JONATHAN MORRELL SMITH
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EDUCATION

Ph.D., Chemistry
Wesleyan University, Middletown, Connecticut
Advisor: Joseph Knee; Thesis: *Zero Electron Kinetic Energy Photoelectron Spectroscopy as A Probe of Molecular Dynamics and Conformation*

B.S., Chemistry,
Bates College, Lewiston, Maine

Postdoctoral Fellow
Yale University, New Haven, Connecticut
Research Director: William Chupka; Collaborators: Pat Vaccaro and Mark Johnson
Massachusetts Institute of Technology, Cambridge, Massachusetts
Research Director: Robert W. Field

EXPERIENCE

Professor of Instruction in Chemistry July 2024 – present
Department of Chemistry
Engaged teacher of data science and introductory through advanced chemistry courses. Mentored undergraduates who have go on to success in PhD, MD, DPharm programs, and industry.

Associate Professor of Instruction in Chemistry September 2008 – June 2024
Department of Chemistry

Director of Data Science First Year July 2021 – present
Temple University, Philadelphia, Pennsylvania
Leading and evolving a Temple science centered program to empower students with data and a Python toolbox to build problem solving skills and support insights from scientific data and beyond.

Visiting Associate Professor of Chemistry (Research) January 2021 - present
Hylleraas Centre for Quantum Molecular Sciences and
Center for Computers in Science Education, University of Oslo
Developing methods to compute dynamics of highly excited molecular species ubiquitous in atmospheric and astrophysical contexts. Leveraging machine learning including neural net and Gaussian process algorithms in novel extension of insight from experimental and computational data.

Visiting Scientist Summer 2008
Massachusetts Institute of Technology, Cambridge, Massachusetts
Collaborator: Robert W. Field
Applied new spectroscopic techniques to explore singlet-triplet coupling.

Associate Professor (with tenure) September 2005 – June 2009
Department of Chemistry

Gustavus Adolphus College, Saint Peter, Minnesota
Innovative and engaging teacher and tenured faculty mentor of over 20 undergraduate research collaborators. Lead collaborative development of successful $1.2 Million (USD) Howard Hughes Medical Institute (HHMI) program.

Visiting Assistant Professor (research appointment) January 2006 – present
Department of Chemistry
University of Minnesota, Minneapolis, Minnesota
Collaborators: Donald Truhlar and Chris Cramer
Deepened computational methodologies and analytic tools to simulate molecular vibrational spectroscopy.

Assistant Professor June 1999 – August 2005
Department of Chemistry
Gustavus Adolphus College, Saint Peter, Minnesota

Visiting Assistant Professor July 1997 - June 1999
Department of Chemistry; Bowdoin College, Brunswick, Maine
Developed engaging teaching and broadened scope of my teaching repertoire.

Visiting Assistant Professor July 1996 – June 1997
Department of Chemistry; Swarthmore College, Swarthmore, Pennsylvania

UNIVERSITY AND PROFESSIONAL SERVICE

Undergraduate Committee Member January 2021 - present
Department of Chemistry, Temple University

Undergraduate Research Coordinator, Fall 2015-June 2018
Department of Chemistry, Temple University

Honors Re-Vision Committee, Provost's Strategic Planning Spring 2009
Committee Member, Temple University

Undergraduate Research Program Spring 2009-Spring 2010
Co-Developer and First Undergraduate Research Director
College of Science and Technology, Temple University

Midwest Undergraduate Computational Chemistry Consortium 2004 - present
Executive Committee

Sigma Xi, Gustavus Adolphus College, Chapter President Fall 2007-Fall 2008

Search Committee Chair, Analytical Chemistry faculty position Fall 2007

Minnesota Science Technology Mathematics and Science Alliance Spring 2006 - 2008
National Science Foundation-Louis Stokes Alliance for Minority Participation (LSAMP), Grant Planning and Implementation Committee

PUBLICATIONS

1. *Collisional Relaxation of Highly Vibrationally Excited Acetylene Mediated by the Vinylidene Isomer. Smith, J. M.; Nikow, M.; Wilhelm, M. J.; Dai, H. L. J Phys Chem A* ***2023****, 127 (42), 8782-8793.*
2. *UV Photolysis of Pyrazine and the Production of Hydrogen Isocyanide.* Wilhelm, M. J.; Petersson, G. A.; Smith, J. M.; Behrendt, D.*; Ma, J.; Letendre, L.; Dai, H. L. The Journal of Physical Chemistry A ***2018*** 122 (46), 9001-9013*

DOI: 10.1021/acs.jpca.8b09179

3. *Is photolytic production a viable source of HCN and HNC in astrophysical environments? A laboratory based feasibility study of methyl cyanoformate*. M.J. Wilhelm, E. Martínez-Núñez, J. González-Vázquez, S. A Vázquez, J.M. Smith, H.-L. Dai, The Astrophysical Journal, **2017**, 849 (1), 15.
4. *Note: Reconstructing interferograms improves spectral SNR*. M.J. Wilhelm, J.M. Smith, H.-L. Dai, Journal of Chemical Physics **2016**, 145 (3), 036101.
5. *Large cross-section for super energy transfer from hyperthermal atoms to ambient molecules*. J. Ma, M.J. Wilhelm, J.M. Smith and H.-L. Dai, Physical Review A **2016,** 93 (4), 040702 (Rapid Communication) https://journals.aps.org/pra/abstract/10.1103/PhysRevA.93.040702.
6. *Predissociation of methyl cyanoformate: The HCN and HNC channels* M.J. Wilhelm, E. Martínez-Núñez, J. González-Vázquez, S.A. Vázquez, J. M. Smith, H.-L. Dai. arXiv preprint arXiv:1606.06230 **2016.**
7. *Spectral reconstruction analysis for enhancing signal-to-noise in time-resolved spectroscopies*. M.J. Wilhelm, J.M. Smith, and H.-L. Dai, Journal of Chemical Physics **2015,** 143 (12), 124204.
8. *Chemical Activation through Super Energy Transfer Collisions.* J.M. Smith, M. Nikow, J. Ma, M.J. Wilhelm, Y.-C. Han, A. R. Sharma, J. M. Bowman, H.-L. Dai, Journal of the American Chemical Society **2014,** 136 (5), 1682-1685.
9. *The lowest quartet-state of the ketenyl (HCCO) radical: Collision-induced intersystem crossing and the vibrational mode,* M.J. Wilhelm, W. McNavage, J.M. Smith, and H.-L. Dai, Chemical Physics **2013,** 422 (0), 290-296
10. *Collisional Energy Transfer from Highly Vibrationally Excited Radicals is Very Efficient,* M.J. Wilhelm, M. Nikow, J.M. Smith, H.-L. Dai, *The Journal of Physical Chemistry Letters*, **2012,** 4 (1), 23-29 [2012 Impact Factor: 6.585]
11. *Photolysis (193 nm) of SO_2: Nascent Product Energy Distribution Examined through IR Emission,* J. Ma, M.J. Wilhelm, J.M. Smith, H.-L. Dai,. *The Journal of Physical Chemistry A* **116**, 166-173 (**2012**).
12. *Strong combination-band IR emission from highly vibrationally excited acetylene,* Matthew Nikow, M.J. Wilhelm, J.M. Smith and H.-L. Dai, *Phys. Chem. Chem. Phys.* **2010,** *12* (12), 2915-2922
13. *Computational and Spectroscopic Investigation of 7 -azaindole Solvation and Intermolecular Interactions,* M. Z. Kamrath*, K.M. Cruse*, N.R. Erickson*, M. B. Beernink*, and J.M. Smith, Abstracts of Papers of American Chemical Society, **233**, PHYS 264, (2007).
14. *Universal solvation models and their applications*, D. G. Truhlar, C.P. Kelly, A. V. Marenich, A. Chamberlin, J.M. Smith, P. Jaque, N. Elmasry, and C. J. Cramer, Abstracts of Papers of American Chemical Society, **233**, COMP 89, (2007).
15. *Cluster-based molecular modeling to enrich the undergraduate chemistry curriculum,* J.M. Smith, Abstracts of Papers of American Chemical Society, **228**, CHED 223 (2004).
16. *Computational chemistry in the physical chemistry curriculum,* J.M. Smith, Abstracts of Papers of American Chemical Society, **222**, PHYS 31, (2001).
17. *Spectroscopic and computational study of charge-transfer in 4-dimethylamino-4'-nitrostilbene,* B. Barker* Y. Soo Hoo*, and J.M. Smith, Abstracts of Papers of American Chemical Society, **222**, PHYS 270, (2001).
18. *Evidence for a Deep Cooper Minimum in the 3s - np Channel of ND_4*, J.M. Smith and W. A.

Chupka, Chemical Physics Letters **250**, 589 (1996).

19. *Molecular Beam Characterization of Hg*-$(NH_3)_n$ n = 1, 2*, J.M. Smith and W. A. Chupka, Abstracts of Papers of American Chemical Society, **212**, 152-PHYS (1996).
20. *Electron Transfer in High n Rydberg States*, J.M. Smith and W. A. Chupka, Journal of Chemical Physics, **103**, 3436 (1995).
21. *Trace Detection of NO_2 by Frequency-Modulation-Enhanced Magnetic Rotation Spectroscopy,* J.M. Smith, J. C. Bloch, R. W. Field, and J. I. Steinfeld, Journal of the Optical Society America B, **12**, 964 (1995).
22. *Intramolecular Relaxation of S_1 Benzene Studied with Picosecond Photoionization and Photoelectron Spectroscopy*, X. Zhang, J. L. Knee, and J.M. Smith, Journal of Chemical Physics, **101,** 1768 (1995).
23. *Threshold Ionization Spectroscopy of the Low Frequency Vibrational Modes of Styrene and Trans-stilbene Cations*, J.M. Smith and J. L. Knee, Laser Chemistry, **14**, 131 (1994).
24. *Picosecond Vibrational Dynamics of Several S_1 Bands in Jet-cooled p-difluorobenzene*, X. Zhang, J.M. Smith, and J. L. Knee, Journal of Chemical Physics, **100**, 2429 (1994).
25. *Aniline-CH_4 S_1 Vibrational Dynamics Studied with Picosecond Photoelectron Spectroscopy,* J.M. Smith, X. Zhang, and J. L. Knee, Journal of Chemical Physics, **99**, 2550 (1993).
26. *Analysis of the Torsional Potential of 9,10-dihydrophenanthrene in Three Electronic States: S_0 , S_1 and Cation Ground State*, J.M. Smith and J. L. Knee, Journal of Chemical Physics, **99**, 38 (1993).
27. *Electronic Spectroscopy of Four Conformations of Jet-Cooled 1,6-dihydroxynaphthalene*, J.M. Smith, X. Zhang, A. Thompson*, C. Lakshminayaran and J. L. Knee, Journal of Physical Chemistry, **97**, 3990 (1993).
28. *Dynamics of High n Molecular Rydberg States with Application to Mass Analyzed Threshold Ionization Spectroscopy*, X. Zhang, J.M. Smith, and J. L. Knee, Journal of Chemical Physics, **99**, 3133 (1993).
29. *High Resolution Zero Electron Kinetic Energy Photoelectron Spectroscopy of Aniline and Aniline van der Waals Complexes*, X. Zhang, J.M. Smith and J. L. Knee, Journal of Chemical Physics, **97**, 2843 (1992).
30. *Laser Photoelectron Spectroscopy of 1- and 2-naphthol: Relative Stability of the Cis and Trans Cation Rotamers*, C. Lakshminarayan, J.M. Smith, and J. L. Knee, Chemical Physics Letters, **182**, 656 (1991).
31. *Picosecond Measurements of Vibrational Dynamics Using Pump-Probe Laser Photoelectron Spectroscopy*, J.M. Smith, C. Lakshminarayan, and J. L. Knee, Journal of Chemical Physics, **93**, 4475 (1990).
32. *Photochemistry in Strongly Absorbing Media*, J. R. Sheets, J.M. Smith, and J. R. Diamond, Journal of Physical Chemistry, **92**, 4922 (1988).

**undergraduate co-author*

TEXT BOOKS

Molecular Physical Chemistry Primer, Jonathan M. Smith, ISBN: 9781942526735, Quantum Curiosity, iBook (2018)

COMPUTER PROGRAMS

https://github.com/laserchemist/datascience	February 2024
https://github.com/laserchemist/spectral_compare	June 2019
https://github.com/laserchemist/GAMESS	December 2018

WebAMBER: Molecular Dynamics Web Front-End, version 0.9 July 2006
B. Magnusson ('05) and J.M. Smith; http://pandora.chem.gac.edu/amber.html
pKa Calculator: Web based calculator, version 1.0 June 2004
M. Klamrath ('07) and J.M. Smith; http://bert.chem.gac.edu/~modeling/kamrath/javacalc.html

COMPUTER LANGUAGES

Fortran, C/C++, Java/Javscript, Python, R, Perl

MAJOR RESEARCH AND CURRICULAR GRANTS

Norwegian Ministry of Education and Research Submitted April 2022
Open World Learning *Denied $436,000*

Fulbright Scholar Finalist - Alternate 2020-2021
Oslo, Norway
High Energy Chemistry: Atmospheric Chemistry Above the Boreal Forest

National Science Foundation-Major Research Instrumentation August 2019-
(#1919571) co-PIs (B. Krueger, J. Gillmore, W. Polik, D. Kohen, July 2022
K. Kuwata and E. Speetzen) *$400,400*
Role: Senior Collaborating Faculty
MRI: Acquisition of a High Performance Computing Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium

National Science Foundation-Major Research Instrumentation September 2010-
(#1039925) co-PI (with W. Polik, D. Kohen, B. Krueger, and K. Kuwata) September 2014
Role: Collaborating consortium Faculty *$299,942*
Acquisition of a Computer Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C)

HHMI Undergraduate Science Program Grant April 2008
Lead co-author and first program director *$1,000,000*

National Science Foundation -RSEC Fellowship Grant January 2006
Simulation of Solvent Effects on Resonance Raman Spectra *$10,161*
University of Minnesota collaborators: Donald Truhlar and Chris Cramer

National Science Foundation-Major Research Instrumentation July 2005
(#0520704), co-PI (with Will Polik, Dani Kohen, Brent Krueger, & Keith Kuwata) *$379,606*
Acquisition of a Computer Cluster for Research, Research Training, and Teaching

National Science Foundation -CCLI July 2003
Molecular Modeling as a Theme in the Undergraduate Chemistry Curriculum *$108,551*

American Chemical Society Petroleum Research Fund Type GB June 2003
Probing the electronic structure and dynamics of stilbene derivatives *$35,000*

Merck/AAAS Undergraduate Science Program May 2003
One of seven biology and chemistry faculty grantees *$60,000*

Camille and Henry Dreyfus Faculty Start-Up Award September 1999
Investigation of Stilbene Derivatives Exhibiting Intramolecular Charge-Transfer: Computational and Spectroscopic Study *$20,000*

INVITED TALKS AND CONFERENCE PARTICIPATION (SELECTED)

Elements of Data Science for STEM Majors is Many Problems Solved
Jonathan Smith, Susan Jansen Varnum, and Michael L. Klein
2023 AAC&U Conference on Transforming STEM Higher Education,
Crystal City, Virginia November 2023

Machine Learning Potential Energy Surfaces
Belinta Naomi Simiyu*, Dr. Jonathan Smith
NOBCChe 50th Annual Meeting, New Orleans, Louisiana September 2023

Machine Learning Potential Energy Surfaces
Belinta Naomi Simiyu*, Dr. Jonathan Smith
Midwest Undergraduate Computational Chemistry Consortium,
Winter Virtual Conference February 2023

Molecular Dynamics on Machine Learning Optimized Potential Energy Surfaces
Jonathan Smith, NKS quantum chemistry and modeling:
virtual autumn meeting November 2020

Theoretical Anharmonic Vibrational Spectroscopy on Machine Learning Optimized Potential Energy Surfaces
Jonathan Smith, University of Oslo, Norway February 2020

Modeling Anharmonic Vibrational Spectroscopy: Mapping Vibrational Spectroscopy onto Molecular Structure and Dynamics May 2019
Jonathan Smith, Hylleraas Spring Meeting, Bardufoss, Norway

Chemical Reaction Dynamics: Insights from Theory and Experiment February 2019
Jonathan Smith, Hylleraas Centre for Quantum Molecular Science,
University of Oslo, Oslo, Norway (Invited Talk)

Theoretical Photolytic Sources of HCN/HNC in the Interstellar Medium August 2017
D. Behrendt and J.M. Smith, Midwest Undergraduate Computational
Chemistry Symposium, University of Illinois at Champaign-Urbana

Non-Norrish type production of HCN in the UV photolysis of asymmetric ketones, August 2016
V. Trunnikova*, S. Rachmil-Etter*, J.M. Smith, M. Wilhelm,
and H.-L. Dai, American Chemical Society, Fall National meeting, Philadelphia

Time resolved infrared emission of highly excited acetylene derivatives August 2016
with an indirect signature of elusive vinylidene species, L. Digiacobbe*,
J.M. Smith, M. Wilhelm, and H.-L. Dai, American Chemical
Society, Fall National meeting, Philadelphia

Efficient Super Energy Transfer Collisions Through Reactive-Complex June 2015
Formation: H + SO_2, J.M. Smith, M. J. Wilhelm, J. Ma, and H.-L. Dai,
70th International Symposium on Molecular Spectroscopy,
University of Illinois, Champaign-Urbana, Illinois

Improving SNR in Time-Resolved Spectroscopies without Sacrificing June 2015
Temporal-Resolution: Application to the UV Photolysis of Methyl Cyanoformate,
M.J. Wilhelm, J.M. Smith, and H.-L. Dai, 70th International Symposium on Molecular
Spectroscopy, University of Illinois, Champaign-Urbana, Illinois

Formation of vibrationally excited acetylene following 193 nm photolysis July 2011

of HBr and H_2S followed be time resolved IR emission,
Dynamics of Molecular Collisions 2011, Snowbird Utah (Poster)

High energy intermediates in combustion reactions: A study of Vinylidene. July 2011
using Born-Oppenheimer molecular dynamics. M. Fennimore* and
J.M. Smith, Midwest Undergraduate Computational Chemistry Symposium,
University of Chicago

2-Dimensional Nanosecond Time-Resolved FTIR Emission Spectroscopy of June 2011
transient radicals, 2D-COS Conference, Sonoma, CA (Invited Talk)

Probing highly vibrationally excited acetylene: Energy transfer December 2010
mediated by acetylene/vinylidene isomerization, Wesleyan University,
Middletown, CT (Invited Talk)

Computational and spectroscopic investigation of 7-azaindole: Solvation July 2007
and intermolecular interactions, (student: Nathan Erickson)
Midwest Undergraduate Computational Chemistry Conference
University of Illinois, Champaign-Urbana, IL

Computational and Spectroscopic Investigation of 7 -azaindole Solvation April 2007
and Intermolecular Interactions, American Chemical Society Spring National
meeting, Chicago.

Midwest Undergraduate Computational Chemistry August 2006
Conference, discussant, Iowa State University, Ames, IA

Computational Analysis of Small Proteins using a Revised Web–AMBER August 2005
Interface, (student: Eddie Gorr) Midwest Undergraduate
Computational Chemistry Conference, University of Minnesota, Minneapolis, MN

Computational and Spectroscopic Approach to Unraveling Protein Structure August 2005
(student: Mike Kamrath), Midwest Undergraduate
Computational Chemistry Conference, University of Minnesota, Minneapolis, MN

Development of a Computational Cluster and Tools August 2004
(student: Brent Magnusson), Midwest Undergraduate
Computational Chemistry Conference, University of Wisconsin, Madison, WI

Cluster-based molecular modeling to enrich the undergraduate August 2004
chemistry curriculum, NSF Catalyzed Innovations Symposium,
228th National American Chemical Society Meeting, Philadelphia, PA

Molecular modeling in the biochemistry curriculum, April 2002
American Society for Biochemistry and Molecular Biology (ASBMB)
Annual Meeting, New Orleans, LA

Twist and Shout, Chemistry Seminar, March 2002
College of Saint Benedict and Saint John's University, St. Joseph, MN

Computational Chemistry and Biology Workshop July 2001
Project Kaleidoscope Summer 2001 Institute, Snowbird, UT,
Workshop Organizer (leader and presenter)

Twist and Shout: Spectroscopic studies on systems, that undergo dramatic October 1999
changes upon absorption of light,
Chemistry Seminar, Carleton College, Northfield MN

Insights from Spectroscopic and Computational Study, February 1999
Chemistry Seminar, Bates College, Lewiston, ME

The Influence of Intermolecular Interactions on the Lifetime September 1993
of High *n* Molecular Rydberg States, European Research Conference,

"Very High Resolution Spectroscopy with Photoelectrons", Giens, France

INVITED REVIEWS

OpenStax Chemistry, Rice University (open source text), lead reviewer	Spring 2016
National Science Foundation, CAREER program reviewer	Fall 2007
Introduction to Molecular Thermodynamics by Robert Hanson University Science Books	November 2006
American Chemical Society Petroleum Research Foundation proposal reviewer	August 2004- present
National Science Foundation, CCLI panel review, Washington, DC	February 2004

PROFESSIONAL MEMBERSHIPS

American Chemical Society; American Association for Advancement of Science (AAAS); Sigma Xi; Project Kaleidoscope, Faculty for the 21st Century, appointed June 2001

STUDENT RESEARCH COLLABORATORS

Temple University: Belinta Naomi Simiyu `26; Tarek Fayed `19; Drew Behrendt `20; Truc Pham `18; Andrei Dzekola `18; Leah Digiacobbe `16; Sam Rachmil-Etter `16 *(PhD candidate, University of Colorado at Boulder, Inaugural ACS undergraduate physical chemistry award winner)*; Viktoriya Trunnikova `16; Oluwaremi Oladeinde `15; Benjamin Datko`13 *(PhD student, University of New Mexico, Chemistry)*; Lynne Huang`12; Nader Anz`12; Mark Fennimore`11*(Quaker Chemical);* Tek Chan `11; Akash Patel `11; Vidhi Sudhani`10 (*D.Ph. Temple)*

University of Oslo: Julie Héron, Phd 2021 (Committee Chair)

Gustavus Adolphus College: Molly Wilker (Beernink) `09 *(PhD, University of Colorado, Chemistry, Assistant Professor Luther College)*; Mark Pedginski `11; Nathaniel Swenson, Gustavus `09, *(PhD student, Northwestern University, Chemistry)*; Nathan Erickson `08; Krista Cruse, `07, (*PhD, Michigan State University, Chemistry; staff scientist at Los Alamos National Laboratory);* Mike Kamrath, Gustavus `07 *(PhD , Yale University `12);* Brent Magnusson `06 (*PhD., Univ. of Tennessee)*; David Baldes `05; Justin Scanlan`04 (*Employed at Bimeda – Osborn, LeSueur, MN)*; Dave Bernhardson `04, (*Ph.D., Yale University, Chemistry)*; Luke Twedt, `04 *(Pharmacy student, U. Minnesota);* Brooks Maki `04, *(Ph.D. student, Northwestern University, Chemistry);* Beau Barker `03, (*Ph.D student, University of Minnesota, Chemistry);* Mike Bradley `02, *(Ph.D., Postdoctoral Fellow, Yale University, Biophysics, National Science Foundation doctoral fellowship awardee)*; Adam Beers`02, (*DMD, University of Minnesota)*; Donnie Berkholz, Univ. of Richmond `04 *(Ph.D. Oregon State University, Computational Structural Biology)*; Margaret Broz `02, Ph.D, *(Ph.D. University of Minnesota, Chemistry)*; Dave Savage `01 (*Ph.D, UCSF, Chemistry, UC Berkeley Chemistry Faculty);* Kelly Devine`01 (*Research Chemist, 3M Corp.);* Yong Soo Hoo `01, *(Ph.D, Chemistry SUNY Stony Brook)*

Bowdoin College: Rachel Niemer, Honors Thesis `99 (Ph.D California Institute of Technology, Chemistry, 2006); Laurie McDonough, Honors Thesis `98 (Ph.D Berkeley Chemistry, 2006)