

DANIEL A. THOMAS

EDUCATION **California Institute of Technology; Pasadena, CA** **2010-2016**

Ph.D. Chemistry, Advisor: J. L. Beauchamp

Dissertation: "Chemical Reaction Dynamics of the Liquid/Vapor Interface Studied by Mass Spectrometry"

University of North Carolina at Chapel Hill; Chapel Hill, NC **2006-2010**

B.S. Chemistry, Advisor: Gary L. Glish

PROFESSIONAL **Assistant Professor of Chemistry** **2020-Present**
EXPERIENCE Department of Chemistry, University of Rhode Island

- Novel instrumentation for cold spectroscopy of ions
- Helium nanodroplet capture of molecular ions and ion clusters stored in an ion trap
- New reagents and methods for the characterization of biomolecular ions
- Investigations of interfacial ion chemistry, with application to atmospheric aerosols
- Spectroscopic interrogation of reaction intermediates captured in helium nanodroplets

Alexander von Humboldt Postdoctoral Fellow **2017-2020**

Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Advisors: Gert von Helden and Gerard Meijer

- Infrared spectroscopy of ions trapped in helium nanodroplets
- Structure and properties of proton-bound dimers, with focus on anharmonicity and nuclear quantum effects
- Spectroscopic interrogation of the reactions of the fluorine anion with carbon dioxide and water in the gas phase
- Variable-temperature infrared spectroscopy of biomolecular ions for thermochemical studies

Postdoctoral Researcher **2016-2017**

Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Advisors: Gert von Helden and Gerard Meijer

- Infrared spectroscopy of ions trapped in helium nanodroplets

Doctoral Researcher **2010-2016**

Division of Chemistry and Chemical Engineering, California Institute of Technology

Advisor: J. L. Beauchamp

- Analysis of chemical processes occurring at the liquid/vapor interface utilizing novel sampling methods coupled with mass spectrometry
- Fundamental studies of reagents for gas-phase free radical sequencing of biomolecules via mass spectrometry

Undergraduate Researcher**2008-2010**

Department of Chemistry, University of North Carolina at Chapel Hill

Advisor: Gary L. Glish

- Investigation of the mechanism of electron capture dissociation mass spectrometry (ECD-MS) in peptides containing histidine residues
- Experimental and theoretical investigation of axial pseudopotentials applied to linear ion traps for improved resolution and sensitivity in quadrupole time-of-flight mass spectrometers

**TEACHING AND
LEARNING****Instructor, CHM 532: Advanced Physical Chemistry****2022**

Department of Chemistry, University of Rhode Island

- Advanced graduate course covering topics including group theory, light-matter interactions, molecular beams, ion spectroscopy, and time-dependent spectroscopy.
- Emphasis on experimental approaches and interpretation of the research literature by applying concepts covered in the course.

Instructor, CHM 507: Graduate Quantum Chemistry**2020-2022**

Department of Chemistry, University of Rhode Island

- Graduate course for all incoming chemistry students, overview of quantum chemistry
- Run with a “flipped” classroom model, complete with notes featuring interactive modules and problems based on research applications

Instructor, CHM 642-644: Graduate Research Presentation**2021, 2023**

Department of Chemistry, University of Rhode Island

- Series of graduate seminar courses designed to develop research presentation skills

Participant, Strategies and Tools for Teaching Workshop**2020**

Office for the Advancement of Teaching and Learning, University of Rhode Island

- Five-day workshop covering best practices in teaching and learning, including course design; inclusive teaching; race, equity, and the learning environment; and effective assessment

Graduate Director, Caltech Project for Effective Teaching**2013-2016**

Center for Teaching, Learning, and Outreach, California Institute of Technology

- Administered certificate of interest program and associated seminar and workshop series to encourage graduate students and postdocs to investigate teaching strategies
- Developed and administered new certificate of practice program that guides participants in best practices in STEM teaching
- Served on the planning committee and for the annual Caltech teaching conference; directed sessions on teaching in laboratory courses (2013), microteaching (2014), and office hour sessions (2015)

Teaching Assistant, Physical Chemistry Laboratory**2010-2014**

Department of Chemistry, California Institute of Technology

- Experiments administered included microwave spectroscopy, 2D-NMR, ion trap mass spectrometry, low-energy electron diffraction, electron spin resonance, diode laser spectroscopy, and single-molecule spectroscopy

Teaching Assistant, Chemical Equilibrium and Analysis Laboratory**2013**

Department of Chemistry, California Institute of Technology

- Taught basic analytical skills including use of volumetric glassware, proper titration procedure, pH meter calibration and utilization, and UV-VIS absorption spectroscopy
- Assisted students in the development of independent projects utilizing standard analytical sample preparation along with HPLC-MS, ICP-MS, GC-MS, and GC-FID systems for sample analysis

Volunteer Tutor, UNC Chemistry Resource Center

2009-2010

Department of Chemistry, University of North Carolina at Chapel Hill

**STUDENT
MENTORSHIP**

Graduate Advisor

2020-2023

Department of Chemistry, University of Rhode Island

- Serving as advisor to four graduate students as of fall 2022

Undergraduate Research Advisor

2020-2023

Department of Chemistry, University of Rhode Island

- Serving as research advisor to three undergraduate students as of spring 2023

Participant, Inclusive Mentoring Workshop

2021

University of Rhode Island

- Six-session workshop covering best practices in mentoring, including effective communication, aligning expectations, equity and inclusion, and power and privilege

Undergraduate Research Mentor

2010-2015

Department of Chemistry, California Institute of Technology

- Served as mentor to ten summer undergraduate research fellows; facilitated project design and oversaw laboratory research

Participant - Research Mentor Development Series

2015

Center for Teaching, Learning, and Outreach, California Institute of Technology

- Attended effective mentoring workshops; topics included knowledge assessment, effective communication, equity and inclusion, and fostering independence

**SCIENCE
OUTREACH**

Community Science Event Volunteer

2015

Center for Teaching, Learning, and Outreach, California Institute of Technology

- Community science events highlight the research of a Caltech faculty member and connect this research to in-class activities for K-12 teachers that fulfill criteria in the next-generation science standards
- Prepared demonstrations of a cloud chamber, a homemade spectrophotometer for tablets and smartphones, and a photosynthesis laboratory activity for events focusing on physics, planetary science, and biology, respectively

High School Science Research Mentor

2013-2015

Department of Chemistry, California Institute of Technology

- Served as mentor to six students from local high schools performing scientific research in the Beauchamp group laboratory, both during the summer and throughout the academic year
- Projects undertaken include novel ionization sources, detection of neurotransmitters, analysis of energy drinks, sunscreen decomposition, and glycan analysis

RESEARCH
FUNDING

American Chemical Society Petroleum Research Fund, 65719-DNI6, “Unraveling the Structural Motifs of Deep Eutectic Solvents by Infrared Action Spectroscopy of Ionic Clusters”, \$110,000. 09/01/2022–08/31/2024

National Science Foundation, MPS Division, CHE-2212926, “LEAPS-MPS: Innovative Approaches to the Structural Characterization of Biomolecular Ions by Mass Spectrometry and Infrared Action Spectroscopy”, \$249,990. 09/01/2022–08/31/2024

HONORS AND
AWARDS

Alexander von Humboldt Postdoctoral Fellowship, 2017–2020

Graduate Mentoring Excellence Award, University of Rhode Island College of Arts and Sciences, 2022

PUBLICATIONS

Accepted Publications:

Schultz, M.; Parker, S. L.; Fernando, M. T.; Wellalage, M. M.; **Thomas, D. A.**, Diserinol Isophthalamide: A Novel Reagent for Complexation with Biomolecular Anions in Electrospray Ionization Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* **2023**, *34* (4), 745-753. <https://doi.org/10.1021/jasms.3c00010>

Taccone, M. I.; **Thomas, D. A.**; Ober, K.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G., Infrared action spectroscopy of the deprotonated formic acid trimer, trapped in helium nanodroplets. *Phys. Chem. Chem. Phys.* **2023**, *25* (15), 10907-10916. <https://doi.org/10.1039/D2CP05409D>

Mucha, E.; **Thomas, D.**; Lettow, M.; Meijer, G.; Pagel, K.; von Helden, G., Spectroscopy of Small and Large Biomolecular Ions in Helium-Nanodroplets. In *Molecules in Superfluid Helium Nanodroplets: Spectroscopy, Structure, and Dynamics*, Slenczka, A.; Toennies, J. P., Eds. Springer International Publishing: Cham, **2022**; pp. 241-280. https://doi.org/10.1007/978-3-030-94896-2_6

Thomas, D. A.; Taccone, M.; Ober, K.; Mucha, E.; Meijer, G.; von Helden, G. Helium Nanodroplet Infrared Action Spectroscopy of the Proton-Bound Dimer of Hydrogen Sulfate and Formate: Examining Nuclear Quantum Effects. *J. Phys. Chem. A*, **2021**, *125*, 9279–9287. <https://doi.org/10.1021/acs.jpca.1c05705>

Greis, K.; Mucha, E.; Lettow, M.; **Thomas, D. A.**; Kirschbaum, C.; Moon, S.; Pardo-Vargas, A.; von Helden, G.; Meijer, G.; Gilmore, K.; Seeberger, P. H.; Pagel, K. The Impact of Leaving Group Anomericity on the Structure of Glycosyl Cations of Protected Galactosides. *ChemPhysChem*, **2020**, *21*, 1905–1907. <https://doi.org/10.1002/cphc.202000473>

Lettow, M.; Grabarics, M.; Greis, K.; Mucha, E.; **Thomas, D. A.**; Chopra, P.; Boons, G.-J.; Karlsson, R.; Turnbull, J. E.; Meijer, G.; Miller, R. L.; von Helden, G.; Pagel, K. Cryogenic Infrared Spectroscopy Reveals Structural Modularity in the Vibrational Fingerprints of Heparan Sulfate Diastereomers. *Anal. Chem.* **2020**, *92*, 10228–10232. <https://doi.org/10.1021/acs.analchem.0c02048>

Thomas, D. A.; Chang, R.; Mucha, E.; Lettow, M.; Greis, K.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G. Probing the Conformational Landscape and Thermochemistry of DNA Dinucleotide Anions *via* Helium Nanodroplet Infrared Action Spectroscopy. *Phys. Chem. Chem. Phys.* **2020**, *22*, 18400–18413. <https://doi.org/10.1039/D0CP02482A>

Lettow, M.; Grabarics, M.; Mucha, E.; **Thomas, D. A.**; Polewski, L.; Freyse, J.; Rademann, J.; Meijer, G.; von Helden, G.; Pagel, K. IR Action Spectroscopy of Glycosaminoglycan

Oligosaccharides. *Anal. Bioanal. Chem.* **2020**, *412*, 533–537. <https://doi.org/10.1007/s00216-019-02327-7>

Marianski, M.; Mucha, E.; Greis, K.; Moon, S.; Pardo, A.; Kirschbaum, C.; **Thomas, D. A.**; Meijer, G.; von Helden, G.; Gilmore, K.; Seeberger, P. H.; Pagel, K. Remote Participation during Glycosylation Reactions of Galactose Building Blocks: Direct Evidence from Cryogenic Vibrational Spectroscopy. *Angew. Chem., Int. Ed.* **2020**, *59*, 6166–6171. <https://doi.org/10.1002/anie.201916245>

Fabijanczuk, K.; Gaspar, K.; Desai, N.; Lee, J.; **Thomas, D. A.**; Beauchamp, J. L.; Gao, J. Resin and Magnetic Nanoparticle-Based Free Radical Probes for Glycan Capture, Isolation, and Structural Characterization. *Anal. Chem.* **2019**, *91*, 15837–15396. <https://doi.org/10.1021/acs.analchem.9b01303>

Thomas, D. A.; Mucha, E.; Lettow, M.; Meijer, G.; Rossi, M.; von Helden, G. Characterization of a trans–trans Carbonic Acid–Fluoride Complex by Infrared Action Spectroscopy in Helium Nanodroplets. *J. Am. Chem. Soc.* **2019**, *141*, 5815–5823. <http://dx.doi.org/10.1021/jacs.8b13542>

Lettow, M.; Mucha, E.; Manz, C.; **Thomas, D. A.**; Marianski, M.; Meijer, G.; von Helden, G.; Pagel, K. The Role of the Mobile Proton in Fucose Migration. *Anal. Bioanal. Chem.* **2019**, *411*, 4637–4645. <http://dx.doi.org/10.1007/s00216-019-01657-w>

Marianski, M.; Seo, J.; Mucha, E.; **Thomas, D. A.**; Jung, S.; Schlögl, R.; Meijer, G.; Trunschke, A.; von Helden, G. Structural Characterization of Molybdenum Oxide Nanoclusters Using Ion Mobility Spectrometry–Mass Spectrometry and Infrared Action Spectroscopy. *J. Phys. Chem. C* **2019**, *123*, 7845–7853. <http://dx.doi.org/10.1021/acs.jpcc.8b06985>
Hans-Joachim Freund and Joachim Sauer Festschrift Issue

Mucha, E.; Marianski, M.; Xu, F.-F.; **Thomas, D. A.**; Meijer, G.; von Helden, G.; Seeberger, P. H.; Pagel, K. Unraveling the Structure of Glycosyl Cations via Cold-Ion Infrared Spectroscopy. *Nat. Commun.* **2018**, *9*, 4174. <http://dx.doi.org/10.1038/s41467-018-06764-3>

Thomas, D. A.; Marianski, M.; Mucha, E.; Meijer, G.; Johnson, M. A.; von Helden, G. Ground-State Structure of the Proton-Bound Formate Dimer by Cold-ion Infrared Action Spectroscopy. *Angew. Chem., Int. Ed.* **2018**, *57*, 10615–10619. <http://dx.doi.org/10.1002/anie.201805436>

Mucha, E.; Lettow, M.; Marianski, M.; **Thomas, D. A.**; Struwe, W. B.; Harvey, D. J.; Meijer, G.; Seeberger, P. H.; von Helden, G.; Pagel, K. Fucose Migration in Intact Protonated Glycan Ions: A Universal Phenomenon in Mass Spectrometry. *Angew. Chem., Int. Ed.* **2018**, *57*, 7440–7443. <http://dx.doi.org/10.1002/anie.201801418>

Thomas, D. A.; Mucha, E.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G. Vibrational Spectroscopy of Fluoroformate, FCO_2^- , Trapped in Helium Nanodroplets. *J. Phys. Chem. Lett.* **2018**, *9*, 2305–2310. <http://dx.doi.org/10.1021/acs.jpclett.8b00664>

Mucha, E.; González Flórez, A. I.; Marianski, M.; **Thomas, D. A.**; Hoffmann, W.; Struwe, W. B.; Hahn, H. S.; Gewinner, S.; Schöllkopf, W.; Seeberger, P. H.; von Helden, G.; Pagel, K. Glycan Fingerprinting via Cold-Ion Infrared Spectroscopy. *Angew. Chem., Int. Ed.* **2017**, *56*, 11248–11251. <http://dx.doi.org/10.1002/anie.201702896>

Thomas, D. A.*; Coggon, M. M.*; Lignell, H.; Schilling, K. A.; Zhang, X.; Schwantes, R. H.; Flagan, R. C.; Seinfeld, J. H.; Beauchamp, J. L. Real-Time Studies of Iron Oxalate-Mediated Oxidation of Glycolaldehyde as a Model for Photochemical Aging of Aqueous Tropospheric Aerosols. *Environ. Sci. Technol.* **2016**, *22*, 12241–12249. <http://dx.doi.org/10.1021/acs.est.6b03588>

*Authors contributed equally

- Desai, N.; **Thomas, D. A.**; Lee, J.; Gao, J.; Beauchamp, J. L. Eradicating Mass Spectrometric Glycan Rearrangement by Utilizing Free Radicals. *Chem. Sci.* **2016**, *7*, 5390-5397. <http://dx.doi.org/10.1039/C6SC01371F>
- Sohn, C. H.; Gao, J.; **Thomas, D. A.**; Kim, T.-Y.; Goddard III, W. A.; Beauchamp, J. L. Mechanisms and Energetics of Free Radical Initiated Disulfide Bond Cleavage in Model Peptides and Insulin by Mass Spectrometry. *Chem. Sci.*, **2015**, *6*, 4550-4560. <http://dx.doi.org/10.1039/C5SC01305D>
- Thomas, D. A.**; Wang, L.; Goh, B.; Kim, E. S.; Beauchamp, J.L. Mass Spectrometric Sampling of a Liquid Surface by Nanoliter Droplet Generation from Bursting Bubbles and Focused Acoustic Pulses: Application to Studies of Interfacial Chemistry. *Anal. Chem.* **2015**, *87*, 3336-3344. <http://dx.doi.org/10.1021/ac504494t>
- Thomas, D. A.**; Sohn, C. H.; Gao, J.; Beauchamp, J. L. Hydrogen Bonding Constrains Free Radical Reaction Dynamics at Serine and Threonine Residues in Peptides. *J. Phys. Chem. A* **2014**, *118*, 8380-8392. <http://dx.doi.org/10.1021/jp501367w>
A. W. Castleman, Jr. Festschrift Issue
- Gao, J.; **Thomas, D. A.**; Sohn, C. H.; Beauchamp, J. L. Biomimetic Reagents for the Selective Free Radical and Acid–Base Chemistry of Glycans: Application to Glycan Structure Determination by Mass Spectrometry. *J. Am. Chem. Soc.* **2013**, *135*, 10684-10692. <http://dx.doi.org/10.1021/ja402810t>
- Mui, W.; **Thomas, D. A.**; Downard, A. J.; Beauchamp, J. L.; Seinfeld, J. H.; Flagan, R. C. Ion Mobility-Mass Spectrometry with a Radial Opposed Migration Ion and Aerosol Classifier (ROMIAC). *Anal. Chem.* **2013**, *85*, 6319-6326. <http://dx.doi.org/10.1021/ac400580u>

**CONFERENCE
PRESENTATIONS**

- New anion microsolvation reagents for the study of biomolecular ions in vacuum. M. Schultz, S. L. Parker, M. T. Fernando, M. M. Wellalage, **D. A. Thomas**. ACS Spring 2023, Indianapolis, IN, 2023. *Invited Oral Presentation*.
- Probing the Conformational Landscape and Thermochemistry of Dinucleotide Anions via Helium Nanodroplet Infrared Action Spectroscopy. **D. A. Thomas**, R. Chang, E. Mucha, M. Lettow, K. Greis, G. Meijer, and G. von Helden. International Symposium on Molecular Spectroscopy, Champaign, IL, 2021. *Oral Presentation (Virtual)*.
- Characterization of the Intriguing Products of Fluoride-Carbon Dioxide Chemistry by Helium Nanodroplet Infrared Action Spectroscopy. **D. A. Thomas**, E. Mucha, M. Lettow, M. Rossi, G. Meijer, and G. von Helden. GRC Conference on Gaseous Ions, Ventura, CA, 2019. *Poster Presentation*.
- Investigating Structure and Thermochemistry of Molecular Ions Using Infrared Action Spectroscopy in He Nanodroplets. **D. A. Thomas**, R. Chang, E. Mucha, G. Meijer, and G. von Helden. GRC Conference on Vibrational Spectroscopy, Biddeford, ME, 2018. *Poster Presentation*.
- Infrared Spectroscopy of Ions Trapped in Helium Nanodroplets: From Baroque Biomolecules to Curious Carboxylates. **D. A. Thomas**, E. Mucha, M. Marianski, S. Gewinner, W. Schöllkopf, G. Meijer, and G. von Helden. Applications of IR Free-Electron Lasers: Latest Developments and Future Directions, Ringberg, Germany, 2018. *Invited Oral Presentation*.
- Vibrational Spectroscopy of Ions Trapped in Helium Nanodroplets: Application to the Analysis of Biomolecules. **D. A. Thomas**, E. Mucha, A. I. González Flórez, K. Pagel, and G. von Helden. Conference on Quantum Fluid Clusters, Innsbruck, Austria, 2017. *Poster Presentation*.

- Exploring Photochemical Oxidation in Liquid Droplets Using Field-Induced Droplet Ionization Mass Spectrometry. **D. A. Thomas** and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2016. *Oral Presentation.*
- A Peer-led Teaching Certificate Program for Post-Graduate STEM Education. **D. A. Thomas**, K. Boyle, and H. Ferguson, POD Network Conference, San Francisco, CA 2015. *Poster Presentation.*
- Finding Sweet Spots in Proteins: Glycan Analysis by Liquid Chromatography Coupled with Gas-Phase Proton-Catalyzed and Free Radical-Initiated Dissociation. **D. A. Thomas**, L. Chen, Jinshan Gao, and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2015. *Poster Presentation.*
- Generating Ions from Droplets without Electric Fields: Mass Spectrometry of Droplets Acoustically Ejected from a Liquid Surface. **D. A. Thomas**, L. Wang, E. S. Kim, and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2014. *Oral Presentation.*
- Studying the Environmental Chemistry of the Liquid/Vapor Interface Using Novel Ionization Techniques Coupled with Mass Spectrometry. **D. A. Thomas**, L. Wang, B. Goh, K. M. Barraza, E. S. Kim, and J. L. Beauchamp, Asilomar Conference on Mass Spectrometry in Environmental Chemistry, Toxicology, and Health, Asilomar, CA, 2013. *Poster Presentation.*
- A Bursting Bubble that Won't Ruin Your 401(k): Sampling the Air-Water Interface with Bursting Bubble Ionization. **D. A. Thomas**, B. Goh, and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2013. *Oral Presentation.*
- Monitoring the Effect of pH Changes on Chemical and Biological Processes at the Air/Water Interfaces Using Field-Induced Droplet Ionization Mass Spectrometry, **D. A. Thomas** and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2012. *Oral Presentation.*
- Hydrogen Bonding Constraints Lead to Unusual Free Radical Chemistry at Serine and Threonine Residues in Peptides, **D. A. Thomas**, C. H. Sohn, and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2011, *Oral Presentation.*
- Study of Radical z Ions Produced by Electron Capture Dissociation (ECD). **Daniel A. Thomas**, N. J. Thompson, T. Baba, and G. L. Glish, American Society for Mass Spectrometry Annual Conference, Salt Lake City, UT, 2010. *Poster Presentation.*
- Probing Electron Capture Dissociation (ECD) Charge Reduced Ions using ECD and Collision-Induced Dissociation (ECD/ECD and ECD/CID). **Daniel A. Thomas**, T. Baba, and G. L. Glish, American Society for Mass Spectrometry Annual Conference, Philadelphia, PA, 2009. *Poster Presentation.*