Contact Information

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Professional Preparation

University of California – Berkeley	Berkeley, CA	Ph.D., Theoretical Chemistry	2008
Iowa State University	Ames, IA	B.S. with distinction, Chemistry	2003

Scientific Appointments

Associate Professor — July 2017 –
Department of Chemistry, University of Utah

Assistant Professor — Aug 2011 – June 2017
Department of Chemistry, University of Utah

Post-Doctoral Associate — Aug 2008 – Jul 2011
Department of Chemistry, Yale University
Research group of Prof. John Tully

Graduate Research Assistant — Aug 2003 – Aug 2008
Department of Chemistry, University of CA – Berkeley
Research group of Prof. Martin Head-Gordon
Thesis: *Dual-Basis Methods for Electronic Structure Theory*

Graduate Student Instructor — Fall 2003, 2004, Spring 2006
Department of Chemistry, University of CA – Berkeley

Undergraduate Research Associate — May – Aug 2002
Georgia Institute of Technology
Research group of Prof. C. David Sherrill

Undergraduate Research Associate — Aug 2002 – May 2003
Iowa State University
Research group of Prof. William S. Jenks

Teaching Assistant — Aug 2002 – May 2003
Iowa State University

Students Mentored

Post-Doctoral Researchers

1. Xiaolu Cheng Fall 2013 – Fall 2017
   New methods for anharmonic vibrational spectroscopy
2. Shervin Fatehi Fall 2013 – Summer 2015
   Multiple-timestep ab initio molecular dynamics
   Currently an assistant professor at the University of Texas – Rio Grande Valley

Graduate Students

1. Jonathan Herr Summer 2012 – Fall 2016
   Water oxidation, Dynamics Methods
2. Nicholas Corbett Spring 2013 – Fall 2015
   Nanoparticle catalysis, Sampling methods
   Currently employed as Quality Engineer at Ultradent
3. Justin Talbot Summer 2014 – Fall 2019
   Oxidized water clusters, Anharmonic vibrational methods, Dynamics methods
   Currently a post-doctoral researcher at UC-Berkeley
4. Diana Reese Summer 2014 – (Defending Spring 2020)
   Metal-dihydrogen complexes and catalysis
   Currently a professor at Dixie State University
5. Elizabeth Christensen Fall 2016 -
   Open-shell water clusters
6. Gabe McDonald Fall 2018 -
   Vibrational Spectroscopy Simulations
7. Asylbek (AJ) Zhanserkeev Fall 2018 -
   Ab Initio Molecular Dynamics
8. Ryan J. Spencer Fall 2020 -
   Reactive Clusters

Undergraduate Students

1. Justin Talbot Fall 2011 – Summer 2014
   Oxidized water clusters, Anharmonic vibrational methods
   Currently a post-doctoral researcher at UC-Berkeley
2. Tyler Rasmussen Summer 2012 -
   Si-H bond activation and the role of electron donation in N-heterocyclic carbenes
   Currently employed at AnvilCorp (Bellingham, WA)
3. Maggie Reid Summer 2012 – Fall 2013
   Hydroxyl radical solvation clusters
   Currently attending graduate school (Tufts)
4. Jordan Meadows Summer 2012 – Fall 2013
   Substituent electron effects on nuclear tunneling in substituted alcohols
   Currently employed by University of Utah Pharmacy

5. Annie Bench Summer 2012 – Summer 2013
   Mechanisms of proton transfer in doubly hydrogen bonded anions
   Currently substitute teaching high school science (Arizona), followed by additional school
6. Zephyr Glass Summer 2012 – Summer 2012
   Hydration effects in water reduction catalysts
7. Justin Park Fall 2012 – Spring 2013
   Cluster models of the second oxidation of water [$OH(H_2O)_n$ ionization]
   Attending graduate school (BYU)
8. Brandon Mitchell Summer 2012 – Spring 2014
   Nuclear motion in hydrogen-storage and σ transition metal complexes
   Currently employed at IM Flash (Lehi, UT)
9. Joemy Ramsay Summer 2012 – Fall 2013
   Mixed time-slicing in path integral methods, H defects in Si
   Currently attending graduate school (Washington)
10. Doo-Hyun Kwon Fall 2012 – Spring 2014
    Hydration effects in water reduction catalysts
    Currently Attending graduate school (BYU)
11. William Gleich Fall 2014 – Spring 2015
    Li^+-water complexes and basis set optimization
    Currently employed at Myriad Genetics (Salt Lake City, UT)
12. Sarah Floris Summer 2015 – Spring 2016
    (REU student, Abilene Christian University)
    Oxidized, mixed water and hydrogen sulfide clusters
    Attending graduate school (Washington) Fall 2016
13. Matthew Wilkinson Summer 2015 –
    Oxidized hydrogen sulfide clusters
    Currently a master's student in Data Science at UVU
14. Jennifer Chlam Summer 2017
    Vibrational spectra of biomolecules
15. Jessica Schulze Spring 2017 – Summer 2017
    Metal-H_2 complexes
16. MacKenzie Ferron Summer 2017
    Metal-H_2 complexes
17. Emily Yang Summer 2019 –
    Vibrational spectra of homatropine analogues
18. Kevin Lutz Spring 2019 –
    Vibrational spectra of metal ion-water complexes

Society Memberships

American Chemical Society
American Physical Society (currently inactive)
American Association for the Advancement of Science (currently inactive)

Honors & Awards

Since 2011
Robert W. Parry Teaching Award, 2019
PCCP Emerging Investigator Lectureship, 2017
Award for Fostering Undergraduate Research Excellence, University of Utah, 2017
ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, 2016
NSF CAREER, 2015
Surface-Hopping Symposium Outstanding Junior Faculty Presentation (ACS San Diego) 2012
ASUU Student Choice Teaching Award 2012

Prior to 2011
Teaching Effectiveness Award 2007 (1 of 13 University-wide)
Outstanding Graduate Student Instructor 2006
Berkeley Travel Award 2006
The Phi Beta Kappa Society
The Honor Society of Phi Kappa Phi
Mortar Board Honor Society
Golden Key International Honour Society
Tau Beta Pi Engineering Honor Society
Iowa State University Senior Chemistry Student of the Year
National Merit Scholar

Journals Refereed

Journal of Chemical Physics
Journal of Physical Chemistry
Journal of the American Chemical Society
Physical Chemistry Chemical Physics
Journal of Chemical Theory and Computation
Journal of Computational Chemistry
Computational and Theoretical Chemistry
Journal of the Electrochemical Society
Molecular Physics
Chemical Physics Letters
International Journal of Quantum Chemistry
Accounts of Chemical Research
Scientific Reports
Proceedings of the National Academy of Sciences

Granting Agencies Refereed

American Chemical Society Petroleum Research Fund (ACS PRF)
Air Force Office of Scientific Research (AFOSR)
National Science Foundation (NSF)

Department of Energy (DOE)

Software Development

Main development within the *Q-Chem* software package (also the back-end program for *Spartan*)

Outreach & Service Activities

Executive Committee Member-at-Large, American Chemical Society (2019-)
Advisory Board, Advancing Mass Spectrometry Conference (2017-)
Co-coordinator, ACS Phys Symposium,
Frontiers in Vibrational Spectroscopy: Theory & Experiment (Orlando, Spring 2019)
Co-coordinator, Utah Quantum Workshop (Park City, Sep 2019)
Co-coordinator, "A Celebration of the First 70 Years of Jack Simons" (Apr 2015)
Co-coordinator, Q-Chem Developers Conference (Philadelphia, Aug 2012)
UofU semi-annual high school teachers' workshop presentation (Sep 2016)
UofU STEM Student Outreach & Engagement, Presentation organized by graduate student JD Herr (Spring 2016)
Science Demonstrations, Edison Elementary School
Judge, Edison Elementary School Science Fair
Judge, Salt Lake Valley Science Fair
"Wonderful World of Quantum Mechanics" Presenter, University of Utah Science Day 2012
Event Coordinator, "Crime Busters" Event, Utah Science Olympiad, 2012, 2013

Committee Service

Department
Undergraduate education committee (2019-)
Teaching mentoring committee (2016-)
Chair, Physical Chemistry Division (2017-)
Graduate recruiting committee (2017-2018)
Graduate admissions committee (2011-2016, 2018)
Physical chemistry seminar coordinator (2011-2016)
Faculty search committee (2011-2012, 2018)

University
Faculty Senate (2019-)
College of Science Council (2018-2020)
College of Science Representative – Teaching and Learning Portfolio committee (2015-)
Crocker Science Curriculum Committee (2018-2019)
Center for High-Performance Computing allocation committee (2014-)
Undergraduate Council (2014-2016)
One Network planning committee (2014)

Presentations, Posters, Conferences

Upcoming

International Invited Talk: World Association of Theoretically Oriented Chemists (WATOC), Vancouver, BC (Aug 2020) [Postponed to 2022]

Invited Talk: Dept of Chemistry, Innsbruck University (June 2021)

Since Aug 2011

73. Invited Talk: *Spectral Signatures of Water Activation by Ions & Radicals*, Idaho State University, Virtual Seminar (Oct 2020)
72. Invited Talk: Department of Energy CTC Meeting (May 2020)
71. Invited Talk: *Spectral Signatures of Water Activation by Ions & Radicals*, Gordon Research Conference ("Molecular & Ionic Clusters"), Ventura, CA (Jan 2020)
70. Invited Talk: *Spectral Signatures of Water Activation by Ions & Radicals*, Utah Quantum Workshop, Park City, UT (Sep 2019)
69. Invited Talk: *Spectral Signatures of Water Activation by Ions & Radicals*, Dynamics of Molecular Collisions, Big Sky, MT (Aug 2019)
68. Poster: Department of Energy CTC Meeting, Gaithersburg, MD (May 2019)
67. Recruiting talk: University of Nebraska – Kearney (Oct 2018)
66. Invited Award Lectureship: EuCheMS Conference, Liverpool, UK (Aug 2018)
65. Invited talk: Gordon Research Conference ("Vibrational Spectroscopy"), Biddeford, ME (Jul 2018)
64. Student invited talk: TheoChem@Boston seminar series – Harvard, MIT, and Boston Universities (Feb 2018)
63. Invited talk: Sanibel Symposium ("Computational Modelling in Mass Spectrometry and Ion Mobility: Methods for Ion Structure and Reactivity Determination") St. Petersburg, FL, Jan 2018
62. Invited talk: Telluride Science Research Center ("New Challenges for Theory in Chemical Dynamics"), Telluride, CO, Jan 2018
61. International Invited talk: Tandem Mass Spectrometry Workshop, Lake Louise, Alberta, Canada, Nov 2017
60. Invited talk: *Quantum Chemistry Approaches for Simulating the Spectroscopy and Dynamics of Biomolecules*, Advancing Mass Spectrometry, Ann Arbor, MI, Jul 2017.
59. Invited talk: *Exploiting Locality for Anharmonic Vibrational Spectroscopy Simulations*, Telluride Science Research Center ("Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Systems"), Telluride, CO, Jul 2017.
58. Invited Conference Session Introduction: Dynamics of Molecular Collisions, Tahoe, CA, Jul 2017.
57. Recruiting talk: Northern Arizona University, *Quantum Chemistry and Molecular Motion* Nov 2016.
56. Recruiting talk: Ft. Lewis College, *Quantum Chemistry and Molecular Motion* Nov 2016.
55. Invited workshop: University of Pittsburgh, *Computational Approaches to Anharmonic Vibrational Spectroscopy* Nov 2016.
54. Invited talk: University of Pittsburgh, *Vibrational Signatures of Electronic Properties in Energy and Biology*, Nov 2016.
53. Invited talk: University of North Carolina, *Vibrational Signatures of Electronic Properties in Energy and Biology* Sept 2016.
52. Invited talk: Duke University, *Vibrational Signatures of Electronic Properties in Energy and Biology* Sept 2016.
51. *Vibrational Signatures of Electronic Properties in Energy and Biology* University of Utah (tenure seminar), Sept 2016.
50. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology* International Society for Theoretical Chemical Physics ("Complex Systems" symposium), Grand Forks, ND, Jul 2016.
49. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology* American Chemical Society

PHYS Division Symposium ("Decoding the spectroscopic signatures of large-amplitude motions: Challenges and opportunities for theory and experiment"), San Diego, CA, Mar 2016.

48. ACS OpenEye Award Poster: *Accelerating Ab Initio Simulations of Molecular Motion* American Chemical Society COMP Division Symposium, San Diego, CA, Mar 2016.
47. International Invited talk: *Reliable Computational Approaches for Vibrational Spectra of Biomolecules* Isolated Biomolecules and Biomolecular Interactions Conference (IBBI16) Oxford, UK Apr 2016.
46. Invited talk: University of Washington, *Vibrational Signatures of Electronic Properties in Energy and Biology*, May 2015.
45. Invited talk: Purdue University, *Vibrational Signatures of Electronic Properties in Energy and Biology*, Feb 2015.
44. Invited talk: Notre Dame University, *Vibrational Signatures of Electronic Properties in Energy and Biology*, Feb 2015.
43. Invited talk: University of Georgia, *Vibrational Signatures of Electronic Properties in Energy and Biology*, Jan 2015.
42. Invited talk: University of Kansas, *Vibrational Signatures of Electronic Properties in Energy and Biology*, Nov 2015.
41. Invited talk: *Ab Initio Molecular Motion and Ionized Water*, US National Institutes of Health (Computational Biophysics Group), Nov 2015.
40. Invited talk (Students' Choice Invitation): *Vibrational Signatures of Electronic Properties in Energy and Biology*, The Ohio State University, Nov 2015.
39. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology*, University of California – San Diego, Oct 2015.
38. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology*, University of California – Los Angeles, Oct 2015.
37. Invited talk: *Ab Initio Molecular Motion and Ionized Water*, University of Southern California, Oct 2015.
36. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology*, California Institute of Technology, Oct 2015.
35. Invited talk: *Ab Initio Molecular Motion and Ionized Water*, University of Illinois – Urbana-Champaign, Oct 2015.
34. Invited talk: *Ab Initio Molecular Motion and Ionized Water*, Iowa State University, Sept 2015.
33. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology*, Kansas State University, Sept 2015.
32. Recruiting talk: *Quantum Chemistry & Molecular Motion*, University of Nebraska – Omaha, Sept 2015.
31. Invited talk: *Vibrational Signatures of Electronic Properties in Energy and Biology*, University of Nebraska – Lincoln, Sept 2015.
30. International Invited talk: *Exploring the Interface of Electronic Structure and Molecular Motion*, IUPAC Congress, Busan, South Korea, Aug 2015.
29. International Invited talk: *New Ab Initio Approaches to Vibrational Spectroscopy*, Mueunjae Symposium on "Chemistry and Light", Mueunjae Institute, POSTECH, South Korea, Aug 2015.
28. Invited talk: American Chemical Society PHYS Division Symposium ("Electronic Structure Theory for Large Systems"), Boston Aug 2015.
27. Invited talk: Q-Chem Developers Meeting, Boston Aug 2015.
26. International Invited talk: *Exploiting the Length- and Timescales of Molecular Interactions* Modeling Many-Body Interactions (MMBI15), Lake Garda House, Italy May 2015.
25. Contributed talk: *Advancing Ab Initio Molecular Dynamics via Multiple-Timestep Methods* American Chemical Society PHYS Division Symposium ("Computational Chemical Dynamics: Advancing our understanding of chemical processes in gas-phase, biomolecular, and condensed-phase systems: A symposium in honor of Donald Truhlar"), Denver, CO, Mar 2015.
24. Invited talk: *Anomalous Vibrational Signatures of Ions and Solvation* American Physical Society National Meeting

("Solvation of Ions and Electrons" Symposium) San Antonio, TX, Mar 2015.

23. Invited talk: *New Ab Initio Approaches to Ion Spectroscopy* Gaseous Ions Gordon Research Conference, Galveston, TX, Mar 2015.
22. Invited talk: *New Computational Techniques for Biomolecular Interactions* Mesilla Chemistry Workshop ("Isolated Biomolecules and Biomolecular Interactions: From the Gas Phase and Towards Solution"), Mesilla, NM, Feb 2015.
21. Invited talk: *Quantum Molecular Motion in Energy and Biology* Wayne State University, Detroit, MI, Nov 2014.
20. Contributed talk: *Vibrational Signatures of Electronic Motion in Oxidized Water.* American Chemical Society PHYS Division Symposium ("Renewable Energy Generation at the Interface Between Theory and Experiment"), San Francisco, CA, Aug 2014.
19. Contributed talk: *Exploring the Interface of Electronic Structure Theory and Chemical Dynamics.* American Chemical Society PHYS Division Symposium ("The Future of Computational Chemistry"), San Francisco, CA, Aug 2014.
18. Contributed talk: *New Approaches to Anharmonic Vibrational Spectroscopy in Large Molecules.* American Chemical Society COMP Division Symposium ("Computational Spectroscopy"), San Francisco, CA, Aug 2014.
17. Invited talk: *Vibrational Signatures of Electronic Motion in Oxidized Water*, International Conference on Chemical Bonding, Kauai, HI, Jul 2014.
16. Invited talk: *New Ab Initio Approaches for Spectroscopy & Dynamics*, Telluride Science Research Center Conference ("Spectroscopy and Dynamics on Multiple Potential Energy Surfaces"), Telluride, CO, Jul 2014.
15. "Hot Topics" Talk: *New Ab Initio Approaches for Spectroscopy & Dynamics*, Gordon Research Conference ("Atomic & Molecular Interactions"), Stonehill, MA, Jul 2014.
14. Invited Honorarium talk: *Spectroscopy & Dynamics with Electronic Structure Theory,* Chemistry Collaborations, Workshops, and Communities of Scholars (cCWCS), Westminster College, Salt Lake City, UT, Jun 2014.
13. Contributed talk: *Accelerated Ab Initio Sampling and Dynamics.* American Chemical Society COMP Division Symposium ("Quantum Chemistry"), Dallas, TX, Mar 2014.
12. Contributed talk: *Signatures of Nuclear and Electronic Motion in Oxidized Water Clusters.* American Chemical Society PHYS Division Symposium ("A little insight goes a long way: A transformative role of theory in spectroscopy"), Dallas, TX, Mar 2014.
11. Contributed talk: *Multiple-Timestep Ab Initio Molecular Dynamics.* American Chemical Society PHYS Division Symposium ("Quantum Mechanics in Many Dimensions), Indianapolis, IN, Sep 2013.
10. Invited talk: *Innovative Approaches to Ab Initio Dynamics and Sampling.* Q-Chem Developers Conference, Indianapolis, IN, Sep 2013.
9. Invited talk: *Accelerated Ab Initio Dynamics and Quantum Sampling.* Telluride Science Research Center Conference ("Quantum Effects in Condensed-Phase Systems"), Telluride, CO, July 2013.
8. Invited talk: *Structure & Dynamics of Water Oxidation.* University of Wisconsin Theoretical Chemistry Institute Seminar Series, Madison, WI, Mar 2013.
7. Recruiting talk: *Structure & Dynamics of Water Oxidation.* BYU-Idaho, Rexburg, ID, Nov 2012.
6. Recruiting talk: *Structure & Dynamics of Water Oxidation.* Southern Utah University, Cedar City, UT, Nov 2012.
5. Recruiting talk: *Structure & Dynamics of Water Oxidation.* University of St. Thomas, St. Paul, MN, Sept 2012.
4. Contributed talk: *Lack-of-electron transfer in water oxidation.* American Chemical Society PHYS Division Symposium ("Electron and Energy Transfer Phenomena"), Philadelphia, PA, Aug 2012.
3. Invited talk: *Beyond Critical Points: Sampling & Dynamics in Q-Chem.* Q-Chem Developers Conference, Philadelphia, PA, Aug 2012.
2. Invited talk: *Fully Quantum Chemistry with Ab Initio Path Integrals.* Telluride Science Research Center Conference ("Spectroscopy and Dynamics on Multiple Potential Energy Surfaces"), Telluride, CO, July 2012.
1. Invited talk: *Fully Quantum Chemistry with Ab Initio Path Integrals.* American Chemical Society PHYS Division Symposium ("Nonadiabatic Dynamics: Surface-hopping and beyond"), San Diego, CA, Mar 2012.

Before Aug 2011

Contributed talk: *The Quantum, Thermal Structure of Protonated Methane and its Isotopologues.* Dynamics of Molecular Collisions Conference, Snowbird, UT, Jul 2011.

Invited talk: *Protons: Nature's Nomads.* Virginia Tech, Blacksburg, VA, Feb 2011.

Invited talk: *Protons: Nature's Nomads.* University of Utah, Salt Lake City, UT, Jan 2011.

Invited talk: *Protons: Nature's Nomads.* University of Washington, Seattle, WA, Jan 2011.

Invited talk: *Protons: Nature's Nomads.* University of Hawaii, Honolulu, HI, Dec 2010.

Invited talk: *Fully Quantum Chemistry: Mechanisms of chemical and biological energy conversion.* Notre Dame University, South Bend, IN, Nov 2010.

Invited talk: *Protons: Nature's Nomads.* Cornell University, Ithaca, NY, Nov 2010.

Poster: *The quantum structure of protonated methane (CH_5^+).* Gordon Research Conference: Atomic and Molecular Collisions, New London, NH, Jul 2010.

Invited talk: *Protons: Nature's Nomads.* University of Alabama, Tuscaloosa, AL, Feb 2009.

Invited talk: *A riddle from the ionosphere reveals how water activation is controlled by the shape of an H-bonded network.* NSF/PIRE Workshop, Pisa, Italy, Jul 2009.

Poster: *Atmospheric water network activation: Delocalized protons and charge migration in $NO^+(H_2O)_{n=1-4}$ clusters.* Dynamics of Molecular Collisions, Snowbird, UT, Jul 2009.

Talk: *Dual basis methods: Energies, derivatives, and non-covalent interactions.* ACS National Meeting, New Orleans, LA, Apr 2008.

Poster: *Cation-π interactions in fullerene systems.* ACS National Meeting, New Orleans, LA, Apr 2008.

Talk: *Circumventing the basis set bottleneck: Dual-basis methods for non-covalent interactions.* MRS National Meeting, San Francisco, CA, Mar 2008.

Poster: *Dual-basis methods for electronic structure theory*. Molecular Quantum Mechanics – Analytic Gradients & Beyond (an international conference in honor of Peter Pulay), Budapest, Hungary, Jun 2007.

Invited Talk: *Recent improvements in SCF methods*. William A. Lester group, Berkeley, CA, Oct 2007.

Poster: *Dual-basis methods for electronic structure theory*. ACS National Meeting, San Francisco, CA, Sept 2006.

Poster: *Dual-basis methods for electronic structure theory*. American Conference on Theoretical Chemistry, Los Angeles, CA, Jul 2005

Courses Taught

Since Aug 2011

Spring 2020 : Chem 7520 – Computational Chemistry (graduate)
Fall 2019 : Chem 1211 – Honors General Chemistry I (undergraduate)
Spring 2019 : Chem 7080 – Chemical Dynamics (graduate)
Fall 2018 : Chem 1211 – Honors General Chemistry I (undergraduate)
Spring 2018 : Chem 7520 – Computational Chemistry (graduate)
Fall 2017 : Chem 1211 – Honors General Chemistry I (undergraduate)
Spring 2017 : Chem 3060 – Quantum Chemistry & Spectroscopy (undergraduate)
Fall 2016 : Chem 7040 – Statistical Thermodynamics (graduate)
Spring 2016 : Chem 3060 – Quantum Chemistry & Spectroscopy (undergraduate)
Spring 2015 : Chem 3060 – Quantum Chemistry & Spectroscopy (undergraduate)
Fall 2014 : Chem 7000 – Quantum Mechanics (graduate)
Spring 2014 : Chem 7520 – Computational Chemistry (graduate)
Fall 2013 : Chem 7040 – Statistical Thermodynamics (graduate)
Spring 2013 : Chem 3060 – Quantum Chemistry & Spectroscopy (undergraduate)
Fall 2012 : Chem 7040 – Statistical Thermodynamics (graduate)
Spring 2012 : Chem 3060 – Quantum Chemistry & Spectroscopy (undergraduate)
Fall 2011 : Chem 7520 – Computational Chemistry (graduate)

Before Aug 2011

Spring 2006 : Quantum Mechanics II Graduate Student Instructor (graduate)
Fall 2004 : Chemistry 1A Head Graduate Student Instructor (undergraduate)
Fall 2003 : Chemistry 1A Graduate Student Instructor (undergraduate)
Spring 2003 : Introductory Chemistry II Teaching Assistant (undergraduate)
Fall 2002 : Introductory Chemistry I Teaching Assistant (undergraduate)

Publications

Since Aug 2011

Manuscripts in Preparation

44. *Persistence of a Delocalized Radical in Larger Clusters of Hydrated Copper (II) Hydroxide*

E. G. Christensen, K. T. Lutz, and R. P. Steele (2021).

43. *Consistent Tracking of Molecular Orbitals in Ab Initio Molecular Dynamics Simulations*

A. J. Zhanserkeev, J. J. Talbot, and R. P. Steele (2021)

Manuscripts under Review

42. *Electronic Structure and Vibrational Signatures of the Delocalized Radical in Hydrated Clusters of Copper ("II") Hydroxide,* $CuOH^+(H_2O)_{0-2}$

E. G. Christensen, K. T. Lutz and R. P. Steele (2021)

Published Articles

41. *Infrared Signatures of Isomer Selectivity and Symmetry Breaking in the* $Cs^+(H_2O)_3$ *Complex Using Many-Body Potential Energy Functions*

M. Riera, J. J. Talbot, R. P. Steele, F. Paesani
J. Chem. Phys. **153**, 044306 (2020).

40. *Stepwise Activation of Water by Open-Shell Interactions,* $Cl(H_2O)_{4-8,17}$

E. G. Christensen and R. P. Steele
J. Phys. Chem. A **124**, 3417-3437 (2020).

39. *Spectroscopic Signatures of Mode-Dependent Tunnel Splitting in the Iodide-Water Binary Complex*

J. J. Talbot, N. Yang, M. Huang, C. H. Duong, A. B. McCoy, R. P. Steele, and M. A. Johnson.
J. Phys. Chem. A **124**, 2991-3001 (2020).

38. *Probing the Partial Activation of Water by Open-Shell Interactions,* $Cl(H_2O)_{1-4}$

E. G. Christensen and R. P. Steele
J. Phys. Chem. A **123**, 8657-8673 (2019).

37. *Nuclear Motion in the Intramolecular Dihydrogen-Bound Regime of an Aminoborane Complex*

D. L. Reese and R. P. Steele
J. Phys. Chem. A **123**, 6547-6563 (2019).

36. *Monitoring Water Clusters 'Melt' Through Vibrational Spectroscopy*

S. E. Brown, A. W. Götz, X. Cheng, R. P. Steele, V. A. Mandelshtam, F. Paesani
JACS **139**, 7082-7088 (2017).

35. *Signatures of Size-Dependent Structural Patterns in Hydrated Copper (I) Clusters,* $Cu^+(H_2O)_{n=1-10}$

J. D. Herr and R. P. Steele
J. Phys. Chem. A **120**, 10252-10263 (2016).

34. *Quantum Molecular Motion in the Mixed Ion-Radical Complex,* $[(H_2O)(H_2S)]^+$

S. D. Floris, J. J. Talbot, M. J. Wilkinson, J. D. Herr and R. P. Steele.
Phys. Chem. Chem. Phys. **18**, 27450-27459 (2016).

33. *Vibrational Signatures of Electronic Properties in Oxidized Water Clusters: Unraveling the anomalous vibrational spectrum of the water dimer cation*

J. Talbot, X. Cheng, J.D. Herr, and R. P. Steele.
JACS **138**, 11936-11945 (2016).

32. *Accelerating Ab Initio Molecular Dynamics Simulations by Linear Prediction Methods*

J. D. Herr and R. P. Steele.
Chem. Phys. Lett. **661**, *42-47* (2016). "Editor's Choice" Article

31. *Ion-Radical Pair Separation in Larger Ionized Water Clusters,* $(H_2O)^+_{n=6-21}$

J. D. Herr and R. P. Steele.
J. Phys. Chem. A **120**, 7225-7239 (2016).

30. *Tuning Vibrational Mode Localization with Frequency Windowing*
X. Cheng, J. J. Talbot, and R. P. Steele.
J. Chem. Phys **145**, 124112 (2016).

29. *Vibrational Signatures of Conformer-Specific Interactions in Protonated Tryptophan*
A.Y. Pereverzev, X. Cheng, N. S. Nagornova, D. Reese, R.P. Steele, O. V. Boyarkin.
J. Phys. Chem. A **120**, 5598-5608 (2016).

28. *Accelerating ab initio path integral simulations via imaginary multiple-timestepping*
X. Cheng,* J.D. Herr,* and R. P. Steele
(*equal authorship)
J. Chem. Theor. Comput. **12** 1627-1638 (2016).

27. *Consecutive charging of a molecule-on-insulator ensemble using single-electron tunnelling methods*
P. Rahe, R. P. Steele, and C. C. Williams.
Nano Letters **16** 911 (2016).

26. *Multiple-timestep ab initio molecular dynamics using an atomic basis set partitioning*
R. P. Steele
J. Phys. Chem. A **119** 12119 (2015).
*Invited Article for "Dynamics of Molecular Collisions XXV: Fifty years of chemical reaction dynamics" Issue

25. *Multiple-timestep ab initio molecular dynamics based on two-electron integral screening*
S. Fatehi and R. P. Steele
J. Chem. Theor. Comput. **11** 884-898 (2015).

24. *Structural progression in clusters of ionized water* $(H_2O)^+_{1-5}$
J. D. Herr, J. Talbot, and R. P. Steele
J. Phys. Chem. A **119** 752-766 (2015)

23. *Multiple environment single system quantum mechanical/molecular mechanical (MESS-QM/MM) calculations. I. Estimation of polarization energies*
A. J. Sodt, Y. Mei, G. König, P. Tao, R. P. Steele, B. R. Brooks, and Y. Shao
J. Phys. Chem. A **119** 1151-1523 (2015).

22. *Efficient anharmonic vibrational spectroscopy for large molecules using local-mode coordinates*
X. Cheng and R. P. Steele
J. Chem. Phys. **141** 104105 (2014).

21. *Nuclear Motion in the σ-Bound Limit of Metal-H_2 Complexes:* $[Mg(H_2)_{n=1-6}]^{2+}$
B. Mitchell and R. P. Steele.
J. Phys. Chem. A **118** 10057-10066 (2014)

20. *Advances in molecular quantum chemistry contained in the Q-Chem 4 program package*
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CAREER Program
$606,515
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Vibrational Signatures of Electronic Properties in Renewable-Energy Catalysis
Department of Energy
Computational Chemical Sciences
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15 Sept 2018 – 14 Sept 2022

Metal-H_2 Complexes vs. Metal Hydrides: Nuclear motion and implications for hydrogenation catalysis
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Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
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Quantum Chemistry for Molecular Motion
Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
4.1 million service units (SUs)
Value of awarded time: **$???,???**
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Quantum Chemistry for Molecular Motion
Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
3.2 million service units (SUs)
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