J. Daniel Gezelter

Professor and Director of Undergraduate Studies
Department of Chemistry and Biochemistry
251 Nieuwland Science Hall (574) 631-7595
University of Notre Dame gezelter@nd.edu
Notre Dame, IN 46556 gezelterlab.org

Education

PhD, Chemistry *University of California at Berkeley*
1995 Research Advisor: William H. Miller

CPS, Chemistry *Churchill College, University of Cambridge*
1990 Research Advisor: Ray Freeman

BS, Chemistry & Philosophy *Duke University*
1989 *cum laude and with Distinction in Chemistry*
Senior Thesis Advisors: Donald B. Chesnut and Richard A. MacPhail

Appointments

Professor *Department of Chemistry & Biochemistry, University of Notre Dame*
2015 - present

Associate Professor *Department of Chemistry & Biochemistry, University of Notre Dame*
2005 - 2015

Assistant Professor *Department of Chemistry & Biochemistry, University of Notre Dame*
1999 - 2005

Postdoctoral Research Scientist *Department of Chemistry, Columbia University*
1996 - 1999 Research Advisor: Bruce J. Berne

Honors, Awards, and Fellowships

2013 Rev. Edmund P. Joyce Award for Excellence in Undergraduate Teaching

2002 NSF Faculty Early Career Development (CAREER) Award

1999 Henry & Camille Dreyfus New Faculty Award

1990-1993 National Science Foundation Graduate Fellowship in Chemistry

1989 Churchill Scholar

Research Interests

- Development of methodology for advanced molecular simulations. Specific interests in: real-space methods for electrostatic interactions, non-equilibrium molecular dynamics, Langevin dynamics for rigid molecular substructures, and coarse-grained modeling for membranes and liquid crystals
- Simulations of mass and energy transport at complex heterogeneous interfaces. Specific interests in: thermal conductivity at metal / ligand / solvent interfaces, vibrational and alloying dynamics in metallic nanoparticles, the behavior of ice / water interfaces, friction and tribology
- Spectroscopy in condensed phases
- Dynamics and thermodynamics of non-equilibrium condensed phases (e.g. glasses and ice polymorphs)
- Open-source scientific software

Professional Memberships

American Chemical Society
American Physical Society

Publications

Key: $ = undergraduate, @ = graduate student, % = post-doc, † = faculty, * = corresponding authors
Citation counts from Web of Science as of September 11, 2017.

1. Suzanne M. Neidhart@ and J. Daniel Gezelter†*, " Reverse Non-Equilibrium Molecular Dynamics Predicts That Thermal Transport is Influenced by Nanoparticle Morphology," submitted to *ACS Nano* (2017).

2. Patrick B. Louden@ and J. Daniel Gezelter†*, "Friction at Ice-I_h / Water interfaces is governed by solid / liquid hydrogen-bonding" submitted to *J. Phys. Chem. C* (2017).
Early version at arXiv: 1501.01056

3. Madan Lamichhane@, Thomas Parsons$, Kathie Newman†, and J. Daniel Gezelter†* "Real Space Electrostatics for Multipoles. III. Dielectric Properties," *J. Chem. Phys.* **145**, 074108 (2016).
DOI: 10.1063/1.4960957, arXiv: 1608.04970
0 citations, IF = 3.1

4. Joseph R. Michalka@, Andrew P. Latham$, and J. Daniel Gezelter †*, "CO-induced restructuring on stepped Pt surfaces: A molecular dynamics study," *J. Phys. Chem. C* **120** (32), pp. 18180-18190, (2016).
DOI: 10.1021/acs.jpcc.6b06619, arXiv: 1608.05833
1 citation, IF=4.8

5. Kelsey M. Stocker@, Suzanne Niedhart@ and J. Daniel Gezelter †*, "Interfacial Thermal Conductance of Thiolate-Protected Gold Nanospheres," *J. Appl. Phys.* **119** (2), 025106 (2016).
DOI: 10.1063/1.4939956, arXiv: 1601.03315
1 citation, IF=2.2

6. Joseph R. Michalka@, and J. Daniel Gezelter†*, "Island Formation on Pt/Pd(557) Surface Alloys in the Presence of Adsorbed CO: A Molecular Dynamics Study," *J. Phys. Chem. C*, 119 (25), pp 14239–14247 (2015).
DOI: 10.1021/acs.jpcc.5b03586
1 citation, IF=4.8

7. Daniel C. Hannah@, J. Daniel Gezelter†, Richard D. Schaller†, and George C. Schatz†*, "Reverse Non-Equilibrium Molecular Dynamics Demonstrates that Surface Passivation Controls Thermal Transport at Semiconductor-Solvent Interfaces," ACS Nano 9 (6), pp 6278–6287 (2015)..
DOI: 10.1021/acsnano.5b01724
2 citations, IF = 12.0

8. J. Daniel Gezelter†*, "Open Source and Open Data Should be Standard Practices," *J. Phys. Chem. Lett.* **6** (7), pp. 1168-1169 (2015).
DOI: 10.1021/acs.jpclett.5b00285
6 citations, IF = 6.7

9. Madan Lamichhane[@], J. Daniel Gezelter[†*], and Kathie Newman[†], "Real Space Electrostatics for Multipoles. I. Development of Methods," *J. Chem. Phys.* **141** (13), 134109 (2014).
DOI: 10.1063/1.4896627
6 citations, IF = 3.1

10. Madan Lamichhane[@], Kathie Newman[†], and J. Daniel Gezelter[†*], "Real Space Electrostatics for multipoles. II. Comparison with the Ewald Sum," *J. Chem. Phys.* **141** (13), 134110 (2014).
DOI: 10.1063/1.4896628
5 citations, IF = 3.1

11. James M. Marr[@] and J. Daniel Gezelter[†*], "Nitrile vibrations as reporters of field-induced phase transitions in 4-cyano-4'-pentylbiphenyl (5CB)," *J. Phys. Chem. B* **118** (28) pp. 8441-8448 (2014)
DOI: 10.1021/jp503235s
0 citations, IF = 3.4

12. Kelsey M. Stocker[@], and J. Daniel Gezelter[†*], "A method for creating thermal and angular momentum fluxes in non-periodic simulations," *J. Chem. Theory Comput.* **10** (5), pp. 1878-1886 (2014)
DOI: 10.1021/ct500221u
4 citations, IF = 5.3

13. Patrick B. Louden[@] and J. Daniel Gezelter[†*], "Simulations of solid-liquid friction at ice-I_h / water interfaces," *J. Chem. Phys.* **139**, 194710 (2013)
DOI: 10.1063/1.4832378
2 citations, IF = 3.1

14. Joseph R. Michalka[@] , Patrick W. McIntyre[$] , and J. Daniel Gezelter[†*], "Molecular Dynamics Simulations of the Surface Reconstructions of Pt(557) and Au(557) under Exposure to CO," *J. Phys. Chem. C* **117**, pp 14579–14587 (2013)
DOI: 10.1021/jp402798n
4 citations, IF = 4.8

15. Kelsey M. Stocker[@] and J. Daniel Gezelter[†*] "Simulations of Heat Conduction at Thiolate-Capped Gold Surfaces: The Role of Chain Length and Solvent Penetration," *J. Phys. Chem. C* 117(15) pp. 7605-7612 (2013)
DOI: 10.1021/jp312734f
10 citations, IF = 4.8

16. Shenyu Kuang[@] and J. Daniel Gezelter[†*], "Velocity Shearing and Scaling RNEMD: a minimally perturbing method for simulating temperature and momentum gradients," *Mol. Phys.* 110, pp. 691-701 (2012)
DOI: 10.1080/00268976.2012.680512
8 citations, IF = 1.6

17. Shenyu Kuang[@] and J. Daniel Gezelter[†], "Simulating Interfacial Thermal Conductance at Metal-Solvent Interfaces: The Role of Chemical Capping Agents," *J. Phys. Chem. C*, **115**(45), pp. 22475-22483, (2011)
DOI: 10.1021/jp2073478
22 citations, IF = 4.8

18. Charles F. Vardeman II[@], Kelsey M. Stocker[@], and J. Daniel Gezelter[†*], "The Langevin Hull: Constant pressure and temperature dynamics for non-periodic systems," *J. Chem. Theory Comput.* 7(4), 834-842 (2011)
DOI: 10.1021/ct100670m
3 citations, IF = 5.3

19. Shenyu Kuang[@] and J. Daniel Gezelter[†*], "A gentler approach to RNEMD: Non-isotropic Velocity Scaling for computing thermal conductivity and shear viscosity," *J. Chem. Phys.* **133**, 164101 (2010)
DOI: 10.1063/1.3499947
13 citations, IF = 3.1

20. Victoria Stodden[%*], David Donoho[†], Sergey Fomel[†], Michael P. Friedlander[†], Mark Gerstein[†], Randy LeVeque[†], Ian Mitchell[†], Lisa Larrimore Ouellette[%], Chris Wiggins[†], Nicholas W. Bramble[%], Patrick O. Brown, Vincent J. Carey, Laura DeNardis[†], Robert Gentleman, J. Daniel Gezelter[†], Alyssa Goodman[†], Matthew G. Knepley[†], Joy E. Moore, Frank A. Pasquale[†], Joshua Rolnick[†], Michael Seringhaus[%], and Ramesh Subramanian[†], "Reproducible Research: Addressing the Need for Data and Code Sharing in Computational Science," *Computing in Science and Engineering* **12**(5) pp. 8-13 (2010)
DOI:10.1109/MCSE.2010.113
0 citations, IF = 1.7

21. Xiuquan Sun[@] and J. Daniel Gezelter[†*], "Langevin Dynamics for Rigid Bodies of Arbitrary Shape," *J. Chem. Phys.* **128**, 24107 (2008)
DOI: 10.1063/1.2936991
21 citations, IF = 3.1

22. Charles F. Vardeman II[@] and J. Daniel Gezelter[†*], "Simulations of laser-induced glass formation in Ag-Cu nanoparticles," *J. Phys. Chem. C*. 112, 3283-3293 (2008)
DOI: 10.1021/jp710063g
6 citations, IF = 4.8

23. Xiuquan Sun[@] and J. Daniel Gezelter[†*], "Dipolar ordering in the ripple phases of molecular-scale models of lipid membranes," *J. Phys. Chem. B*. **112**, pp. 1968- 1975 (2008)
DOI: 10.1021/jp0762020
16 citations, IF = 3.4

24. Xiuquan Sun[@] and J. Daniel Gezelter[†*], "Spontaneous Corrugation of Dipolar Membranes," *Phys. Rev. E* **75**, 031602 (2007)
DOI: 10.1103/PhysRevE.75.031602
2 citations, IF = 2.3

25. Christopher J. Fennell[@] and J. Daniel Gezelter[†*], "Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics," *J. Chem. Phys.*, **124**, 234104 (2006)
DOI: 10.1063/1.2206581
249 citations, IF = 3.1

26. Christopher J. Fennell[@] and J. Daniel Gezelter[†*], "Computational free energy studies of a new ice polymorph which exhibits greater stability than Ice Ih," *J. Chem. Theory Comput.* **1**, pp. 662-667 (2005)
DOI: 10.1021/ct050005s
20 citations, IF = 5.3

27. Matthew A. Meineke[@], Charles F. Vardeman II[@], Teng Lin[@], Christopher J. Fennell[@] and J. Daniel Gezelter[†*], "OOPSE: An Object-Oriented Parallel Simulation Engine for Molecular Dynamics," *J. Comput. Chem.* **26**, pp. 252-271 (2005)
DOI: 10.1002/jcc.20161
28 citations, IF = 3.6

28. Charles F. Vardeman II[@], Patrick F. Conforti[$], Megan M. Sprague[$], and J. Daniel Gezelter[†*], "Breathing Mode Dynamics and Elastic Properties of Gold Nanoparticles," *J. Phys. Chem. B* (2005)
DOI: 10.1021/jp051575r
7 citations, IF = 3.4

29. Christopher J. Fennell[@] and J. Daniel Gezelter[†*], "On the structural and transport properties of the Soft Sticky Dipole (SSD) and related single-point water models," *J. Chem. Phys.* 120, 9175-9184 (2004)
DOI: 10.1063/1.1697381
19 citations, IF = 3.1

30. Tomohiro Shibata[@], Bruce A. Bunker[†*], Zhenyuan Zhang[%], Dan Meisel[†*], Charles F. Vardeman II[@], and J. Daniel Gezelter[†*], "Size Dependent Spontaneous Alloying of Au-Ag Nanoparticles," *J. Am. Chem. Soc.* **124**, 11898-11996 (2002)
DOI: 10.1021/ja026764r
292 citations, IF = 11.4

31. Matthew A. Meineke[@] and J. Daniel Gezelter[†*], "A Random Sequential Adsorption model for the differential coverage of Gold (111) surfaces by two related Silicon phthalocyanines, *J. Phys. Chem. B.* **105**, 6515-6519 (2001)
DOI: 10.1021/jp010985m
6 citations, IF = 3.4

32. Charles F. Vardeman II[@] and J. Daniel Gezelter[†*], "Comparing models for diffusion in supercooled liquids: The eutectic composition of the Ag-Cu alloy, *J. Phys. Chem. A*, **105**, 2568-2574 (2001)
DOI: 10.1021/jp0035784
11 citations, IF = 2.8

33. Eran Rabani[%], J. Daniel Gezelter[%], and B.J. Berne[†*], "Response to 'Comment on "Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function"'," *Phys. Rev. Lett.* **85**, 467 (2000)
DOI: 10.1103/PhysRevLett.85.467
5 citations, IF = 7.7

34. Eran Rabani[%], J. Daniel Gezelter[%], and B.J. Berne[†*], "Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function" *Phys. Rev. Lett.* **82**, 3649 (1999)
DOI: 10.1103/PhysRevLett.82.3649
55 citations, IF = 7.7

35. J. Daniel Gezelter[%], Eran Rabani[%], and B.J. Berne[†*], "Calculating the hopping rate for diffusion in molecular liquids: CS_2," *J. Chem. Phys.* **110**, 3444 (1999)
DOI: 10.1063/1.478211
22 citations, IF = 3.1

36. J. Daniel Gezelter%, Eran Rabani%, and B.J. Berne†*, "Response to 'Comment on a Critique of the Instantaneous Normal Mode (INM) Approach to Diffusion'," *J. Chem. Phys.* **109**, 4695 (1998)
DOI: 10.1063/1.477081
20 citations, IF = 3.1

37. Eran Rabani%, J. Daniel Gezelter%, and B.J. Berne†*, "Calculating the hopping rate for self-diffusion on rough potential energy surfaces: cage correlations," *J. Chem. Phys.* **107**, 6867 (1997)
DOI: 10.1063/1.474927
77 citations, IF = 3.1

38. J. Daniel Gezelter%, Eran Rabani%, and B.J. Berne†*, "Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?" *J. Chem. Phys.* 107, 4618 (1997)
DOI: 10.1063/1.474822
82 citations, IF = 3.1

39. J. Daniel Gezelter@ and William H. Miller†*, "Dynamics of the Photodissociation of Triplet Ketene," *J. Chem. Phys.* **104**, 3546 (1996)
DOI: 10.1063/1.471059
23 citations, IF = 3.1

40. J. Daniel Gezelter@ and William H. Miller†*, "Resonant features in the energy dependence of the rate of ketene isomerization," *J. Chem. Phys.* **103**, 7868 (1995)
DOI: 10.1063/1.470204
34 citations, IF = 3.1

41. Simon W. North@, David A. Blank@, J. Daniel Gezelter@, Cheryl A. Longfellow@, and Yuan T. Lee†*, "Evidence for Stepwise Dissociation Dynamics of Acetone at 248 nm and 193 nm," *J. Chem. Phys.* **102**, 4447 (1995)
DOI: 10.1063/1.469493
193 citations, IF = 3.1

42. Thomas D. Sewell@, Donald L. Thompson†, J. Daniel Gezelter@, and William H. Miller†*, "Some problems of correcting the zero-point energy problem in classical trajectories," *Chem. Phys. Lett.* **193**, 512 (1992)
DOI: 10.1016/0009-2614(92)85841-W
50 citations, IF = 2.0

43. J. Daniel Gezelter@ and Ray Freeman†*, "Use of Neural Networks to Design Shaped Radio-Frequency Pulses," *J. Magn. Reson.* **90**, 397 (1990)
DOI: 10.1016/0022-2364(90)90149-4
27 citations, IF = 2.3

Publications as Software

OpenMD OpenMD is an open source parallel molecular dynamics engine that is the group's major research workhorse. (See openmd.org for more details) It has had more than **4,830** external downloads and is actively used by other research groups, notably at Southampton University (UK), Texas A&M, the University of Pittsburgh, University of Akron, Beijing University of Chemical Technology, University of Nevada at Reno, the Slovak Academy of Sciences, University of Texas El Paso, and the Los Alamos National Laboratory.

Algorithms from this program also appear in other major simulation codes (e.g. LAMMPS, and DL_POLY)

Jmol Jmol is an open source molecular dynamics viewer that originated in my lab. I was the lead developer from 1998-2002, and contribute occasionally now. Jmol has seen more than **1,178,423** downloads as an application, and *millions* more as an embedded structure viewer for chemical journals, the protein data bank and many other sites. (See jmol.sf.net for more details.) It has also been independently cited 328 times.

Jmol has evolved into *one of the most widely-used scientific software tools*.

Tilted RSA Tilted RSA is a program which performs Random Sequential Adsorption simulations on models for molecules adsorbing onto Gold surfaces. See github.com/GezelterLab/tiltedRSA for more details.

xyz2pov This is a general purpose program which generates graphical inputs to ray-tracing programs from the results of a molecular simulation. See github.com/GezelterLab/xyz2pov for more details.

Research Support

Current Awards

2014 *Real space electrostatics and non-equilibrium molecular dynamics for nanoscale transport*
NSF CHE-1362211, 7/1/2014 - 6/30/2018, $447,121 (sole-PI)

2016 *CDS&E: Method Development for Coupled Charge and Thermal Transport in Molecular Simulations*
NSF CHE-1663773, 8/1/2017 - 7/31/2020, $450,000 (sole-PI)

Completed Research Support

2012 *Design of Nanocatalysts for Selective Production of Liquid Fuels from Alternative Energy Sources: Experimental Studies and Advance Molecular Simulations*
Notre Dame SEI, $65,000, co-PI with Franklin Tao

2011 *Surface restructuring of model metal catalysts under reaction conditions: experiment and theory*
Notre Dame SEI, $65,000, co-PI with Franklin Tao

2009 *Computational Methods for Simulating Metal Nanoparticle-solvent interfaces*
NSF CHE-0848243, 8/15/2009 - 7/31/2014, $400,000 (sole-PI)

2003 *CAREER: Dynamics of Model Biological Membranes and Glass Formation in Liquid Metals*
NSF CHE-0134881, 6/19/2003 - 6/18/2008, $465,000 (sole-PI)

2002 *Acquisition of a High Performance Computing System*
NSF DMR-0079647, $320,000 (co-PI with Olaf Wiest, Laszlo Barabasi, Ed Maginn, and Mark Stadtherr)

2002 *New Faculty Award*
Camille and Henry Dreyfus Foundation, $40,000 (sole-PI)

2000 *The OpenScience Project*
Alfred P. Sloan Foundation, $30,000 (sole-PI) + $2,700 in additional private donations

Invited Lectures and Addresses

2017 "Real-Space Electrostatics," Chemical Dynamics in Complex Environments (Chem-DICE) meeting, Telluride Science Research Center, Telluride, CO

2017 "Non-Equilibrium Molecular Dynamics for Nanoscale Thermal Transport," Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, MI

2017 "Code as a Research Product: Open Source for Open Science," SIAM Conference on Computational Science & Engineering, Atlanta, GA

2016 "Simulating thermal transport at Nanoparticle Interfaces," Computational Materials Chemistry symposium at the Midwest regional ACS meeting, Manhattan, KS

2016 "Simulating thermal transport at Nanoparticle Interfaces," Thermal Transport at the Nanoscale workshop, Telluride Science Research Center, Telluride, CO

2015 "Friction at Water / Ice-I_h interfaces: Do the Facets of Ice Have Different Hydrophilicity?" Chemical Dynamics in Complex Environments (Chem-DICE) meeting, Telluride Science Research Center, Telluride, CO

2014 "Code as a Research Product: Open Source for Open Science," NIAID/NIH Bioinformatics Festival, Bethesda, MD, April 8, 2014

2014 "Thermal transport at metal nanoparticle interfaces: ligand and curvature effects," University of Nevada, Reno, NV, March 28, 2014.

2013 "Simulating heat conduction at thiolate-capped gold surfaces: chain length, solvent penetration, and surface curvature," Chemical Dynamics in Complex Environments (Chem-DICE) meeting, Telluride Science Research Center, Telluride, CO

2013 "Simulating heat conduction at thiolate-capped gold surfaces: chain length, solvent penetration, and surface curvature," Thermal Transport at the Nanoscale, Telluride Science Research Center, Telluride, CO

2012 "Dynamics at the nanoscale: modeling what goes on at the surfaces of metallic nanoparticles," Grand Valley State University, Grand Rapids, MI

2012 "Simulating mass and heat transport at the interfaces of metallic nanoparticles," Telluride Nanomaterials Conference, Telluride Science Research Center, Telluride, CO

2012 "Dynamics at the nanoscale: chemically-realistic modeling of interfacial transport," Southern Illinois University, Carbondale, IL

2010 "Open Science, Reproducible Experiments, and Experimental Archives," Archive '10 workshop on Archiving Experiments to Raise Scientific Standards. University of Utah, Salt Lake City, UT

2010 "Interesting phase behavior exhibited by coarse-grained models for lipids and water," Department of Physics, Indiana University Purdue University, Indianapolis, IN

2009 "Rippled Membranes and the Condensed Phases of Water," Andrews University, Berrien Springs, MI

2008 "From Open Source to Open Science," Open Access conference, Braga, Portugal

2008 "Real-space alternatives to the Ewald sum for electrostatic interactions," Telluride workshop on Many-Body Interactions, Telluride, CO

2008 "From Open Source to Open Science," New Communication Channels for Biology Workshop, La Jolla, CA

2008 "Rippled Membranes and Imaginary Ice: Surprises from Molecular Dynamics," Chemistry Department Seminar, Virginia Commonwealth University, Richmond, VA

2008 "Rippled Membranes and Imaginary Ice: Surprises from Molecular Dynamics," Chemistry Department Seminar, Boston College, Boston, MA

2007 "Rippled Membranes and Imaginary Ice: Surprises from Molecular Dynamics," Chemistry Department Capstone Seminar Series, Northeastern Illinois University, North Park, IL

2007 "Glass formation in bimetallic nanoparticles," Condensed Matter Seminar, Department of Physics, University of Notre Dame

2007 "Rippled Membranes and Imaginary Ice: Surprises from Molecular Dynamics," Chemistry Department Seminar, University of Memphis, Memphis, TN

2007 "Avoiding the Bottleneck in Molecular Dynamics Simulations," Department of Chemical and Biomolecular Engineering, University of Notre Dame

2005 "(The Math Underlying) Computer Simulations of Water Phase Transitions," Applied Math Seminar, Department of Mathematics, University of Notre Dame

2004 "Simulations of slow condensed phases: Rippled Membranes and Imaginary Ice," Chemistry Department Seminar, University of Kansas, Lawrence, KS

2004 "Anomalous Dynamics in Metallic Glasses and Core-Shell Nanoparticles," Inorganic Chemistry Seminar Series, Department of Chemistry, University of Notre Dame, Notre Dame, IN

2003 "Simulations of slow condensed phases: Metallic Glasses, Alloying & Vibrating Nanoparticles," and
"Simulations of slow condensed phases: Rippled Membranes (with a side of water)," Joint Harvard, MIT, and Boston University theoretical chemistry seminar series, Cambridge, MA

2003 "Mesoscale Models for Phospholipid Simulations," CERC3 Workshop on Computer Modelling of Chemical and Biological Systems, Porto, Portugal

2003 "Anomalous Dynamics in Metallic Nanoparticles," Theoretical Chemistry Institute Seminar, University of Wisconsin, Madison, WI

2002 "Anomalous Dynamics in Metallic Nanoparticles," Joint Georgia Tech and Emory University Chemical Physics Lecture Series, Atlanta, GA

2001 "Dynamics of Diffusion in Metallic Glasses and in Bimetallic Core-Shell Nanoparticles," Departmental Seminar in Chemical Engineering, University of Notre Dame, Notre Dame, IN

2001 "The alloying mechanism in bimetallic core-shell nanoparticles," Midwest Theoretical Chemistry Conference, Minneapolis, MN

2001 "Random Sequential Adsorption on surfaces and the Dynamics of Diffusion in Metallic Glasses," Physical Chemistry seminar series, Department of Chemistry, University of Notre Dame, Notre Dame, IN

2001 "Cage correlations and Continuous-time Random Walks in a model glass-former," Miller Chemical Dynamics Conference, Berkeley, CA

2001 "A Reductionist Model for Ripple Phase Formation in Phospholipid Membranes," 2001 Mesilla meeting on Biomembranes, Mesilla, NM

1999 "Self-Diffusion in Condensed Phases: Hopping Times & Cage Correlations," NIDDK Chemical Physics Seminar, National Institutes of Health

1998 "Self-Diffusion in Condensed Phases: Hopping Times & Cage Correlations," Department of Chemistry & Biochemistry, University of Notre Dame

1997 "Diffusion in Condensed Phases: Instantaneous Normal Modes of Cage Correlations?" Department of Chemistry, Iowa State University

---

Contributed Lectures & Addresses

2014 "Molecular dynamics methodologies for nanoscale transport," Department of Chemistry, University of Notre Dame, October 14, 2014

2012 "Developing gentler approaches to reverse nonequilibrium molecular dynamics (RNEMD) for computing transport properties," ACS national meeting, San Diego

2012 "Simulating interfacial thermal conductance at metal-solvent interfaces: The role of chemical capping agents," ACS national meeting, San Diego

2010 "Constant pressure and temperature dynamics for non-periodic systems using the convex hull," ACS national meeting, San Francisco, CA

2009 "Real-Space Alternatives to the Ewald Sum for Electrostatic Interactions," 2009 ACS Great Lakes Regional Meeting, Lincolnshire, IL

2007 "Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long range electrostatics," ACS national meeting, Chicago, IL

1999 "Catalyzing Open Source development in science: The OpenScience Project," OpenSource / OpenScience conference at Brookhaven National Labs

1999 "On the Cage-correlation Function," CECAM workshop on the INM Approach to Dynamics in Liquids, Lyon, France.

1997 "Instantaneous Normal Modes and The Cage-Correlation Function," Enrico Fermi summer school on Computer Simulation of Rare Events in Condensed Phases, Lerici, Italy

Teaching

In the Notre Dame Department of Chemistry and Biochemistry, the typical teaching load for research-active faculty is 1 full course per semester, with faculty sometimes taking on responsibility for additional one-credit seminar courses. During my time at Notre Dame, my teaching responsibilities have been split between the following courses:

Undergraduate Courses

Chemistry 113/114, 10171
General Chemistry I and II
144-240 students per section
Spring 2006, Fall 2006, 2007, and 2010

These are one-semester (3 credit + lab + tutorial), freshman-level service classes that are requirements for most science, engineering, and pre-professional majors. The courses cover the fundamental principles governing chemical structure and reactivity, including the quantum mechanical structure of atoms, models of chemical bonding, chemical equilibrium, acidity and basicity, thermochemistry and thermodynamics. They are accompanied by laboratory work and by a tutorial section.

Chemistry 20262
Mathematical Methods for the Chemical Sciences
37-42 students per section
Spring 2012 & 2013

This is a one-semester, 3 credit, sophomore-level class that is required for all chemistry and biochemistry majors. It was originally developed to enhance the mathematical background of students leading up to the physical chemistry sequence that is taken in the junior year. The class provides chemistry and biochemistry majors with mathematical background, chemical context, and problem-solving methods for problems that involve multivariate calculus, differential equations, linear algebra, and probability and statistics. All of the teaching materials (including some in-class computational labs) are available online.

Chemistry 30321 / 30322
Physical Chemistry I and II
25-46 students per section
Fall 2003, 2004, 2011, 2012
Spring 2004, 2014

This is a two-semester sequence (6 credits + lab) taken by all junior-level chemistry and biochemistry majors. The physical chemistry sequence is a set of challenging courses in the fundamentals of physical chemistry, including chemical thermodynamics, kinetics and the elements of atomic and molecular structure. For pedagogical reasons, Notre Dame reverses the topic ordering compared with other institutions, placing an emphasis on the microscopic theory (quantum mechanics) in the first semester, and then building on this with the macroscopic theories (statistical mechanics, thermodynamics and chemical kinetics) in the following semester.

Chemistry 40426
The Chemistry of Fermentation and Distillation
13 students per section
Fall 2015, 2016, 2017

This is a one-semester (4 credit) science elective that is an overview of the chemical and physical processes that take place during the fermentation and distillation of alcoholic beverages. It provides the chemical concepts needed to understand the molecules, reactions, separations, and physical transformations during the production of wine, beer, and distilled spirits, but it also discusses fermentation in a broader culinary, cultural, and industrial context. Hands-on activities include: chemical analysis of sugars, sulfites, and titratable acidity of starting materials, initiation and monitoring of a fermentation process, distillation of a multicomponent solution, and analysis of the distillate at multiple stages of the process. Students also have the opportunity to tour off-campus facilities, including a working winery and distillery.

Graduate Courses

Chemistry 60641
Statistical Mechanics I
10-20 students per section
Spring 2001, 2005, and 2011
Fall 2009 2013, and 2014

Statistical mechanics is a core course for physical chemistry and chemical engineering graduate students. The topics covered include: the foundations of statistical mechanics, including introductions to chemically relevant ensembles; thermodynamics; partition functions; chemical equilibria; quantum statistics; spin glasses and chemical kinetics. The students who enroll in this course are highly motivated and have a deep background in a related area. Final projects in the class are directly related to research that is ongoing at Notre Dame. For example, to illustrate the properties of the Ising spin model, students are asked to model chains of quantum cellular automata (QCA) devices with this model. The course also covers topics not traditionally covered in basic statistical mechanics courses such as liquid theory, glassy materials, protein folding, and computer simulation methods.

Chemistry 60642
Statistical Mechanics II
5-10 students per section
Spring 2007, 2008, 2009, and 2016

This is an advanced graduate course aimed at physical chemistry and chemical engineering graduate students. The topics covered include: spin-lattice models, atomic and continuum models for fluids, free energy perturbation theories, electron transfer, quantum statistical mechanics, rare event sampling, path integral theories, tunneling, Ising/Quantum correspondence and biased Monte Carlo methods.

Chemistry 60649
Quantum Mechanics I
7-12 students per section
Fall 1999, 2000, 2001, and 2008

This is a chemically oriented survey of quantum mechanics at an intermediate level. The subjects that are discussed include quantum mechanical operators, commutator relations, angular momentum, central field problems, harmonic oscillators, and approximation methods. It is the core course that all entering physical chemistry graduate students take to prepare for research, although advanced undergraduates also occasionally enroll.

Chemistry 90650 / 40650
Computational Chemistry
15-20 students per section
Spring 2002, 2010, 2015, 2017
Fall 2005

This class is taught to a mixed group of graduate & undergraduate students from organic chemistry, biochemistry, physical chemistry, and across the college of engineering. The course is an overview of the fundamental theory, methodology, and applications of computational chemistry. Topics include simulation techniques such as molecular dynamics and Monte Carlo.

Every fourth meeting of the class is a hands-on practical lab. The computer labs cover a wide range of topics, including operating systems, text editors, programming, and software packages such as Avogadro, OpenMD, and Packmol. In addition to impacting the students at Notre Dame, the course web site allows students at other universities to teach themselves about computer simulation and assists professors designing similar courses at other universities.

This version of the course emphasized force-field based approaches such as molecular modeling, molecular dynamics, Monte Carlo sampling, and minimization methods. For a final project, the students were asked to utilize these techniques on a molecule related to their own research.

Other Courses

I have taught various one-semester seminar courses (CHEM 23201/23202) which are one-credit offerings that give our undergraduate majors a chance to hone their presentation skills. These seminar courses often have a theme, and in Spring 2010, the theme chosen was *Science 2.0*. This theme allowed us to cover some big picture topics in modern science like Open Access publishing; Open Data and data archiving; intellectual property distinctions for papers, data and code; pre- and post-publication peer review; scholarly metrics; the third and fourth legs (simulation and big data), and social networking for science. This course was repeated in the Fall of 2015 and 2017.

In Spring 2014, I was placed in charge of the supervised teaching experience for one of the GAANN fellows, Paul Johns. Paul was given primary lecturing responsibilities for a second-semester physical chemistry course for three students who were out of sequence from the normal physical chemistry curriculum. Paul used lecture notes and problem sets that I prepared in advance and had meetings with me before each lecture. He was coached in effective lecture pacing and student engagement and was observed in the classroom. Paul was eventually responsible for creating assignments and exam questions himself, and became quite self-sufficient during the semester.

In Spring 2002, I was responsible for a half semester of CHEM 324 (Physical Chemistry for Engineers) that was team-taught with Dennis Jacobs.

Courses in which I have given guest lectures include many of the courses listed above as well as an ACMS class taught by Mark Alber.

Advising & Mentoring

Post-doctoral Researchers

Dr. Jayashree Saha Dr. Saha is now an Associate Professor of Physics at Calcutta University, India
1999-2001

Doctoral Dissertations Directed

Dr. Christopher Fennell *Development of Molecular Dynamics Techniques for the Study of Water and Biochemical Systems*
2007
After a post-doc with Ken Dill at UCSF & Stony Brook, Chris started his career as an Assistant Professor of Chemistry at Oklahoma State University in 2013

Dr. Shenyu Kuang *Atomistic Simulations of Nanoscale Transport Phenomena*
2012
Shenyu is now a Research & Development Engineer at Synopsys in Boston.

Dr. Teng Lin *Molecular Dynamics Methodology and Simulations of Phospholipid Bilayers and Liquid Crystals*
2006
Teng is now the Director of Business Development at Schrödinger, Inc.

Dr. Madan Lamichhane *Development and Applications of Real-Space Electrostatic Interaction Methods for Charge-Multipoles in Condensed Phase Environments (co-advised with Kathie Newman)*
2016
Madan is now a Analytic Scientist II at FICO in San Diego.

Dr. James Marr *Atomic Force Microscopy and Raman Spectroscopy Experiments with Molecular Dynamics for the Study of Field-dependent Chemical and Morphological Changes (co-advised with Zac Schultz)*
2014
James is currently a post-doctoral research scientist at the NIST Center for Nanoscale Science and Technology

Dr. Matthew Meineke *Statistical Mechanics Simulations of Surface Coverage and Phospholipid Bilayers*
2004
Matt is now a Clinical Radiation Physicist, at the Ohio State University Wexner Medical Center.

Dr. Joseph Michalka *Adsorbate Induced Reconstructions of Metal Surfaces*
2016
Joseph is now an Assistant Professor of Chemistry at Southern Baptist University in Bolivar, MO

Dr. Kelsey Stocker *Development and Application of Non-periodic and Non-equilibrium Molecular Dynamics Simulation Methods*
2014
After a post-doc with George Schatz at Northwestern, Kelsey started her career as an Assistant Professor of Chemistry at Suffolk University in Boston in 2016.

Dr. Xiuquan Sun *Algorithms for Modeling the Dynamics and Phase Transitions of Lipid Bilayers*
2008
Xiuquan was a post-doctoral researcher with Liem Dang at PNNL (2008-2012), and is currently living in Bellevue, WA.

Dr. Charles F. Vardeman II *Computational Studies of Metallic Glasses and Nanoparticles*
2009
Chuck is now a Computational Scientist at the Center for Research Computing and Research Assistant Professor in Computer Science and Engineering at the University of Notre Dame.

Masters Theses Directed

Kyle Daily *2006*	*Size-dependent Cutoff Methods: A Statistical, Dynamic, and Structural Comparison* Kyle is now a Secondary Physical Sciences Teacher at Mount Calvary Christian School in Elizabethtown, PA.
Dr. Chunlei Li *2010*	*Computational Studies of Beetle Anti-freeze Protein Binding to Ice I_h* Chunlei transferred to the Applied & Computational Mathematics and Statistics (ACMS) program and earned his PhD with Mark Alber in 2014. He is now a data scientist at eBay.
Changsen Xu *2001*	*Reaction Path Hamiltonian Analysis of Dynamical Solvent Effects on Claisen Rearrangement and a Random Matrix Theory for Liquid Vibrational Densities of States (co-advised with Sharon Hammes-Schiffer)* Changsen is now a Senior Python Programmer for Atmel in Shanghai City, China
Yang Zheng *2005*	*Size-dependent Cutoff Methods for Molecular Dynamics* Yang is now a Lead Reporting Analyst for Stanford Hospital & Clinics

Undergraduate Research Students Advised

Heather Chiarello	*BS (2013), currently at the University of Pennsylvania School of Dental Medicine*
Dr. Dan Combest	*BS (Wash. U, St. Louis, 2004), PhD from WUSTL in 2012.* *Dan is now CFD Engineer and Code developer at ENGYS in St. Louis*
Dr. Patrick Conforti	*BS (2003), PhD from Penn State in 2008.* *Patrick is now a Senior Scientist at Spectral Sciences, Inc.*
Dr. Peter DeCarlo	*BS (2001), PhD from the University of Colorado, Boulder in 2007. Peter is now an Associate Professor in the Department of Civil, Architectural, and Environmental Engineering at Drexel University*
Kenneth Fletcher	*BS (Andrews University, 2008) MS (University of Michigan, 2011), Ken is now a Laboratory Technician at Great Lakes Scientific.*
Erik Helgesen	*BS (2012), currently a documentary and landscape photographer in Columbus, Ohio.*
Patrick Holvey	*BS (2010), J.D. from NYU School of Law in 2015, currently a judicial law clerk at the U.S. District Court for the Eastern District of Texas*
Andrew Latham	*BS (2017), currently in the PhD program in Chemistry at MIT*
Patrick McIntyre	*BS (2013), currently at the Indiana University School of Dentistry*
Jennifer (Morton) O'Mahony	*BS (2008), M.S. in Industrial Engineering from the University of Pittsburgh in 2014, currently an Industrial Engineer at Cleaveland/Price Inc.*
Thomas Parsons	*BS (2016), currently in the PhD program in Chemistry at MIT*
Dr. Christie (Puglis) Francia, OD	*BS (2008), OD from the Southern College of Optometry in 2012. Christie is now an optometrist for Wing Eyecare in Cincinnati, Ohio*
Megan Sprague	*BS (2003), attended graduate school in chemistry at the University of Wisconsin, Megan is currently Adjunct Instructor of Chemistry at Heartland Community College in Normal, Illinois*
Jenna Stevens	*BS (2007), current whereabouts unknown*

Awards to Gezelter graduate students:

- **Chris Fennell** was awarded the 2006 *Rohm and Haas award for Outstanding Graduate Research*
- **Teng Lin** was awarded the 2005-2006 *Center for Applied Mathematics (CAM) fellowship*
- **Joseph Michalka** was awarded the *Best Contributed Talk* award at the 2015 Midwest Theoretical Chemistry Conference
- **Suzanne Neidhart** was awarded the *Journal of Physical Chemistry Best Student Poster Award* at the 2017 Midwest Theoretical Chemistry Conference
- **Matt Meineke** (2003), **Chris Fennell** (2005) and **Charles Vardeman** (2008) were awarded *CRC/SGI awards in Computational Science and Visualization*
- **Matt Meineke** (2001), **Chris Fennell** (2002), **Teng Lin** (2003), **Charles Vardeman** (2007), **Kelsey Stocker** (2010) , and **Joseph Michalka** (2014) were awarded *Outstanding Graduate Student Teaching* awards from the Kaneb Center for Teaching and Learning
- **Kyle Daily** (2006) and **Joseph Michalka** (2011) were awarded the department's *Emil T. Hoffman Award* for outstanding teaching in the first year program
- **Kelsey Stocker** was awarded the department's 2012 *Rudy Bottei Graduate Teaching Award*
- **Chris Fennell** (2002) and **Charles Vardeman** (2006) were awarded the department's *Jeremiah P. Freeman teaching award*

Awards to Gezelter undergraduate research students:

- **Christie (Puglis) Francia** was awarded the 2007 Wiech Research Fellowship
- **Andrew Latham** was awarded the 2017 Outstanding Chemistry Research Award
- **Thomas Parsons** was awarded the 2015 Wiech Award, and the 2016 Outstanding Biochemistry Research Award.

Students presently under direction:

Hemanta Bhattarai	*3rd year Physics graduate student, co-advised with Kathie Newman*
Suzanne Niedhart	*4th year Chemistry graduate student*
Soren Holm	*Senior Chemistry with Computing major*
Patrick Louden	*6th year Chemistry graduate student*

Thesis committees served on:

Chemistry & Biochemistry (40 students)

Marcus Arieno, Steven Asiala, Cory Aires, Clyde Daly, Bipasha Deb, Danyal Floisand, Thomas Frederick, Ivan Gregoretti, Xin Gu, Song Guo, Brandon Haines, Eric Hansen, Min Hu, Xiaosong Hu, Shanghui Huang, Elsa Kieken, Kevin Koh, Wenguang Lin, Xin Liu, Tierney Miller, Patty Maazouz, Ruth Nelson, Hristina Petrova, Julia Philip, Delphine Picot, Carrie Miller, Xiangdong Qin, Rebecca Quardokus, Cecilia Quinteros, Heath Rose, Daniel Scott, Mary Sherman, Zachary Terranova, Rachel Thompson, Pierre Tran, Xuan Wang, Yuliang Wang, Kun Yao, Li Zeng, Jonathan Zintsmaster

Chemical & Biomolecular Engineering (14 students):

Solomon Assefa, Anshumaan Bajpai, Jason Bray, Samir Budhathoki, Cesar Cadena, David Eike, Timothy Morrow, Andrew Paluch, Eliseo Rimoldi, Jindal Shah, Prasad Sarangapani, David Schmidt, Surya Tiwari, Brian Yoo

Physics (2 students):

Laura Kinnaman, Danielle McDermott

Aerospace & Mechanical Engineering (2 students):

Gianluca Puliti, Xingfei Wei

Computer Science & Engineering (1 student):

Scott Hampton

As outside chair (13 students):

Istvan Albert (Physics), Sung-Jae Cha (Biological Sciences), Aaron Couture (Physics), Hattie Dambroski (Biological Sciences), Rachel Getman (CBE), Saivenkataraman Jayaraman (CBE), Yingxin Jiang (CSE), Manish Kelkar (CBE), Laurent Thiers (CBE), Marc Ma (CSE), Jason Quinn (Physics), Istvan Robel (Physics), Rebecca Weber (Mathematics)

Service

Departmental Service

2015-present	**Director of Undergraduate Studies**
2006-2007, 2012-2015	**Physical/Analytical Chemistry Group Coordinator (Group Leader)**
1999-present	**Departmental Web Team**
2006-2011	**Director of Graduate Admissions** Increased the size of the incoming graduate class from 23 to 47 students, became *more selective* (36% → 27%), achieved *higher yields* (25% → 43%), all while *increasing the quality* of incoming graduate classes
2006	**Member of Committee on Appointments and Promotions**
2001-2002	**Physical chemistry representative to the Graduate Studies Committee**
2004-2005, 2011-2012	**Physical chemistry representative to the Undergraduate Studies Committee**
1999-2000, 2006-2011	**Physical chemistry representative of the Graduate Admissions Committee**
2003-2004	**Physical chemistry representative of the Lectures Committee**
2000, 2002, 2004, 2010	**Member of various physical chemistry faculty search committees**

University or College Service

2000-present	**Faculty advisor for (and member of) the Notre Dame Bagpipe Band**
2013-present	**Member of the Learning Management Guidance Council**
2006-2011	**Member of the CRC Faculty Advisory Committee**
1999-2005	**Member of the Committee on Technical Computing**
2006-2009	**Member of the Search Committee for the CRC Director**
2008-2010	**Member of the College of Science Computing Committee**
2007, 2009, 2011-2012	**Member of the University Committee on Academic Technologies (UCAT)**
2000-2005	**Campus representative for the Churchill Scholarship**
2006-present	**Founding co-organizer of the Notre Dame Theory "Super-Group"**

Service to the profession

1999-Present **Director of the Open Science Project**
(See openscience.org for more details)
Founding member of the Open Science movement, participant in many Open Science workshops and panels, invited to present at the OSTP / White House *Open Science Champions of Change* event on June 20, 2013

2016 **Workshop Organizer**
Thermal Transport at the Nanoscale, held at the Telluride Science Research Center, Telluride, CO

2011 **Conference Organizer**
43rd Midwest Theoretical Chemistry Conference, held on the campus of the University of Notre Dame

1999-Present **Reviewer** for journals including the *Journal of Physical Chemistry, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Chemical Physics Letters, Physical Review E, Journal of Cheminformatics,* and *Journal of Molecular Structure: THEOCHEM*

2002-2004 **Grant reviewer and panelist** for the National Institute of General Medical Sciences (NIGMS) at the NIH

2002-Present **Member, NSF Grant review panels** (and ad hoc reviewer) - CHE, OCI, CDS&E programs

2008 **Speaker and Panelist** at the *New Communication Channels for Biology* workshop sponsored by the California Institute for Telecommunication and Information Technology (CalIT2)

2009 **Speaker and Panelist** at the Kauffman Innovation Roundtable on *Sharing Data and Code in Computational Science* at the Yale Information Society Project

2010 **Speaker and Panelist** at the NSF-sponsored workshop on *Archiving Experiments to Raise Scientific Standards*

2014 **Invited Speaker** on *Open Science* at the NIAID Bioinformatics and Computational Biosciences Festival

Community Service

2009 **Chemistry Presenter for Ms. Wizard Day**
2010 **Chemistry Presenter for College Mentors for Kids**
2012 **Presenter for the CRC Summer Scholars program**

Media Reports

An interesting Open Science story that featured our comments:
Brian Owens: "Montreal institute going 'open' to accelerate science," *Science* **2016**, 351, 239
science.sciencemag.org/content/351/6271/329.full

This was also featured on techdirt (a widely-read tech industry web magazine):
Glynn Moody: "Beyond Open Access And Open Data: Open Science – And No Patents," *techdirt* **2016.**
www.techdirt.com/articles/20160129/09420033460/beyond-open-access-open-data-open-science-no-patents.shtml

Rose Eveleth: "Free Access to Science Research Doesn't Benefit Everyone," *The Atlantic*, December 22, 2014.

www.theatlantic.com/technology/archive/2014/12/free-access-to-science-research-doesnt-benefit-everyone/383875/

Antony Funnell: "Open Science" *Future Tense*, broadcast on February 4, 2010.
www.abc.net.au/radionational/programs/futuretense/open-science/3100152

Vincent Kiernan: "The 'Open-Source Movement' Turns Its Eye to Science" *The Chronicle of Higher Education*, **46**(11), A51-A52, November 1999.
chronicle.com/article/The-Open-Source-Movement-/3254

Gregory V. Wilson: "A Natural Home for Open Source," *Dr. Dobbs Journal*, December 1999.
www.drdobbs.com/a-natural-home-for-open-source/184411210

Gregory V. Wilson and Pete Beckman: "Open Source Meets Big Iron," *Dr. Dobbs Journal*, June 2000.
www.drdobbs.com/open-source-meets-big-iron/184404131

Bernadette Toner: "Petition Urges Public Funding Agencies to Formally Endorse Open Source Software," *BioInform* **5**, 1-10 (2001).
www.genomeweb.com/informatics/petition-urges-public-funding-agencies-formally-endorse-open-source-software

Stephen Adler: "Open Source / Open Science 1999," *Linux Journal* **70**, 2000.
www.linuxjournal.com/article/3739