women's University Seoul; Ohio State University; Purdue University; Katholieke Universiteit Leuven; University of Chemistry and Technology Prague; Arizona State University

National
Ludwig-Maxmilians-Universität München; Freie Universität Berlin; Helmholtz-Zentrum Berlin; Albert-Ludwigs-Universität Freiburg; Heidelberg Institute for Theoretical Studies (HITS); Heinrich-Heine-Universität Düsseldorf; Universität Duisburg-Essen; Technische Universität Darmstadt, Max-Planck-Institut für Kohlenforschung; Martin-Luther-Universität Halle-Wittenberg, Universität Paderborn

32 Contributed Conference Presentations (summary)

16 talks	General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung); Symposium on Theoretical Chemistry (STC); Telluride Science Research Center (TSRC) Workshop: Vibrational Dynamics; International Workshop on Optical Terahertz Science and Technology (OTST); WE-Heraeus-Seminar: Exploring Solvation Science; Molecular Graphics and Modeling Society (MGMS) meeting; Condensed Matter Days; Faltertage
16 posters	Gordon Research Conferences/Seminars (GRC/GRS): Water & Aqueous Solutions, Chemistry & Physics of Liquids; Annual Meeting of the Biophysical Society; General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung); Symposium on Theoretical Chemistry (STC); International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz)

Invited Talks / Conferences (detailed list)

14. invited by **Prof. Christian Ochsenfeld**
    Triennial Congress of the **World Association of Theoretical and Computational** (WATOC)
    Solvation and solvent-mediated driving forces:
    Spatially resolved information from detailed atomistic trajectories
    27th of August – 1st of September 2017, Munich, Germany

13. invited by **Prof. Andrea Markelz**
    253rd **American Chemical Society** (ACS) **National Meeting**
    Symposium: Long-range Correlated Motions in Proteins
    Spectral analysis of correlated protein and protein-water vibrations in molecular dynamic simulations
    2nd – 6th of April 2017, San Francisco, CA, USA

12. invited by **Prof. Roland Netz**
    SFB/CRC 1114 conference: „Scaling Cascades in Complex Systems"
    Freie Universität Berlin
    Connecting local solvent dynamics to thermodynamic properties
    27th – 29th of March 2017, Berlin, Germany

11. invited by **Prof. Dor Ben-Amotz**
Telluride Science Research Center (TSRC) **workshop:**
Interfacial molecular and electronic structure and dynamics
3D-2PT: Analyzing the thermodynamics of solvation via intermolecular vibrations
18th – 22nd of July 2016, Telluride, CO, USA

10. invited by **Dr. Martin Weik, Prof. John Straub** and **Prof. Douglas J. Tobias**
Telluride Science Research Center (TSRC) **workshop: Protein dynamics**
Thermodynamic properties of water solvating biomolecular surfaces
3rd – 8th of April 2016, Les Houches, France

9. invited by **Prof. Douglas J. Tobias**
American Physical Society (APS) **March Meeting**
Session: Water at Biological Interfaces
Thermodynamic properties of water solvating biomolecular surfaces
14th – 18th of March 2016, Baltimore, MD, USA

8. invited by **Prof. Alenka Luzar**
Pacifichem 2015
Symposium: Recent Advances in Dynamics of Confined Liquids
Water in the pocket: Exploring local entropies and dynamics of water confined on biomolecular surfaces in atomistic simulations
15th – 20th of December 2015, Honolulu, Hawaii, USA

7. invited by **Dr. Ali Hassanali**
Workshop on Water at the Interface between Biology, Chemistry, Physics and Materials Science
The dynamic footprint of biomolecules in their local solvation environment
5th – 9th of October 2015, Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy

6. invited by **Prof. Sihyun Ham**
15th **KIAS Conference on Protein Structure and Function**
Interactions of proteins with their solvating environment
17th – 19th of September 2015, Korea Institute for Advanced Study (KIAS), Seoul, Republic of Korea

5. invited by **Prof. Dr. Dominik Marx**
CECAM-Jülich School on Computational Trends in Solvation and Transport in Liquids
Biomolecular solvation
23rd – 27th of March 2015, Jülich Sompercomputing Centre, Jülich, Germany

4. invited by **Prof. Douglas J. Tobias**
Gordon Research Conference (GRC) **on Water & Aqueous Solutions 2014**
Correlated vibrations of proteins and their hydration water
27th of July – 1st of August 2014, Holderness, NH, USA

3. invited by **Dr. Martin Weik, Prof. John Straub** and **Prof. Douglas J. Tobias**
Telluride Science Research Center (TSRC) **workshop: Protein dynamics**
Correlations in protein and solvent dynamics studied with atomistic molecular dynamics simulations
18th – 23rd of May 2014, Les Houches, France

2. invited by **Prof. Dr. Ana-Nicoleta Bondar**
CECAM workshop: Coupling between protein, water, and lipid dynamics in complex biological systems
Dynamics of a fast activating G-protein coupled receptor in extended simulations
24th – 27th of September 2013, Lausanne, Switzerland

1. invited by **Prof. Dor Ben-Amotz**
243rd **American Chemical Society (ACS) National Meeting**
Symposium: Water-mediated chemical assembly
Correlated intermolecular motion in solvation water of biomolecules
25th – 29th of March 2012, San Diego, CA, USA

Invited Talks / Seminars (detailed list)

26. invited by **Prof. Dr. Thomas Kühne**
GdCh Kolloquium of the Department of Chemistry, **Universität Paderborn**
Disentangling thermodynamic driving forces using atomistic simulations
22nd of May 2017, Paderborn, Germany

25. invited by **Dr. Jan Heyda**
    Department of Physical Chemistry, **University of Chemistry and Technology, Prague**
    Extracting solvation entropies and free energies from equilibrium intermolecular vibrations
    4th of November 2016, Prague, Czech Republic
24. invited by **Prof. Jeremy Harvey**
    Department of Chemistry, **Katholieke Universiteit Leuven**
    Mini-symposium solutions and solvation: a computational viewpoint
    Vibrations in the water hydrogen bond network
    18th of August 2016, Leuven, Belgium
23. invited by **Prof. Dr. Nico van der Vegt**
    Computational Physical Chemistry, **Technische Universität Darmstadt**
    Simulating solvation: Understanding native biomolecular environments in atomistic detail
    15th of June 2016, Darmstadt, Germany
22. invited by **Prof. Dr. Eckhard Spohr**
    Department of Chemistry, **Universität Duisburg-Essen**
    What local water dynamics can tell us about solvation thermodynamics?
    13th of April 2016, Essen, Germany
21. invited by **Prof. Damien Laage**
    Ecole Normale Supérieure Paris
    Thermodynamic properties of water solvating biomolecular surfaces
    31st of March 2016, Paris, France
20. invited by **Prof. Dor Ben-Amotz**
    Department of Chemistry, **Purdue University**
    Thermodynamic properties of water solvating biomolecular surfaces
    12th of January 2016, West Lafayette, IN, USA
19. invited by **Prof. Heather Allen**
    Department of Chemistry, **Ohio State University**
    Thermodynamic properties of water solvating biomolecular surfaces
    11th of January 2016, Columbus, OH, USA
18. invited by **Prof. Francesco Paesani**
    Department of Chemistry, **University of California, San Diego**
    Thermodynamic properties of water solvating biomolecular surfaces
    8th of January 2016, San Diego, CA, USA
17. invited by **Prof. Douglas J. Tobias**
    Department of Chemistry, **University of California, Irvine**
    Thermodynamic properties of water solvating biomolecular surfaces
    7th of January 2016, Irvine, CA, USA
16. invited by **Prof. Dr. Daniel Sebastiani**
    Department of Chemistry, **Martin-Luther-Universität Halle-Wittenberg**
    The dynamic footprint of biomolecules in their local solvation environment
    19th of November 2015, Halle, Germany
15. invited by **Prof. Sihyun Ham**
    Sookmyung Women's University Seoul
    Biomoleular Solvation
    14th of September 2015, Seoul, Republic of Korea
14. invited by **Prof. Dr. Roland Netz**
    Department of Theoretical Physics, **Freie Universität Berlin**
    Biomolecular stability and dynamics in the context of the solvating environment
    16th of July 2015, Berlin, Germany
13. invited by **Prof. Dr. Gerhard Stock**
    Department of Physics, **Albert-Ludwigs-Universität Freiburg**
    Analyzing the effects of the solvating environments on proteins in simulations
    17th of July 2014, Freiburg, Germany

12. invited by **Prof. Dr. Rebecca Wade**
Heidelberg Institute for Theoretical Studies (HITS)
Monte Carlo sampling of flexible proteins and polymers in many-molecule systems
15th of July 2014, Heidelberg, Germany

11. invited by **Prof. Dr. Joachim Dzubiella**
Soft Matter and Functional Materials Institute, **Helmholtz-Zentrum Berlin**
Analyzing the interactions between bimolecular solutes and their solvating environment
20th of June 2014, Berlin, Germany

10. invited by **Prof. Dr. Christel Marian**
Department of Theoretical Chemistry, **Heinrich-Heine-Universität Düsseldorf**
Coupled solute-solvent dynamics in biomolecular solutions
28th of May 2014, Düsseldorf, Germany

9. invited by **Dr. Martin Weik**
Insitute de Biologie Structurale (IBS)
Understanding the influence of the solvating environment on biomolecular properties
16th of May 2014, Grenoble, France

8. invited by **Dr. Jens Kortmann**
School of Medicine, **Stanford University**
Molecular dynamics simulations and the role of solvation in biological processes
6th of May 2013, Palo Alto, CA, USA

7. invited by **RESOLV Cluster of Excellence**
Max-Planck-Institut für Kohlenforschung
Role of collective vibrations for solute-solvent interactions of proteins and enzymes
27th of February 2013, Mülheim an der Ruhr, Germany

6. invited by **Prof. Mounir Tarek**
Équipe de Chimie et Biochimie Théoriques, **Université Henri Poincaré Nancy**
Vibrations in water at THz frequencies and membrane protein dynamics at timescales from ps to μs
— Insights from various molecular dynamics approaches
30th of June 2011, Nancy, France

5. invited by **Prof. Dr. Ana-Nicoleta Bondar**
Theoretical Molecular Biophysics, **Freie Universität Berlin**
Membrane protein dynamics in different lipid environments:
Native membranes vs. reconstitution in artificial lipid bilayers studied with molecular dynamics simulations
6th of June 2011, Berlin, Germany

4. invited by **Prof. Mark Sherwin**
Institute for Terahertz Science and Technology, **University of California, Santa Barbara**
Tuning in on the frequencies of the hydrogen bond network of water
28th of April 2011, Santa Barbara, CA, USA

3. invited by **Prof. Dr. Walter Thiel**
Department of Theoretical Chemistry, **Max-Planck-Institut für Kohlenforschung**
Water seen through terahertz glasses
14th of July 2010, Mülheim an der Ruhr, Germany

2. invited by **Prof. Douglas J. Tobias**
Department of Chemistry, **University of California, Irvine**
Water seen through terahertz glasses
— Picosecond dynamics and THz vibrational modes in water and aqueous solutions
29th of March 2010, Irvine, CA, USA

1. invited by **Prof. Dr. Paul Tavan** and **Dr. Gerald Mathias**
Biomolecular Optics, **Ludwig-Maximilians-Universität** (LMU) **München**
Vibrational modes of water in ab initio molecular dynamics simulations
10th of July 2009, Munich, Germany

Contributed Talks (detailed list)

16. **52nd · Symposium on Theoretical Chemistry** (STC)
Solvation thermodynamics probed by intermolecular vibrations in molecular dynamics simulations
26th – 29th of September 2016, Bochum, Germany

15. **115th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
Thermodynamic properties of water solvating biomolecular surfaces
5th – 7th of May 2016, Rostock, Germany

14. **Molecular Graphics and Modeling Society Meeting: Exploring Mechanisms in Biology – Theory and Experiment**
Understanding molecules in their natural habitat
– How the solvating environment affects protein dynamics and stability
25th – 27th of November 2015, Singapore

13. **572th WE-Heraeus-Seminar: "Exploring Solvation Science"**
Resolving anisotropic distributions of correlated vibrational motion in protein hydration water
27th – 30th of October 2014, Bad Honnef, Germany

12. **50th · Symposium on Theoretical Chemistry** (STC)
Spatial resolution of long-ranged dynamical coupling between proteins and hydration water
14th – 18th of September 2014, Vienna, Austria

11. **Condensed Matter Days 2014** (CMD 25 – JMC 14)
Tracking correlations of vibrational motion from biomolecular solutes into the surrounding solvent
24th – 29th of August 2014, Paris, France

10. **113th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
Analyzing coupled solute/solvent dynamics via correlated vibrational motion in protein hydration shells
29th – 31st of May 2014, Hamburg, Germany

9. **Telluride Science Research Center** (TSRC) **workshop: Vibrational Dynamics**
Intermolecular vibrations in water and aqueous solutions
25th – 29th of July 2011, Telluride, CO, USA

8. **International Workshop on Optical Terahertz Science and Technology** (OTST) **2011**
Solvation water of biomolecules seen through THz glasses
13th – 17th of March 2011, Santa Barbara, CA, USA

7. **AirUCI workshop**
Ions in motion: Intermolecular vibrations of solvated ions in the far infrared
19th – 20th of January 2011, Laguna Beach, CA, USA

6. **21st Faltertage**
Solvation water of biomolecules seen through terahertz glasses
15th – 17th of October 2010, Regensburg, Germany

5. **Gordon Research Conference** (GRC) **on Water & Aqueous Solutions**
Invited short talk: Water seen through terahertz glasses
8th – 13th of August 2010, Holderness, NH, USA

4. **HLRB2 Workshop for Supercomputer Users**
Statistically converged properties of water from ab initio molecular dynamics simulations
8th – 9th of December 2009, Garching, Germany

3. **108th Annual Meeting of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
THz vibrational modes in ab initio water simulations
21st – 23rd of May 2009, Köln, Germany

2. **63rd OSU International Symposium on Molecular Spectroscopy 2008**
Probing hydrogen bond network vibrations in carbohydrate solvation shells at THz frequencies
16th – 20th of June 2008, Columbus, OH, USA
(presented by S. Ebbinghaus)

1. **106th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
Characteristics of solvation water around carbohydrates and proteins
17th – 19th of May 2007, Graz, Austria

Posters (detailed list)

16. **116th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
Quantifying the thermodynamic cost of protein desolvation
25th – 27th of May 2017, Kaiserslautern, Germany

15. **Gordon Research Conference** (GRC) **on Water & Aqueous Solutions**
    3D-2PT: Spatially resolved solvent entropies from molecular dynamics simulations
    31st of July – 5th of August 2016, Holderness, NH, USA
14. **51st Symposium on Theoretical Chemistry** (STC)
    Resolving the effects of solute-solvent interactions with spatial resolution in atomistic molecular dynamics simulations
    20th – 24th of September 2015, Potsdam, Germany
13. **114th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
    Exploring correlated solute-solvent dynamics in biomolecular solvation environments
    14th – 16th of May 2015, Bochum, Germany
12. **Gordon Research Conference** (GRC) **on Water & Aqueous Solutions**
    Resolving coupled protein-water motions in time and space
    27th of July – 1st of August 2014, Holderness, NH, USA
11. **Gordon Research Conference** (GRC) **on Chemistry & Physics of Liquids**
    Correlated vibrational dynamics in protein hydration water
    4th – 9th of August 2013, Holderness, NH, USA
10. **57th Annual Meeting of the Biophysical Society**
    GPCR activation on the microsecond timescale in MD simulations
    2nd – 6th of February 2013, Philadelphia, PA, USA
9. **Gordon Research Conference** (GRC) **on Water & Aqueous Solutions**
    Vibrational coupling between biomolecules and hydration water
    12th – 17th of August 2012, Holderness, NH, USA
8. **56th Annual Meeting of the Biophysical Society**
    Microsecond dynamics of the G-protein coupled receptor squid rhodopsin in atomistic detail
    25th – 29th of February 2012, San Diego, CA, USA
7. **110th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
    Sensing solvation effects:
    Which properties of water are most sensitive to the presence of biomolecular solutes
    2nd – 4th of June 2011, Berlin, Germany
6. **35th International Conference on Infrared, Millimeter and Terahertz Waves** (IRMMW-THz)
    Solvation water of biomolecules seen through terahertz glasses III
    5th – 10th of September 2010, Rome, Italy
5. **Gordon Research Conference** (GRC) **on Water & Aqueous Solutions (Poster Prize)**
    Solvation water of biomolecules seen through terahertz glasses II
    8th – 13th of August 2010, Holderness, NH, USA
4. **Leopoldina Symposium:**
    The complexity connecting biomolecular structure and solvation dynamics
    Solvation water of biomolecules seen through terahertz glasses I
    25th – 27th of May 2010, Bochum, Germany
3. **44th Symposium on Theoretical Chemistry** (STC)
    Solvation water dynamics of biological compounds on the picosecond timescale
    23rd – 27th of September 2008, Ramsau am Dachstein, Austria
2. **107th General Assembly of the German Bunsen Society for Physical Chemistry** (Bunsentagung)
    Water confined in nanoporous Metal Organic Frameworks
    1st – 3rd of May 2008, Saarbrücken, Germany
1. **International Bunsen Discussion Meeting "Exploring THz Spectroscopy" (Poster Prize)**
    In the grasp of biomolecules:
    Dynamic properties of solvation water around sugars, proteins and nucleic acids
    1st – 4th of April 2007, Bad Honnef, Germany