

Nadja Heine

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Education

- 2010 – 2014 **Ph.D. Physics (summa cum laude)**
Freie Universität Berlin
Thesis: “Vibrational Spectroscopy of Gaseous Hydrogen-Bonded Clusters: On the Role of Isomer-Specificity and Anharmonicity”
Supervisors: Prof. G. Meijer, Prof. K.R. Asmis
- 2008 – 2010 **M.Sc. Chemistry**
Freie Universität Berlin
Thesis: “Time-Resolved Photoelectron Spectroscopy of Chromophores in Solution”
Supervisor: Prof. E. Rühl
- 2004 – 2008 **B.Sc. Chemistry**
Freie Universität Berlin
Thesis: “Optical Levitation of Microparticles and NEXAFS Measurements of Salts”
Supervisor: Prof. E. Rühl

Research Experience

- 2015 – pres **Postdoctoral Research Fellow**, Supervisors: Dr. H. Bluhm, Dr. K.R. Wilson
Lawrence Berkeley National Laboratory, Berkeley, USA
 - Measured heterogeneous oxidation of organic particles using aerosol mass spectrometry and velocity map imaging.
 - Employed stochastic kinetics models to determine the mechanism of organic particle oxidation.
 - Facilitated external user access to synchrotron-VUV beamlines at the Advanced Light Source.
- 2010 – 2014 **Graduate Researcher**, Supervisor: Prof. K.R. Asmis, Prof. G. Meijer
Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany
 - Developed, designed and implemented an ion trap triple mass spectrometer.
 - Characterized the structure of mass-selected and thermalized hydrogen-bonded clusters in the gas phase using infrared (IR) photodissociation spectroscopy.
 - Performed IR/IR isomer-specific measurements of protonated water clusters with a free electron laser.
- 2009 – 2010 **Research Assistant**, Supervisor: Dr. T. Schultz
Max-Born-Institute, Berlin, Germany
 - Characterized a new experimental setup for ultrafast dynamic processes in a liquid microjet.
 - Determined the vertical binding energy of solvated electrons in solution using fs time-resolved photoelectron spectroscopy.

- 2008 – 2010 **Research Assistant**, Supervisor: Prof. V. Nordmeier
Freie Universität Berlin, Berlin, Germany
◦ Developed interactive laboratory experiments ([examples](#)).
- 2007 – 2008 **Research Assistant**, Supervisor: Prof. E. Rühl
Freie Universität Berlin, Berlin, Germany
◦ Built a flow tube mass spectrometer for synthesis of free Cl and ClO radicals.
◦ Performed NEXAFS experiments on free Cl, ClO radicals and salts.

Teaching Experience

- 2009 – 2010 **Teaching Assistant**, Physical Chemistry Laboratory Course
Freie Universität Berlin, Berlin, Germany
◦ Introduced interactive lab experiments in a weekly seminar.
- 2008 – 2009 **Teaching Assistant**, Chemistry Laboratory Course and Seminar for Biologists and Vet. Medicine Students
Freie Universität Berlin, Berlin, Germany
◦ Supervised laboratory courses with focus on basic chemical experiments.
◦ Held lecture in general chemistry on a weekly basis.

Honors and Awards

- 2016 Wolfgang-Paul-Studienpreis (DGMS)
2016 Travel Grant, German Academic Exchange Service (DAAD)
2015 Feodor Lynen Research Fellowship, Alexander von Humboldt Foundation
2014 Summa cum laude (high honors) awarded for doctoral thesis

Professional Associations

- German Society for Mass Spectrometry (DGMS)
American Chemical Society (ACS)
American Association for Aerosol Research (AAAR)
German Chemical Society (GDCh)

Publications

- 2016 T. Wende, **N. Heine**, T.I. Yacovitch, K.R. Asmis, D.M. Neumark, L. Jiang, “Probing the Microsolvation of a Quaternary Ion Complex: Gas Phase Vibrational Spectroscopy of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_{n=0-8}$ ”, *Phys. Chem. Chem. Phys.* **18** 267–77 .
- 2015 **N. Heine**, M.R. Fagiani, and K.R. Asmis, “Disentangling the Contribution of Multiple Isomers to the Infrared Spectrum of the Protonated Water Heptamer”, *J. Phys. Chem. Lett.* **6** 2298–2304.
- S.-T. Sun, L. Jiang, J.-W. Liu, **N. Heine**, T.I. Yacovitch, T. Wende, D.M. Neumark, K. R. Asmis, and Z.-F. Liu, “Interactions between a Dihydrogen Phosphate Ion and Water Molecules Probed by Infrared Multiphoton Dissociation Spectroscopy and First Principles Calculations”, *Phys. Chem. Chem. Phys.* **17** 25714–25724.

- C.T. Wolke, F.S. Menges, N. Totsch, O. Gorlova, J.A. Fournier, G.H. Weddle, M.A. Johnson, **N. Heine**, T.K. Esser, H. Knorke, K.R. Asmis, A.B. McCoy, "Thermodynamics of Water Dimer Dissociation in the Primary Hydration Shell of the Iodide Ion with Temperature-Dependent Vibrational Predissociation Spectroscopy", *J. Phys. Chem. A* **119** 1859–1866.
- N. Heine**, K.R. Asmis, "Cryogenic Ion Trap Vibrational Spectroscopy of Hydrogen-Bonded Clusters Relevant to Atmospheric Chemistry", *Int. Rev. Phys. Chem.* **34** 1–34.
- 2014 J.A. Fournier, C.T. Wolke, C.J. Johnson, M.A. Johnson, **N. Heine**, S. Gewinner, W. Schöllkopf, T.K. Esser, M.R. Fagiani, H. Knorke, K.R. Asmis, "Site-specific spectral signatures of water molecules in the "magic" $\text{H}_3\text{O}^+(\text{H}_2\text{O})_{20}$ and $\text{Cs}^+(\text{H}_2\text{O})_{20}$ clusters in the regions of the OH(D) stretches and low frequency librations ($215\text{--}1000\text{ cm}^{-1}$)", *Proc. Natl. Acad. Sci. USA* **111** 18132–7.
- G.B.S. Miller, T.K. Esser, H. Knorke, S. Gewinner, W. Schöllkopf, **N. Heine**, K.R. Asmis, E. Uggerud, "Spectroscopic Identification of a Bidentate Binding Motif in the Anionic Magnesium- CO_2 Complex ($[\text{ClMgCO}_2]^-$)", *Angew. Chem. Int. Ed.* **53** 14407–10.
- N. Heine**, E.G. Kratz, R. Bergmann, D.P. Schofield, K.R. Asmis, K.D. Jordan, A.B. McCoy, "Vibrational Spectroscopy of the Water-Nitrate Complex in the O-H Stretching Region", *J. Phys. Chem. A* **118** 8188–97.
- N. Heine**, T.I. Yacovitch, F. Schubert, C. Brieger, K.R. Asmis, D.M. Neumark, "Infrared Photodissociation Spectroscopy of Microhydrated Nitrate-Nitric Acid Clusters $\text{NO}_3^-(\text{HNO}_3)_m(\text{H}_2\text{O})_n$ ", *J. Phys. Chem. A* **118** 7613–22.
- L. Jiang, S.-T. Sun, **N. Heine**, J.-W. Liu, T.I. Yacovitch, T. Wende, Z.-F. Liu, D.M. Neumark, K.R. Asmis, "Large Amplitude Motion in Cold Monohydrated Dihydrogen Phosphate Anion $\text{H}_2\text{PO}_4^-(\text{H}_2\text{O})$: Infrared Photodissociation Spectroscopy combined with Ab Initio Molecular Dynamics Simulations", *Phys. Chem. Chem. Phys.* **16** 1314–1318.
- 2013 T.I. Yacovitch, **N. Heine**, C. Brieger, T. Wende, C. Hock, D.M. Neumark, and K.R. Asmis, "Vibrational Spectroscopy of Bisulfate/Sulfuric Acid/Water Clusters: Structure, Stability and IRMPD Intensities", *J. Phys. Chem. A* **117** 7081–7090.
- N. Heine**, M.R. Fagiani, M. Rossi, T. Wende, G. Berden, V. Blum, K.R. Asmis, "Isomer-Selective Detection of Hydrogen-Bond Vibrations in the Protonated Water Hexamer", *J. Am. Chem. Soc.* **135** 8266–8273.
- 2012 T.I. Yacovitch, **N. Heine**, C. Brieger, T. Wende, C. Hock, D.M. Neumark, K.R. Asmis, "Communication: Vibrational Spectroscopy of Atmospherically Relevant Acid Cluster Anions: Bisulfate versus Nitrate Core Structures", *J. Chem. Phys.* **136** 241102–(1–4).
- 2011 T.I. Yacovitch, T. Wende, L. Jiang, **N. Heine**, G. Meijer, D.M. Neumark, K.R. Asmis, "Infrared Spectroscopy of Hydrated Bisulfate Anion Clusters: $\text{HSO}_4^-(\text{H}_2\text{O})_{1-16}$ ", *J. Phys. Chem. Lett.* **2** 2135–2140.
- 2010 F. Buchner, A. Lübcke, **N. Heine**, T. Schultz, "Time-Resolved Photoelectron Spectroscopy of Liquids", *Rev. Sci. Instrum.* **81** 113107–113112 (2010).

A. Lübcke, F. Buchner, **N. Heine**, I.V. Hertel, T. Schultz, “Time-Resolved Photoelectron Spectroscopy of Solvated Electrons in Aqueous NaI Solution”, *Phys. Chem. Chem. Phys.* **12** 14629–14634.

Selected Conference and Seminar Presentations

- 2015 **American Association for Aerosol Research (AAAR): Annual Conference 2015.** “Formation of Highly Oxidized Multifunctional Organic Compounds in the OH-Initiated Heterogeneous Oxidation of Squalene under Environmental Conditions”, poster.
- 2014 **Gordon Research Conference: Molecular and Ionic Clusters.** “Structure and Microsolvation of Atmospheric Anions”, hot topic talk.
Deutsche Physiker Tagung. “Characterization of a 6 K Ring-Electrode Ion-Trap used for IR Photodissociation Experiments”, poster.
- 2013 **Institute for Atmospheric and Environmental Sciences, Goethe Universität Frankfurt.** “Vibrational Spectroscopy of Atmospherically Relevant Clusters”, invited talk.
Bunsentagung. “Vibrational Spectroscopy of Atmospherically Relevant Clusters: $\text{NO}_3^- (\text{HNO}_3)_m (\text{H}_2\text{O})_n$ ”, hot topic talk.
Deutsche Physiker Tagung. “Vibrational Spectroscopy of Atmospherically Relevant Cluster Anions: Mixed Clusters”, talk.
Deutsche Physiker Tagung. “A 6 K Ion Trap Triple Mass Spectrometer for Isomer-Selective IR/IR Photodissociation Experiments”, poster.
Symposium on Size Selected Cluster. “Vibrational Spectroscopy of Atmospherically Relevant Cluster Anions”, hot topic talk.
Symposium on Size Selected Cluster. “Isomer-Selective Double Resonance Spectroscopy: Isolating the Spectral Signatures of $\text{H}^+(\text{H}_2\text{O})_7$ Isomers”, poster.
- 2012 **European Aerosol Conference.** “Microhydration of Conjugate Base Anions Probed by Gas Phase Vibrational Spectroscopy ”, poster.
Deutsche Physiker Tagung. “Isomer-Selective IR/IR Double Resonance Spectroscopy: Isolating the Spectral Signatures of $\text{H}^+(\text{H}_2\text{O})_6$ Isomers”, talk.
Gordon Research Conference: Molecular and Ionic Clusters. “Isomer-Selective IR/IR Double Resonance Spectroscopy: Isolating the Spectral Signatures of $\text{H}^+(\text{H}_2\text{O})_6$ Isomers”, hot topic talk.
- 2011 **Clustertreffen.** “The Effect of Anharmonic Coupling on the IR Spectra of Microhydrated Nitrate Ions”, poster.
Deutsche Physiker Tagung. “The Effect of Anharmonic Coupling on the IR Spectra of Microhydrated Nitrate Ions”, talk.

List of References

Provided on request.