

## Curriculum Vitae

### Education

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- 09/2010 **Dr. rer. nat.** (equivalent to PhD) (*summa cum laude*)  
*Ruhr-University Bochum, Germany*
- 10/2004 – 02/2006 **Preparational Course for fast-track PhD** (*instead of M.Sc.*) (*1.1, magna cum laude*)  
*Ruhr-University Bochum, Germany*
- 09/2004 **Bachelor of Science in Biochemistry** (*1.1, magna cum laude*)  
*Ruhr-University Bochum, Germany*
- 10/2001 – 09/2004 **Undergraduate Studies in Biochemistry**  
*Ruhr-University Bochum, Germany*

### Professional Experience

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- from 10/2017 **Assistant Professor** (tenure-track)  
*School of Molecular Sciences, Arizona State University, Tempe, AZ, USA*
- 08/2013 – 09/2017 **RESOLV Early Career Research Group Leader**  
*Theoretical Chemistry, Max-Planck-Institut für Kohlenforschung,  
Mülheim an der Ruhr, Germany*  
Host: Prof. Dr. Walter Thiel
- 11/2010 – 07/2013 **Postdoctoral Researcher**  
*Department of Chemistry, University of California, Irvine, USA*  
Host: Prof. Douglas J. Tobias
- 02/2006 – 09/2010 **Graduate Research Studies**  
*Department of Physical Chemistry II, Ruhr-University Bochum, Germany*  
Thesis: "Properties of Water at Terahertz Frequencies and Picosecond Timescales"  
Supervisor: Prof. Dr. Martina Havenith
- 12/2004 – 02/2006 **Undergraduate Research Assistant**  
*Department of Physical Chemistry II, Ruhr-University Bochum, Germany*
- 06/2004 – 09/2004 **Bachelor Thesis**  
*Department of Physical Chemistry II, Ruhr-University Bochum, Germany*  
Thesis: "Study of potential surfaces for the description of intermolecular vibrations"  
Supervisor: Prof. Dr. Martina Havenith

### Research Stays

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- 04/2010 *Department of Structural Biology, Weizmann Institut, Rehovot, Israel*  
Host: Prof. Dr. Irit Sagi
- 06/2006 – 09/2006 *Department of Chemistry, University of Nevada, Reno, USA*  
Host: Prof. David M. Leitner

### Awards

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- 08/2011 **Postdoctoral scholarship** (24 months)  
*German National Academy of Sciences Leopoldina*
- 07/2011 **Peter A. Salamon Award**  
*Telluride Science Research Center, Telluride, CO, USA*
- 08/2010 **Victoria Buch Memorial Poster Prize**  
*Gordon Research Conference on Water & Aqueous Solutions  
Holderness, NH, USA*
- 06/2009 **Participant of the 59<sup>th</sup> Meeting of the Nobel Laureates**  
*Lindau, Germany*

01/2008	<b>Doctoral Scholarship</b> (30 months) <i>German National Academic Foundation (Studienstiftung des deutschen Volkes)</i>
04/2007	<b>PCCP Poster Prize</b> <i>International Bunsen Discussion Meeting: "Exploring THz spectroscopy" Bad Honnef, Germany</i>
02/2007	<b>Fellowship</b> of the Ruhr-University Research School <i>Ruhr-University Bochum, Germany</i>
06/2006	<b>Short-term doctoral fellowship</b> (4 months) <i>German Academic Exchange Service (DAAD)</i>
<b>Service</b>	
06/2018	co-Organizer: Les Houches/TSRC Workshop on Protein Dynamics 2018 (with Martin Weik, Paul Schanda and James Fraser)
since 2016	Proposal referee <i>Swiss National Science Foundation; National Science Center, Poland</i>
08/2014	Chair of the Gordon Research Seminar on Water & Aqueous Solutions Cluster of Excellence RESOLV
10/2014 – 09/2017	Speaker: Early Career Researcher Board Member: RESOLV Executive Board
10/2013 – 10/2014	Member: Early Career Researcher Board Member: Graduate School of Solvation Science Board
since 2010	Journal referee (53 manuscripts + revisions): <i>Biophys J, J Am Chem Soc, J Phys Chem B, J Phys Chem Lett, J Chem Theory Comput, J Chem Phys, J Comput Chem, Phys Chem Chem Phys, Sci Rep, Vib Spectrosc, Chem Phys, ChemPhysChem, Europhys Lett</i>
since 2011	Society Memberships <i>Biophysical Society, USA (2011–2015); American Physical Society (since 2015), American Chemical Society (since 2016)</i>

## Publications

- Peer-reviewed** citations (google scholar): **2225** / h-index: **17** (10/2017)
- 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)
  - 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.jpbc.7b07526)
  - 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). citations: **1**
  - 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). citations: **2**
  - Hydration dynamics of a peripheral membrane protein*  
O. Fiset, C. Päslock, R. Barnes, J. Isas, R. Langen, M. Heyden, S. Han and L. Schäfer  
**J Am Chem Soc** 138, 11526-11535 (2016). citations: **3**
  - 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). citations: **8**
24. Molecular dynamics simulations of a powder model of the intrinsically disordered protein tau  
Y. Fichou, M. Heyden, G. Zschaler, M. Weik and D. J. Tobias  
**J Phys Chem B** 119, 12580-12589 (2015). citations: **4**
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). citations: **13**
22. Curvature dependence of hydrophobic hydration dynamics  
R. G. Weiss, M. Heyden and J. Dzubiella  
**Phys Rev Lett** 114, 187802 (2015). citations: **6**
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). citations: **71**
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). citations: **62**
19. Resolving anisotropic distributions of correlated vibrations in protein hydration water  
M. Heyden  
**J Chem Phys** 141, 22D509 (2014). citations: **6**  
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). citations: **57**
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). citations: **46**
15. Terahertz absorption of dilute aqueous solutions  
M. Heyden, D. J. Tobias and D. V. Matyushov  
**J Chem Phys** 137, 235103 (2012). citations: **31**
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). citations: **22**
13. Assembly and stability of  $\alpha$ -helical membrane proteins  
M. Heyden, J. A. Freites, M. B. Ulmschneider, S. H. White and D. J. Tobias  
**Soft Matter** 8, 7742-7752 (2012). citations: **17**
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). citations: **111**

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). citations: **47**
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 citations: **142**
8. *Combining THz spectroscopy and MD simulations to study protein-hydration coupling*  
M. Heyden and M. Havenith  
**Methods** 52, 74-83 (2010). citations: **100**
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). citations: **202**
6. *Characterization of interfacial water in MOF-5 (Zn<sub>4</sub>(O)(BDC)<sub>3</sub>)  
— 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). citations: **61**
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). citations: **195**
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). citations: **134**
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). citations: **465**
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). citations: **334**
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). citations: **41**

#### 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  
23<sup>rd</sup> 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 – 9<sup>th</sup> 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

citations: 5

#### 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*  
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

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##### 40 invited talks (summary)

##### 13 invited Lectures at International Conferences (+1 scheduled)

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; Pacificchem; 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*  
27<sup>th</sup> of August – 1<sup>st</sup> of September 2017, Munich, Germany
13. invited by **Prof. Andrea Markelz**  
253<sup>rd</sup> **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*  
2<sup>nd</sup> – 6<sup>th</sup> 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*  
27<sup>th</sup> – 29<sup>th</sup> 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*  
18<sup>th</sup> – 22<sup>nd</sup> 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*  
3<sup>rd</sup> – 8<sup>th</sup> 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*  
14<sup>th</sup> – 18<sup>th</sup> of March 2016, Baltimore, MD, USA
8. invited by **Prof. Alenka Luzar**  
**Pacificchem 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*  
15<sup>th</sup> – 20<sup>th</sup> 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*  
5<sup>th</sup> – 9<sup>th</sup> of October 2015, Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy
6. invited by **Prof. Sihyun Ham**  
15<sup>th</sup> **KIAS Conference on Protein Structure and Function**  
*Interactions of proteins with their solvating environment*  
17<sup>th</sup> – 19<sup>th</sup> 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*  
23<sup>rd</sup> – 27<sup>th</sup> 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*  
 27<sup>th</sup> of July – 1<sup>st</sup> 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*  
 18<sup>th</sup> – 23<sup>rd</sup> 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*  
 24<sup>th</sup> – 27<sup>th</sup> of September 2013, Lausanne, Switzerland
1. invited by **Prof. Dor Ben-Amotz**  
**243<sup>rd</sup> American Chemical Society (ACS) National Meeting**  
 Symposium: Water-mediated chemical assembly  
*Correlated intermolecular motion in solvation water of biomolecules*  
 25<sup>th</sup> – 29<sup>th</sup> 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*  
 22<sup>nd</sup> 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*  
 4<sup>th</sup> 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*  
 18<sup>th</sup> 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*  
 15<sup>th</sup> 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?*  
 13<sup>th</sup> of April 2016, Essen, Germany
21. invited by **Prof. Damien Laage**  
**Ecole Normale Supérieure Paris**  
*Thermodynamic properties of water solvating biomolecular surfaces*  
 31<sup>st</sup> of March 2016, Paris, France
20. invited by **Prof. Dor Ben-Amotz**  
 Department of Chemistry, **Purdue University**  
*Thermodynamic properties of water solvating biomolecular surfaces*  
 12<sup>th</sup> 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*  
 11<sup>th</sup> 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*  
 8<sup>th</sup> 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*  
 7<sup>th</sup> 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*  
 19<sup>th</sup> of November 2015, Halle, Germany
15. invited by **Prof. Sihyun Ham**  
**Sookmyung Women's University Seoul**  
*Biomolecular Solvation*  
 14<sup>th</sup> 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*  
 16<sup>th</sup> 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*  
 17<sup>th</sup> 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*  
 15<sup>th</sup> 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*  
 20<sup>th</sup> 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*  
 28<sup>th</sup> 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*  
 16<sup>th</sup> 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*  
 6<sup>th</sup> 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*  
 27<sup>th</sup> 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*  
 30<sup>th</sup> 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*  
 6<sup>th</sup> 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*  
28<sup>th</sup> 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*  
14<sup>th</sup> 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*  
29<sup>th</sup> 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*  
10<sup>th</sup> of July 2009, Munich, Germany

#### **Contributed Talks (detailed list)**

16. **52<sup>nd</sup> · Symposium on Theoretical Chemistry (STC)**  
*Solvation thermodynamics probed by intermolecular vibrations in molecular dynamics simulations*  
26<sup>th</sup> – 29<sup>th</sup> of September 2016, Bochum, Germany
15. **115<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Thermodynamic properties of water solvating biomolecular surfaces*  
5<sup>th</sup> – 7<sup>th</sup> 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*  
25<sup>th</sup> – 27<sup>th</sup> of November 2015, Singapore
13. **572<sup>th</sup> WE-Heraeus-Seminar: “Exploring Solvation Science”**  
*Resolving anisotropic distributions of correlated vibrational motion in protein hydration water*  
27<sup>th</sup> – 30<sup>th</sup> of October 2014, Bad Honnef, Germany
12. **50<sup>th</sup> · Symposium on Theoretical Chemistry (STC)**  
*Spatial resolution of long-ranged dynamical coupling between proteins and hydration water*  
14<sup>th</sup> – 18<sup>th</sup> 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*  
24<sup>th</sup> – 29<sup>th</sup> of August 2014, Paris, France
10. **113<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Analyzing coupled solute/solvent dynamics via correlated vibrational motion in protein hydration shells*  
29<sup>th</sup> – 31<sup>st</sup> of May 2014, Hamburg, Germany
9. **Telluride Science Research Center (TSRC) workshop: Vibrational Dynamics**  
*Intermolecular vibrations in water and aqueous solutions*  
25<sup>th</sup> – 29<sup>th</sup> 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*  
13<sup>th</sup> – 17<sup>th</sup> of March 2011, Santa Barbara, CA, USA
7. **AirUCI workshop**  
*Ions in motion: Intermolecular vibrations of solvated ions in the far infrared*  
19<sup>th</sup> – 20<sup>th</sup> of January 2011, Laguna Beach, CA, USA
6. **21<sup>st</sup> Faltertage**  
*Solvation water of biomolecules seen through terahertz glasses*  
15<sup>th</sup> – 17<sup>th</sup> of October 2010, Regensburg, Germany

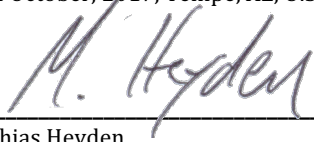
5. **Gordon Research Conference (GRC) on Water & Aqueous Solutions**  
*Invited short talk: Water seen through terahertz glasses*  
8<sup>th</sup> – 13<sup>th</sup> of August 2010, Holderness, NH, USA
4. **HLRB2 Workshop for Supercomputer Users**  
*Statistically converged properties of water from ab initio molecular dynamics simulations*  
8<sup>th</sup> – 9<sup>th</sup> of December 2009, Garching, Germany
3. **108<sup>th</sup> Annual Meeting of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*THz vibrational modes in ab initio water simulations*  
21<sup>st</sup> – 23<sup>rd</sup> of May 2009, Köln, Germany
2. **63<sup>rd</sup> OSU International Symposium on Molecular Spectroscopy 2008**  
*Probing hydrogen bond network vibrations in carbohydrate solvation shells at THz frequencies*  
16<sup>th</sup> – 20<sup>th</sup> of June 2008, Columbus, OH, USA  
(presented by S. Ebbinghaus)
1. **106<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Characteristics of solvation water around carbohydrates and proteins*  
17<sup>th</sup> – 19<sup>th</sup> of May 2007, Graz, Austria

#### Posters (detailed list)

16. **116<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Quantifying the thermodynamic cost of protein desolvation*  
25<sup>th</sup> – 27<sup>th</sup> of May 2017, Kaiserslautern, Germany
15. **Gordon Research Conference (GRC) on Water & Aqueous Solutions**  
*3D-2PT: Spatially resolved solvent entropies from molecular dynamics simulations*  
31<sup>st</sup> of July – 5<sup>th</sup> of August 2016, Holderness, NH, USA
14. **51<sup>st</sup> Symposium on Theoretical Chemistry (STC)**  
*Resolving the effects of solute-solvent interactions with spatial resolution in atomistic molecular dynamics simulations*  
20<sup>th</sup> – 24<sup>th</sup> of September 2015, Potsdam, Germany
13. **114<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Exploring correlated solute-solvent dynamics in biomolecular solvation environments*  
14<sup>th</sup> – 16<sup>th</sup> of May 2015, Bochum, Germany
12. **Gordon Research Conference (GRC) on Water & Aqueous Solutions**  
*Resolving coupled protein-water motions in time and space*  
27<sup>th</sup> of July – 1<sup>st</sup> of August 2014, Holderness, NH, USA
11. **Gordon Research Conference (GRC) on Chemistry & Physics of Liquids**  
*Correlated vibrational dynamics in protein hydration water*  
4<sup>th</sup> – 9<sup>th</sup> of August 2013, Holderness, NH, USA
10. **57<sup>th</sup> Annual Meeting of the Biophysical Society**  
*GPCR activation on the microsecond timescale in MD simulations*  
2<sup>nd</sup> – 6<sup>th</sup> of February 2013, Philadelphia, PA, USA
9. **Gordon Research Conference (GRC) on Water & Aqueous Solutions**  
*Vibrational coupling between biomolecules and hydration water*  
12<sup>th</sup> – 17<sup>th</sup> of August 2012, Holderness, NH, USA
8. **56<sup>th</sup> Annual Meeting of the Biophysical Society**  
*Microsecond dynamics of the G-protein coupled receptor squid rhodopsin in atomistic detail*  
25<sup>th</sup> – 29<sup>th</sup> of February 2012, San Diego, CA, USA
7. **110<sup>th</sup> 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*  
2<sup>nd</sup> – 4<sup>th</sup> of June 2011, Berlin, Germany
6. **35<sup>th</sup> International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz)**  
*Solvation water of biomolecules seen through terahertz glasses III*  
5<sup>th</sup> – 10<sup>th</sup> 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*  
8<sup>th</sup> – 13<sup>th</sup> 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*  
25<sup>th</sup> – 27<sup>th</sup> of May 2010, Bochum, Germany
3. **44<sup>th</sup> Symposium on Theoretical Chemistry (STC)**  
*Solvation water dynamics of biological compounds on the picosecond timescale*  
23<sup>rd</sup> – 27<sup>th</sup> of September 2008, Ramsau am Dachstein, Austria
2. **107<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung)**  
*Water confined in nanoporous Metal Organic Frameworks*  
1<sup>st</sup> – 3<sup>rd</sup> 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*  
1<sup>st</sup> – 4<sup>th</sup> of April 2007, Bad Honnef, Germany

9<sup>th</sup> of October, 2017, Tempe, AZ, U.S.A.



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Matthias Heyden