Contact Information

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Professional Preparation

University of California – Berkeley	Ph.D., Theoretical Chemistry	2008
Iowa State University	B.S. with Distinction, Chemistry	2003

Scientific Appointments

Associate Professor	The University of Utah Dept of Chemistry	2017 – current
Assistant Professor	The University of Utah Dept of Chemistry	2011 – 2017
Post-Doctoral Associate	Yale University Dept of Chemistry (Prof. John Tully)	2008 – 2011
Graduate Research Assistant	University of California – Berkeley Dept of Chemistry (Prof. Martin Head-Gordon)	2003 – 2008
Graduate Student Instructor	University of California – Berkeley Dept of Chemistry	2003, 2004, 2006
Undergraduate Research Associate	Georgia Institute of Technology Dept of Chemistry (Prof. David Sherrill)	2002
Undergraduate Research Associate	Iowa State University Dept of Chemistry (Prof. William Jenks)	2002 – 2003
Teaching Assistant	Iowa State University Dept of Chemistry	2002 – 2003

Students Mentored

Post-Doctoral Researchers	Current Position	Years in Group
Xiaolu Cheng	Staff Scientist A-Alpha Bio	2013-2017
Shervin Fatehi	Assistant Professor of Chemistry University of TX – Rio Grande Valley	2013-2015

Graduate Students	Current Position	Years in Group
Ryan Spencer		2020 – current
Asylbek (A.J.) Zhanserkeev	Post-doctoral Researcher NIST	2018 – 2023
Gabe McDonald	Nuclear Engineer & Officer U.S. Navy	2018 – 2021 (MS)

Austin Gillespie (MSSST Program)	High School Chemistry Teacher Brighton High School	2018 – 2019 (MS)
Elizabeth Christensen	Researcher & Project Manager Silvester & Co.	2016 – 2021
Diana Reese	Assistant Professor of Chemistry Utah Tech University	2014 – 2020
Justin Talbot	Post-Doctoral Researcher University of California – Berkeley	2014 – 2019
Nicholas Corbett	Chief Science Officer Canyon Labs	2013 – 2015 (MS)
J.D. Herr	Lead Data Scientist Perpay, Inc.	2012 – 2016

Undergraduate Students	**Current Position**	**Years in Group**
Emily Yang	Researcher Gentex	2019 – 2023
Matthew Laskowski	Attending graduate school Fall 2023 (B.S., Univ. Maryland, 2022)	2021 – 2023 (REU)
Kevin Lutz	Senior Certified Pharmacy Technician Walgreens	2019 – 2023
MacKenzie Ferron	Chemistry Lab Technician Xenon Pharmaceuticals	2017
Jessica Schulze	Ph.D., Penn State JAS Consulting	2017
Jennifer Chlam	OD/MS Student, Ohio State	2017 (REU)
Matthew Wilkinson	M.S., Utah Valley University Data Engineer, Amplify Consulting	2015 – 2017
Sarah Floris	Senior Data Engineer Clinical Trial Media	2015 – 2016 (REU)
William Gleich	DevOps Engineer Proofpoint	2012 – 2013
Doo-Hyun Kwon	Ph.D., BYU Investigator, Computational Chemistry & Molecular Design, GSK	2012 – 2014
Joemy Ramsay	M.S., University of Washington Ph.D., University of Utah Post-Doctoral Fellow, Huntsman Cancer Inst.	2012 – 2013
Brandon Mitchell	Senior Process Engineer Micron Technology	2012 – 2014
Justin Park	Ph.D., BYU Formulation Chemist, Autoliv	2012 – 2013
Annie Bench	Science Teacher	2012 – 2013
Jordan Meadows	Pharm.D., University of Utah Pharmacist, University of Utah	2012 – 2013
Maggie Reid	M.S. & M.P.H., Tufts University Ph.D. Student, University of Colorado - Denver Sr. Statistical Analyst, CIDA/CAIANH	2012 – 2014

Tyler Rasmussen	Process Engineer Anvil Corporation	2012 – 2014
Justin Talbot	Post-Doctoral Researcher University of California - Berkeley	2011 – 2014

Honors & Awards

2019 Robert W. Parry Teaching Award
2017 PCCP Emerging Investigator Lectureship
2017 Award for Fostering Undergraduate Research Excellence, The University of Utah
Before Tenure Review
2016 ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry
2015 NSF CAREER
2012 Surface-Hopping Symposium Outstanding Junior Faculty Award (San Diego ACS)
2012 ASUU Student Choice Teaching Award
Before Aug 2011
2007 Teaching Effectiveness Award, University of California – Berkeley
2006 Outstanding Graduate Student Instructor
2006 Berkeley Travel Award
2003 Senior Chemistry Student of the Year, Iowa State University
2000-3 Phi Beta Kappa, Phi Kappa Phi, Mortar Board, Golden Key International, and Tau Beta Pi Honor Societies
1999 National Merit Scholar

Journals Refereed

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

Granting Agencies Refereed

Department of Energy (DOE)	Site review, *ad hoc* reviews
National Science Foundation (NSF)	Panel review, *ad hoc* reviews

Air Force Office of Scientific Research (AFOSR)	*Ad hoc* reviews
ACS Petroleum Research Fund (PRF)	*Ad hoc* reviews

Software Development

Electronic structure & dynamics:	Q-Chem software package
Vibrational stimulations:	In-house, currently developed package

Outreach & External Service Activities

2023-2025	American Conference on Theoretical Chemistry co-chair
2019-2023	Executive Committee member-at-large, American Chemical Society Physical Division
2015-current	Michael Wormit Award Selection Committee (Q-Chem)
2023-current	Nick Besley Award Selection Committee (Q-Chem)
2017-2021	Advisory Board, Advancing Mass Spectrometry Conference
2019	Co-coordinator, ACS Phys Symposium (Orlando, FL, Spring) "Frontiers in Vibrational Spectroscopy: Theory & Experiment"
2019	Co-coordinator, Utah Quantum Workshop (Park City, UT)
2018	Summer Enrichment Program lecture, The University of Utah
2014, 2017	MSSST lecture, The University of Utah
2011-2017	Science Demonstrations, Edison Elementary School
2012-2017	Science Fair Judge, Edison Elementary School
2016-2017	Science Fair Judge, Salt Lake Valley Science Fair
2016	Semi-annual High School Teachers' Workshop lecture, The University of Utah
2016	STEM Student Outreach & Engagement, The University of Utah

Before Tenure Review

2015	Co-coordinator, "A Celebration of the First 70 Years of Jack Simons" (Salt Lake City, UT)
2012	Co-coordinator, Q-Chem Developers Workshop (Philadelphia, PA)
2012-2013	Event Coordinator, Utah Science Olympiad
2012	Science Day Presenter, The University of Utah

Service

Department

2022-current	Associate Chair and Director of Graduate Studies
2022-current	Chair, Graduate Education Committee
2019-2022	Undergraduate Education Committee
2017-2019	Chair, Physical Chemistry Division
2017-2018	Graduate Recruiting Committee
2011-2016, 2018	Graduate Admissions Committee
2011-2016	Physical Chemistry Seminar Coordinator
2011-2012, 2018, 2020	Faculty Search Committee

University

2022-current	Benefits Advisory Committee (Faculty representative)
2014-current	Center for High-Performance Computing Allocation Committee
2021-2022	Academic Senate Executive Committee
2019-2022	Academic Senate
2015-2022	Teaching & Learning Portfolio Committee (College of Science representative)
2018-2020	College of Science Council
2014-2016	Undergraduate Council
2014	One Network Planning Committee

Courses Taught

2024 (Planned)	Spring	CHEM 7520: Computational Chemistry Laboratory		Graduate
2023	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2023	Spring	CHEM 7080: Chemical Dynamics		Graduate
2022	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2022	Spring	CHEM 7520: Computational Chemistry Laboratory		Graduate
2021	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2021	Spring	CHEM 7080: Chemical Dynamics		Graduate
2020	Fall	CHEM 1211: Honors General Chemistry I	(1 section, online)	Undergraduate
		CHEM 1210: General Chemistry I	(5 sections, online)	Undergraduate
2020	Spring	CHEM 7520: Computational Chemistry Laboratory		Graduate
2019	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2019	Spring	CHEM 7080: Chemical Dynamics		Graduate
2018	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2018	Spring	CHEM 7520: Computational Chemistry Laboratory		Graduate
2017	Fall	CHEM 1211: Honors General Chemistry I		Undergraduate
2017	Spring	CHEM 3060: Quantum Chemistry & Spectroscopy		Undergraduate
2016	Fall	CHEM 7040: Statistical Thermodynamics		Graduate

Before Tenure Review

2016	Spring	CHEM 3060: Quantum Chemistry & Spectroscopy		Undergraduate
2015	Fall	(pre-tenure relief)		
2015	Spring	CHEM 3060: Quantum Chemistry & Spectroscopy		Undergraduate
2014	Fall	CHEM 7000: Quantum Mechanics		Graduate
2014	Spring	CHEM 7520: Computational Chemistry Laboratory		Graduate
2013	Fall	CHEM 7040: Statistical Thermodynamics		Graduate
2013	Spring	CHEM 3060: Quantum Chemistry & Spectroscopy		Undergraduate
2012	Fall	CHEM 7040: Statistical Thermodynamics		Graduate
2012	Spring	CHEM 3060: Quantum Chemistry & Spectroscopy		Undergraduate
2011	Fall	CHEM 7520: Computational Chemistry Laboratory		Graduate

Before Aug 2011

University of California - Berkeley

2006	Spring	Quantum Mechanics II (Graduate Student Instructor)	Graduate
2004	Fall	Chemistry 1A (Head Graduate Student Instructor)	Undergraduate
2003	Fall	Chemistry 1A (Graduate Student Instructor)	Undergraduate

Iowa State University

2003	Spring	Introductory Chemistry II (Undergraduate Teaching Assistant)	Undergraduate
2002	Fall	Introductory Chemistry I (Undergraduate Teaching Assistant)	Undergraduate

Presentations, Posters, & Conferences

84	Invited Virtual Seminar	TBD	*(Upcoming)*	Virginia Commonwealth University	Richmond, VA
83	Invited Seminar	2024 Jun	*(Upcoming)*	Telluride Science Research Center (Spectroscopy & Dynamics of Coupled Anharmonic Vibrations of Floppy Systems)	Telluride, CO
82	Invited Seminar	2024 Jan	*Good Vibrations: New insights from simulations of infrared spectroscopy*	Brigham Young University	Provo, UT
81	RPT Seminar	2023 Sep	*Good Vibrations: New methods for the simulation of anharmonic spectroscopy*	University of Utah	Salt Lake City, UT
80	Invited Conference	2023 Jul	*Taming the Beast: New Developments & Demonstrations of Anharmonic Vibrational Simulations for Larger Chemical Systems*	Dynamics of Molecular Collisions	Snowbird, UT
79	Invited Conference	2022 Jul	*New Local-Mode Approaches for Anharmonic Vibrational Spectroscopy Simulations*	Telluride Science Research Center (Spectroscopy & Dynamics of Coupled Anharmonic Vibrations of Floppy Systems)	Telluride, CO
--	International Invited Conference	2022 Jul	*Invited 2020 Conference postponed to 2022 due to COVID Withdrew due to lack of virtual option	World Association of Theoretically Oriented Chemists (WATOC)	Vancouver, BC
78	Contributed Conference	2022 Mar	*Exploiting Locality in Anharmonic Vibrational Simulations*	ACS National Meeting (John Stanton Symposium)	San Diego, CA
77	International Invited Virtual Seminar	2021 Dec	*Spectral Signatures of Water Activation by Ions & Radicals*	Queen's University	Ontario, Canada
76	International Invited Virtual Seminar	2021 Jun	*Spectral Signatures of Water Activation by Ions & Radicals*	Innsbruck University	Innsbruck, Austria
75	Invited Virtual Seminar	2020 Oct	*Spectral Signatures of Water Activation by Ions & Radicals*	Idaho St. University	Pocatello, ID
74	Invited Virtual Conference	2020 May	*Spectral Signatures of Water Activation by Ions & Radicals*	DOE CTC Meeting	Gaithersburg, MD
73	Invited Conference	2020 Jan	*Spectral Signatures of Water Activation by Ions & Radicals*	Gordon Research Conference (Molecular & Ionic Clusters)	Ventura, CA
72	Invited Seminar	2019 Dec	*Spectral Signatures of Water Activation by Ions & Radicals*	Westminster College	Salt Lake City, UT
71	Recruiting Seminar	2019 Nov	*Spectral Signatures of Water Activation by Ions & Radicals*	BYU-Idaho Visit to UofU	Salt Lake City, UT

70	Invited Conference	2019 Sep	*Spectral Signatures of Water Activation by Ions & Radicals*	Utah Quantum Workshop	Park City, UT
69	Invited Conference	2019 Aug	*Spectral Signatures of Water Activation by Ions & Radicals*	Dynamics of Molecular Collisions	Big Sky, MT
68	Poster	2019 May	*Vibrational Signatures of Electronic Properties in Renewable Energy Catalysis*	DOE CTC Meeting	Gaithersburg, MD
67	Recruiting Seminar	2018 Oct	*Quantum Chemistry & Molecular Motion*	University of Nebraska – Kearney	Kearney, NE
66	International Invited Award Lectureship	2018 Aug	*From Electrons to Molecular Vibrations…and Back*	EuCheMS Conference	Liverpool, UK
65	Invited Conference	2018 Jul	*Spectral Signatures of Water Activation by Ions & Radicals*	Gordon Research Conference (Vibrational Spectroscopy)	Biddeford, ME
64	Student-Invited Seminar	2018 Feb	*Exploiting Time and Length Scales in Quantum Simulations of Spectroscopy & Dynamics*	TheoChem@Boston Seminar Series (Harvard, MIT, Boston U)	Boston, MA
63	Invited Conference	2018 Jan	*Vibrational Signatures of Electronic Properties in Molecules*	Sanibel Symposium (Computational Modelling in Mass Spectrometry and Ion Mobility)	St. Petersburg, FL
62	Invited Conference	2018 Jan	*Exploiting Time and Length Scales for Accelerated AIMD Simulations*	Telluride Science Research Center (New Challenges for Theory in Chemical Dynamics)	Telluride, CO
61	International Invited Talk	2017 Nov	*Probing Ion Structure with New Quantum Simulations*	Lake Louise Mass Spectrometry Workshop	Alberta, Canada
60	Invited Conference	2017 Jul	*Quantum Chemistry Approaches for Simulating the Spectroscopy & Dynamics of Biomolecules*	Advancing Mass Spectrometry	Ann Arbor, MI
59	Invited Conference	2017 Jul	*Exploiting Locality for Anharmonic Vibrational Spectroscopy Simulations*	Telluride Science Research Center (Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Systems)	Telluride, CO
58	Invited Presenting Chair	2017 Jul	*Bimolecular Collision Dynamics*	Dynamics of Molecular Collisions	Tahoe, CA
57	Recruiting Seminar	2016 Nov	*Quantum Chemistry & Molecular Motion*	Northern Arizona University	Flagstaff, AZ
56	Recruiting Seminar	2016 Nov	*Quantum Chemistry & Molecular Motion*	Ft. Lewis College	Durango, CO
55	Invited Workshop	2016 Nov	*Computational Approaches to Anharmonic Vibrational Spectroscopy*	University of Pittsburgh	Pittsburgh, PA

Before Tenure Review

54	Invited Seminar	2016 Nov	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Pittsburgh	Pittsburgh, PA
53	Invited Seminar	2016 Sep	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of North Carolina	Chapel Hill, NC
52	Invited Seminar	2016 Sep	*Vibrational Signatures of Electronic Properties in Energy & Biology*	Duke University	Durham, NC
51	Tenure Seminar	2016 Sep	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Utah	Salt Lake City, UT
50	Invited Conference	2016 Jul	*Vibrational Signatures of Electronic Properties in Energy & Biology*	International Society for Theoretical Chemical Physics	Grand Forks, ND
49	Invited Conference	2016 Mar	*Vibrational Signatures of Electronic Properties in Energy & Biology*	ACS National Meeting PHYS Division (Decoding the spectroscopic signatures of large-amplitude motion)	San Diego, CA
48	Award Poster	2016 Mar	*Accelerating Ab Initio Simulations of Molecular Motion*	OpenEye Award ACS Spring COMP Division	San Diego, CA
47	International Invited Conference	2016 Mar	*Reliable Computational Approaches for Vibrational Spectra of Biomolecules*	Isolated Biomolecules and Biomolecular Interactions (IBBI)	Oxford, UK
46	Invited Seminar	2015 May	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Washington	Seattle, WA
45	Invited Seminar	2015 Feb	*Vibrational Signatures of Electronic Properties in Energy & Biology*	Purdue University	W. Lafayette, IN
44	Invited Seminar	2015 Feb	*Vibrational Signatures of Electronic Properties in Energy & Biology*	Notre Dame University	South Bend, IN
43	Invited Seminar	2015 Jan	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Georgia	Athens, GA
42	Invited Seminar	2015 Nov	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Kansas	Lawrence, KS
41	Invited Seminar	2015 Nov	*Ab Initio Molecular Motion and Ionized Water*	National Institutes of Health Computational Biophysics Group	Bethesda, MD
40	Student-Invited Seminar	2015 Nov	*Vibrational Signatures of Electronic Properties in Energy & Biology*	Ohio State University	Columbus, OH
39	Invited Seminar	2015 Oct	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of California – San Diego	San Diego, CA

38	Invited Seminar	2015 Oct	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of California – Los Angeles	Los Angeles, CA
37	Invited Seminar	2015 Oct	*Ab Initio Molecular Motion and Ionized Water*	University of Southern California	Los Angeles, CA
36	Invited Seminar	2015 Oct	*Vibrational Signatures of Electronic Properties in Energy & Biology*	California Institute of Technology	Pasadena, CA
35	Invited Seminar	2015 Oct	*Ab Initio Molecular Motion and Ionized Water*	University of Illinois	Urbana-Champaign, IL
34	Invited Seminar	2015 Sep	*Ab Initio Molecular Motion and Ionized Water*	Iowa State University	Ames, IA
33	Invited Seminar	2015 Sep	*Vibrational Signatures of Electronic Properties in Energy & Biology*	Kansas State University	Manhattan, KS
32	Recruiting Seminar	2015 Sep	*Quantum Chemistry & Molecular Motion*	University of Nebraska – Omaha	Omaha, NE
31	Invited Seminar	2015 Sep	*Vibrational Signatures of Electronic Properties in Energy & Biology*	University of Nebraska	Lincoln, NE
30	International Invited Conference	2015 Aug	*Exploring the Interface of Electronic Structure and Molecular Motion*	IUPAC Congress	Busan, South Korea
29	International Invited Conference	2015 Aug	*New Ab Initio Approaches to Vibrational Spectroscopy*	Mueunjae Symposium on Chemistry & Light (POSTECH)	Pohang, South Korea
28	Invited Conference	2015 Aug	*Exploring the Interface of Electronic Structure and Molecular Dynamics*	ACS National Meeting	Boston, MA
27	Invited Conference	2015 Aug	*New Ab Initio Approaches to Vibrational Spectroscopy*	Q-Chem Developers Meeting	Boston, MA
26	International Invited Conference	2015 May	*Exploiting the Length- and Timescales of Molecular Interactions*	Modeling Many-Body Interactions (MMBI15)	Lake Garda, Italy
25	Contributed Conference	2015 Mar	*Advancing Ab Initio Molecular Dynamics via Multiple-Timestep Methods*	ACS National Meeting PHYS Symposium (Don Truhlar Symposium)	Denver, CO
24	Invited Conference	2015 Mar	*Anomalous Vibrational Signatures of Ions and Solvation*	APS National Meeting (Solvation of Ions and Electrons)	San Antonio, TX
23	Invited Conference	2015 Mar	*New Ab Initio Approaches to Ion Spectroscopy*	Gordon Research Conference (Gaseous Ions)	Galveston, TX
22	Invited Conference	2015 Feb	*New Computational Techniques for Biomolecular Interactions*	Mesilla Chemistry Workshop	Mesilla, NM
21	Invited Seminar	2014 Nov	*Quantum Molecular Motion in Energy and Biology*	Wayne State University	Detroit, MI
20	Contributed Conference	2014 Aug	*Vibrational Signatures of Electronic Motion in Oxidized Water*	ACS National Meeting PHYS Symposium	San Francisco, CA

19	Contributed Conference	2014 Aug	*Exploring the Interface of Electronic Structure Theory and Chemical Dynamics*	ACS National Meeting PHYS Symposium	San Francisco, CA
18	Contributed Conference	2014 Aug	*New Approaches to Anharmonic Vibrational Spectroscopy in Large Molecules*	ACS National Meeting COMP Symposium	San Francisco, CA
17	Invited Conference	2014 Jul	*Vibrational Signatures of Electronic Motion in Oxidized Water*	International Conference on Chemical Bonding	Kauai, HI
16	Invited Conference	2014 Jul	*New Ab Initio Approaches for Spectroscopy & Dynamics*	Telluride Science Research Center (Spectroscopy & Dynamics on Multiple Potential Energy Surfaces)	Telluride, CO
15	"Hot Topics" Conference	2014 Jul	*New Ab Initio Approaches for Spectroscopy & Dynamics*	Gordon Research Conference (Atomic & Molecular Interactions)	Stonehill, MA
14	Invited Honorarium Conference	2014 Jun	*Spectroscopy & Dynamics with Electronic Structure Theory*	Chemistry Collaborations, Workshops, and Communities of Scholars Westminster College	Salt Lake City, UT
13	Contributed Conference	2014 Mar	*Accelerated Ab Initio Sampling and Dynamics*	ACS National Meeting COMP Symposium	Dallas, TX
12	Contributed Conference	2014 Mar	*Signatures of Nuclear and Electronic Motion in Oxidized Water Clusters*	ACS National Meeting PHYS Symposium	Dallas, TX
11	Contributed Conference	2013 Sep	*Multiple-Timestep Ab Initio Molecular Dynamics*	ACS National Meeting PHYS Symposium	Indianapolis, IN
10	Invited Conference	2013 Sep	*Innovation Approaches to Ab Initio Dynamics and Sampling*	Q-Chem Developers Conference	Indianapolis, IN
9	Invited Conference	2013 Jul	*Accelerated Ab Initio Dynamics and Quantum Sampling*	Telluride Science Research Center (Quantum Effects in Condensed-Phase Systems)	Telluride, CO
8	Invited Seminar	2013 Mar	*Structure & Dynamics of Water Oxidation*	University of Wisconsin Theoretical Chemistry Institute Seminar Series	Madison, WI
7	Recruiting Seminar	2012 Nov	*Structure & Dynamics of Water Oxidation*	BYU-Idaho	Rexburg, ID
6	Recruiting Seminar	2012 Nov	*Structure & Dynamics of Water Oxidation*	Southern Utah University	Cedar City, UT
5	Recruiting Seminar	2012 Sep	*Structure & Dynamics of Water Oxidation*	University of St. Thomas	St. Paul, MN
4	Contributed Conference	2012 Aug	*Lack-of-Electron Transfer in Water Oxidation*	ACS National Meeting PHYS Symposium	Philadelphia, PA

3	Invited Conference	2012 Aug	*Beyond Critical Points: Sampling & Dynamics in Q-Chem*	Q-Chem Developers Conference	Philadelphia, PA
2	Invited Seminar	2012 Jul	*Fully Quantum Chemistry with Ab Initio Path Integrals*	Telluride Science Research Center (Spectroscopy and Dynamics on Multiple Potential Energy Surfaces)	Telluride, CO
1	Invited Seminar	2012 Mar	*Fully Quantum Chemistry with Ab Initio Path Integrals*	ACS National Meeting PHYS Symposium	San Diego, CA
Before Aug 2011					
	Contributed Seminar	2011 Jul	*The Quantum, Thermal Structure of Protonated Methane and its Isotopologues*	Dynamics of Molecular Collisions	Snowbird, UT
	Invited Seminar	2011 Feb	*Protons: Nature's Nomads*	Virginia Tech	Blacksburg, VA
	Invited Seminar	2011 Jan	*Protons: Nature's Nomads*	University of Utah	Salt Lake City, UT
	Invited Seminar	2011 Jan	*Protons: Nature's Nomads*	University of Washington	Seattle, WA
	Invited Seminar	2010 Dec	*Protons: Nature's Nomads*	University of Hawaii	Honolulu, HI
	Invited Seminar	2010 Nov	*Fully Quantum Chemistry: Mechanisms of Chemical and Biological Energy Conversion*	Notre Dame University	South Bend, IN
	Invited Seminar	2010 Nov	*Protons: Nature's Nomads*	Cornell University	Ithaca, NY
	Contributed Poster	2010 Jul	*The Quantum Structure of Protonated Methane*	Gordon Research Conference (Atomic and Molecular Interactions)	New London, NH
	Invited Seminar	2009 Feb	*Protons: Nature's Nomads*	University of Alabama	Tuscaloosa, AL
	International Invited Seminar	2009 Jul	*A Riddle from the Ionosphere Reveals How Water Activation is Controlled by the Shape of an H-bonded Network*	NSF/PIRE Workshop	Pisa, Italy
	Contributed Poster	2009 Jul	*Atmospheric Water Network Activation: Delocalized Protons and Charge Migration in* $NO^+(H_2O)_{n=1-4}$	Dynamics of Molecular Collisions	Snowbird, UT
	Contributed Conference	2008 Apr	*Dual-Basis Methods: Energies, Derivatives, and Non-Covalent Interactions*	ACS National Meeting COMP Symposium	New Orleans, LA
	Contributed Poster	2008 Apr	*Cation-π Interactions in Fullerene Systems*	ACS National Meeting	New Orleans, LA
	Contributed Conference	2008 Mar	*Circumventing the Basis Set Bottleneck: Dual-Basis Methods for Non-Covalent Interactions*	MRS National Meeting	San Francisco, CA

International Contributed Poster	2007 Jun	*Dual-Basis Methods for Electronic Structure Theory*	Molecular Quantum Mechanics – Analytic Gradients and Beyond (Peter Pulay Conference)	Budapest, Hungary
Invited Seminar	2007 Oct	*Recent Improvements in SCF Methods*	William A. Lester Group	Berkeley, CA
Contributed Poster	2006 Sep	*Dual-Basis Methods for Electronic Structure Theory*	ACS National Meeting	San Francisco, CA
Contributed Poster	2005 Jul	*Dual-Basis Methods for Electronic Structure Theory*	American Conference on Theoretical Chemistry	Los Angeles, CA

Publications

Manuscripts in Preparation

Converged Anharmonic Vibrational Spectroscopy for Large Molecules: Combining multilevel and local-mode simulation methods
A. A. Zhanserkeev,* R. J. Spencer,* and R. P. Steele
(2024)

The Surprising Locality of Many-Body Interactions in Vibrational Couplings
A. A. Zhanserkeev,* R. J. Spencer,* and R. P. Steele
(2024)

Converging the n-Mode Representation of Molecular Potentials via Local-Mode Vibrations
R. J. Spencer, E. L. Yang, and R. P. Steele
(2024)

Manuscripts in Revision

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Manuscripts under Review

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Revised Manuscripts under Review

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Accepted Articles

52 Infrared multiple photon dissociation spectra of cesiated complexes of the aliphatic amino acids: Challenges for conformational-space calculations by density functional theory
P. B. Armentrout, R. P. Steele, B. C. Stevenson, R. M. Jones, J. Martens, G. Berden, J. Oomens
Int. J. Mass. Spectrom. (In press, 2024)

Published Articles

51 Pitfalls of the n-Mode Representation of Vibrational Potentials
E. L. Yang, R. J. Spencer, J. J. Talbot, and R. P. Steele
J. Chem. Phys. **159** 204104 (2023)

50 Accelerating Anharmonic Vibrational Simulations via Local-Mode, Multilevel Methods
A. A. Zhanserkeev, E. L. Yang, and R. P. Steele
J. Chem. Theor. Comput. **19** 5572-5585 (2023)

49 Accelerating and Stabilizing the Convergence of Vibrational Self-Consistent Field Calculations via the Direct Inversion of the Iterative Subspace (vDIIS) Algorithm
E. L. Yang, R. J. Spencer, and R. P. Steele

J. Chem. Phys. **159** 084103 (2023)

48 Persistence of a Delocalized Radical in Larger Clusters of Hydrated Copper (II) Hydroxide, $CuOH^+(H_2O)_{3-7}$
E. G. Christensen, K. T. Lutz, R. J. Spencer, and R. P. Steele
J. Phys. Chem. A **127** 6647-6659 (2023)

47 Structural, Thermodynamic, and Spectroscopic Evolution in the Hydration of Copper (II) Ions, $Cu^{2+}(H_2O)_{2-8}$
E. G. Christensen and R. P. Steele
J. Phys. Chem. A **127** 6660-6676 (2023)

46 Molecular Motion in the Interconverting σ-H_2, Di-, and Tri-hydride Regimes, $Mo(PH_3)_5H_2$
D. L. Reese and R. P. Steele
J. Phys. Chem. A. **126**, 6834-6848 (2022)

45 Software for the Frontiers of Quantum Chemistry: An overview of developments in the Q-Chem 5 package
E. Epifanovsky, (220 total authors, including R. P. Steele)
J. Chem. Phys. **155**, 084801 (2021).

44 Adiabatic Orbital Tracking in Ab Initio Molecular Dynamics
A. A. Zhanserkeev, J. J. Talbot and R. P. Steele
J. Chem. Theor. Comput. **17**, 4675-4685 (2021).

43 Role of Ligand-Bound CO_2 in the Hydrogenation of CO_2 to Formate with a (PNP)Mn Catalyst
K. Schlenker, E. G. Christensen, A. A. Zhanserkeev, G. R. McDonald, E. L. Yang, K. T. Lutz, R. P. Steele, R. T. VanderLinden, C. T. Saouma
ACS Catalysis **11**, 8358-8369 (2021).

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
J. Phys. Chem. A **125**, 3631-3645 (2021).

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
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Research Funding

Exploiting Locality for Enhanced Simulations of Anharmonic Vibrational Spectroscopy [Pending]
National Science Foundation
Chemical Theory, Models, and Computational Methods (CTMC)
$699,952 Requested
01 April 2024 – 31 March 2028

Disentangling Many-Body Effects and Couplings in Vibrational Spectra of Aqueous Clusters
National Science Foundation
Chemical Structure, Dynamics, and Mechanisms (CSDM-A)
$789,413 [Utah Portion: $382,529]
26 April 2021 – 25 April 2024

Vibrational Signatures of Electronic Properties in Renewable-Energy Catalysis
Department of Energy
Computational Chemical Sciences (CCS)
$600,000
15 Sept 2018 – 14 Sept 2022 [Under No-Cost Extension until Sept 2023]

Award for Fostering Undergraduate Research Excellence
The University of Utah
College of Science
$20,000
24 March 2017 [Unrestricted time window]

CAREER: New Methods for Dynamical Quantum Chemistry
National Science Foundation
Chemical Theory, Models, and Computational Methods
CAREER Program
$606,515
1 April 2015 – 31 Mar 2020

Metal-H_2 Complexes vs. Metal Hydrides: Nuclear motion and implications for hydrogenation catalysis
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$110,000
1 Sept 2015 – 31 Aug 2017 [Extended to Aug 2018]

Chemistry in Action via Anharmonic Spectroscopy
University of Utah Vice President for Research
Seed Grant [*Generated proof-of-concept for current DOE grant]
$28,000
1 July 2013 – 30 June 2014

Exploring the Interface of Quantum Chemistry and Molecular Motion
Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
6.8 million core hours
Value of awarded time: **$29,840.56**
1 Oct 2021 – 31 Dec 2022

Quantum Chemistry for Molecular Motion
Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
3.2 million service units (SUs)
Value of awarded time: **$51,164.50**
1 Oct 2019 – 30 Sept 2020

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Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
4.1 million service units (SUs)
Value of awarded time: **$71,532.66**
1 Oct 2017 – 30 Sept 2018

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Extreme Science and Engineering Discovery Environment (XSEDE) [Funded by NSF]
4.1 million service units (SUs)
Value of awarded time: **$145,315**
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