J. Daniel (Dan) Gezelter

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Education and Training

1996 – 1999	Postdoctoral Research Scientist, Department of Chemistry, Columbia University Advisor: Bruce J. Berne
1995	Ph.D., Chemistry, University of California at Berkeley Advisor: William H. Miller
1990	CPS, Chemistry, Churchill College, University of Cambridge Advisor: Ray Freeman, FRS
1989	B.S., Chemistry & Philosophy, Duke University, *cum laude* and with distinction in chemistry Advisors: Richard A. MacPhail and Donald B. Chestnut

Academic Positions

2015 – present	Professor, Department of Chemistry and Biochemistry, University of Notre Dame
2005 – 2015	Associate Professor, Department of Chemistry and Biochemistry, University of Notre Dame
1999 – 2005	Assistant Professor, Department of Chemistry and Biochemistry, University of Notre Dame

Leadership Appointments

2025 – present	Chair, Department of Chemistry and Biochemistry, University of Notre Dame
2023 – 2025	Senior Associate Dean for Education and Undergraduate Programs, College of Science, University of Notre Dame
2020 – 2023	Associate Dean for Undergraduate Studies, College of Science, University of Notre Dame
2015 – 2020	Director of Undergraduate Studies, Department of Chemistry and Biochemistry, University of Notre Dame
2006 – 2011	Director of Graduate Admissions, Department of Chemistry and Biochemistry, University of Notre Dame

Awards and Honors

2023	Provost's Award for Teaching Excellence in the Core Curriculum
2020	Shilts / Leonard Award for Outstanding Teaching in the College of Science
2020	Rev. Edmund P. Joyce Award for Excellence in Undergraduate Teaching
2018 – 2019	Faculty Fellow, Kaneb Center for Teaching Excellence
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	National Science Foundation Graduate Fellowship in Chemistry
1989	Churchill Scholar

Key Accomplishments in University Leadership

Senior Associate Dean for Education and Undergraduate Programs
College of Science, University of Notre Dame (2023-present)

The Senior Associate Dean for Education and Undergraduate Programs directs all undergraduate affairs of the College of Science, and oversees curriculum for five departments, four non-departmental majors, three centers which offer minors, and dual degree programs with three other colleges. This role oversees academic records (including graduation lists), undergraduate advising, course approvals, teaching evaluations, undergraduate research, and upkeep and replacement of laboratory equipment in the teaching labs. It is the main contact in the College of Science for the Registrar's office, the Study Abroad office, and with a number of committees that operate out of the Provost's office (core curriculum, academic code and policy, honor code, university advising), and with various IT initiatives including the learning management software. This role also oversees interdisciplinary majors (Neuroscience and Behavior, Science-Business, and Science-Computing) as well as all advising done inside the College of Science. The Assistant Dean for Advising, and the Directors of the Galvin Scholars program, Undergraduate Research, the Digital Visualization Theater, and the Neuroscience and Behavior program all report to the Senior Associate Dean.

College of Science Overview and Leadership:

- Oversight of undergraduate programs in five departments (ACMS, Biological Sciences, Chemistry & Biochemistry, Physics & Astronomy, Mathematics), 6 centers, and 18 institutes.
- Supported 281 faculty members, 700 graduate students, and 1,900 undergraduates, helping them to bring in $83 million in extramural research funding last year (~37% of the University's total funding).
- Supported the Center for Health Sciences Advising in achieving an annual 79-85% medical school acceptance rate, among the highest in the country.
- Committed to maintaining and expanding Notre Dame's success as a leading undergraduate institution, particularly as we serve a more complex student population.

Examples of Key Accomplishments:

- Portfolio includes oversight of interdisciplinary majors, such as the Neuroscience and Behavior major, and undergraduate advising for the College of Science.
- Helped the College of Science secure a commitment for 6 new faculty lines and 4 teaching post-docs in Neuroscience and Behavior.
- Helping benchmark and review curriculum for the cross-college Neuroscience and Behavior major.
- Introduced Student Research @ Notre Dame (STRAND), an undergraduate research matching program aimed at improving access to student research.
- Served as the academic lead on the 'Huddles' pilot project to implement and study peer-facilitated study groups in General Chemistry.
- Helping the Mathematics and Physics and Astronomy departments support transformation of their foundational courses to meet the needs of an increasingly complex student body.
- Oversaw new initiatives in mathematics, notably a required mathematics placement test, pre-calculus course, and re-leveling process for students incorrectly placed in math courses.
- Expanded the Galvin Scholars Program to better support underrepresented students in STEM fields.

Fundraising and Donor Relations:

- Contributed to fund-raising efforts with the Notre Dame Science Advisory Council, particularly for the endowment of the Galvin Scholars Program.
- Met with donors annually at council meetings and during individual donor visits, in collaboration with the Director of Academic Advancement.

Associate Dean for Undergraduate Studies
College of Science, University of Notre Dame (2020-2023)

The Associate Dean for Undergraduate Studies directs undergraduate affairs of the College of Science, and oversees curriculum for five departments, four non-departmental majors, three centers which offer minors, and dual degree programs with three other colleges. This role oversees academic records (including graduation lists), undergraduate advising, course approvals, teaching evaluations, undergraduate research, and upkeep and replacement of laboratory equipment in the teaching labs. It is the main contact in the College of Science for the Registrar's office, the Study Abroad office, and with a number of committees that operate out of the Provost's office (core curriculum, academic code and policy, honor code, university advising), and with various IT initiatives including the learning management software.

Examples of Key Accomplishments:

- Served on the Faculty Task Force for Instructional Continuity and the Advisory Committee on the Academic Code and Policy (ACACP), overseeing the academic response to the pandemic.
- Helped implement rapid transitions to hybrid/online learning, new academic policies (credit/no-credit), expanded classroom use, and a new online winter term during the Covid-19 pandemic.
- Led the College of Science response for two successful accreditation exercises (Higher Learning Commission and ABET).
- Oversaw the expansion of the Galvin scholars program to 320 students (80 / cohort).

Leadership and Impact:

- Managed a portfolio impacting 1,900 students, resolving complex academic and interpersonal issues through a prepared, honest, and empathetic approach.
- Focused on creating environments where both students and faculty can flourish.

Committee on Under-Resourced Student Success (2023):

- Collaborated with Provost Emeritus Tom Burish and dean-level leadership to study and propose twelve data-driven recommendations for improving support for under-resourced students at Notre Dame.
- Key outcomes: implemented a summer bridge program, expanded peer-facilitated study groups, increased financial aid, and helping to restructure foundational coursework to better support under-resourced students.

Development and Leadership of the *Mary E. Galvin Science & Engineering Scholars* Program
College of Science, University of Notre Dame (2017- present)

- Addressed significant retention issues for students coming from high schools without strong AP STEM programs. Many of these students are first-generation and Pell-eligible students.
- Co-created the Galvin Scholars Program aimed at improving the foundational courses in science and math for these students.
- Implemented key program features: smaller class sizes, graded active learning classes, reduced first-semester course load, online summer math refresher, and mentoring programs.
- Created and taught the Galvin Scholars General Chemistry courses, meeting five days per week to provide intensive instruction and support.
- Improved student retention by 14% over a matched control group, with scholars outperforming peers by a *full grade point* in challenging courses like Organic Chemistry and Engineering Physics.
- Helped raise $15 million in endowment funds to support five teaching faculty lines, program directorship, and research and internship opportunities for 65 students annually.

Director of Undergraduate Studies
Department of Chemistry and Biochemistry, University of Notre Dame (2015-2020)

The Director of Undergraduate Studies manages curriculum and advising for a department, coordinates service teaching with client departments, and ensures the relevance and effectiveness of undergraduate degree programs. Responsibilities include reviewing and recommending curriculum changes, advising majors, overseeing pre-registration and registration, recommending student awards, and approving new undergraduate courses and programs

Examples of Key Accomplishments:
- Chaired the departmental curriculum committee, which impacts a large portion of the campus due to Chemistry's role as a service department.
- Led restructuring of the chemistry coursework from a 2-2 (General - Organic) to a 1-2-1 (General - Organic - Inorganic) sequence, affecting half of the student population.
- Reorganized the physical chemistry curriculum to a quantum-first approach and developed a separate physical chemistry track for biochemistry majors.
- Co-developed the Chemistry of Fermentation and Distillation course, now highly popular with both students and faculty.

Director of Graduate Admissions
Department of Chemistry and Biochemistry, University of Notre Dame (2006-2011)

The Director of Graduate Admissions oversees recruitment strategies, maintains relationships with feeder schools, provides program information to applicants, and arranges applicant visits to the graduate program.

Examples of Key Accomplishments:
- Oversaw the growth of the graduate program from 130 to 180 Ph.D. students, with incoming class sizes increasing from an average of 27 to 47 students.
- Increased selectivity (admissions rate improved from 36% to 27%) while also boosting yield (admitted students accepting offers grew from 35% to 43%).
- Managed the admissions process for approximately 400 graduate applicants annually.
- Coordinated recruitment weekends, wrote departmental and university fellowship nominations, and facilitated advisor meetings.
- Collaborated with graduate admissions and graduate studies committees to recruit a high-quality applicant pool from a range of undergraduate institutions.
- Established feeder school relationships with local institutions, such as Grand Valley State University, leading to a steady stream of strong graduate students.
- Enhanced the reputation and visibility of the department through recruiting efforts, contributing to increased research output, stronger teaching, and overall institutional recognition.

University Service and Leadership

2024 – present	Academic Council (and chair of the Undergraduate Studies Committee), University of Notre Dame
2024 – 2025	Computational Biophysics Faculty Search Committee
2024 – present	Academic Lead, Student Research @ Notre Dame *(STRAND)* project
2024 – 2025	Academic Lead, *Huddles* Peer-Facilitated Study Group pilot program
2023 – 2024	ND-LEAD program, University of Notre Dame
2022 – 2023	Provost's committee on *Promoting Success of Students From Lower-Resourced Backgrounds*
2022 – present	Advisory Board, Glynn Family Honors Program, University of Notre Dame

2020 – 2025	Core Curriculum Committee, University of Notre Dame
2020 – 2025	Advisory Committee on the Academic Code and Policies, University of Notre Dame
2020 – present	Deans and Chairs Committee, College of Science, University of Notre Dame
2020 – 2025	Chair, College Council, College of Science, University of Notre Dame
2020 – 2025	Goldwater Scholars Selection Committee, University of Notre Dame
2020 – 2021	Provost's Working Group on the Forms and Structures of a Notre Dame Education
2020 – 2021	Learning Management System (LMS) Succession Committee, University of Notre Dame
2020 – 2021	Faculty Task Force on Instructional Continuity, University of Notre Dame
2020 – 2021	Strategic Plan Working Group, College of Science
2020 – 2021	General Chemistry Teaching Faculty Search Committee
2020 – 2021	Theoretical Chemistry Faculty Search Committee
2020	Valedictorian Selection Committee, University of Notre Dame
2020	Physical Chemistry Seminar Coordinator, Department of Chemistry & Biochemistry
2020	Member of Committee on Appointments / Committee on Reappointments, Promotions, and Tenure (CA/CRPT) Executive Committee, Department of Chemistry & Biochemistry
2020	Undergraduate Studies Committee, Department of Chemistry & Biochemistry
2018 – 2021	Core Curriculum Subcommittee on Science and Technology, University of Notre Dame
2018 – 2020	Learning Management Guidance Council, University of Notre Dame
2018 – 2019	Faculty Fellow, Kaneb Center for Teaching Excellence, University of Notre Dame
2017 – present	Design & Implementation of the *Mary E. Galvin Science & Engineering Scholars* program
2015 – 2020	Director of Undergraduate Studies, Department of Chemistry and Biochemistry
2012 – 2015	Physical/Analytical Chemistry Group Coordinator (Group Leader)
2011 – 2012	University Committee on Academic Technologies (UCAT), University of Notre Dame
2011 – 2012	Undergraduate Studies Committee, Department of Chemistry & Biochemistry
2009	University Committee on Academic Technologies (UCAT), University of Notre Dame
2006 – 2011	Center for Research Computing Faculty Advisory Committee, University of Notre Dame
2006 – 2011	Graduate Admissions Committee, Department of Chemistry & Biochemistry
2006 – 2009	Search Committee for the Center for Research Computing (CRC) Director, University of Notre Dame
2008 – 2010	College of Science Computing Committee
2007	University Committee on Academic Technologies (UCAT), University of Notre Dame
2006 – 2011	Director of Graduate Admissions, Department of Chemistry & Biochemistry
2006	Committee on Appointments and Promotions, Department of Chemistry & Biochemistry
2006 – present	Co-organizer of the Notre Dame Theory "Super-Group," University of Notre Dame
2006 – 2007	Physical / Analytical Chemistry Group Coordinator (Group Leader)
2004 – 2005	Undergraduate Studies Committee, Department of Chemistry & Biochemistry
2003 – 2004	Physical Chemistry Seminar Coordinator, Department of Chemistry & Biochemistry
2001 – 2002	Graduate Studies Committee, Department of Chemistry & Biochemistry
2000 – 2005	Campus representative for the Churchill Scholarship, University of Notre Dame
2000 – 2010	Member of four Physical Chemistry faculty search committees, Department of Chemistry & Biochemistry, chair of two of these search committees.
2000 – present	Faculty advisor for (and member of) the Notre Dame Bagpipe Band
1999 – 2020	Department of Chemistry and Biochemistry Web Team
1999 – 2005	Committee on Technical Computing, University of Notre Dame
1999 – 2000	Graduate Admissions Committee, Department of Chemistry & Biochemistry

Professional Service and Leadership

2024	Workshop Organizer, *Structure and Dynamics of Ice Surfaces*, Telluride Science Research Center, Telluride, CO

2022-24	Symposium co-organizer, *Chemistry of Ice*, ACS National Meeting, Spring 2024
2020	Workshop Organizer, *Structure and Dynamics of Ice Surfaces*, Telluride Science Research Center, Telluride, CO
2019	Workshop Organizer, *Thermal Transport at the Nanoscale*, Telluride Science Research Center, Telluride, CO
2019	Conference Organizer, 51st Midwest Theoretical Chemistry Conference
2016	Workshop Organizer, *Thermal Transport at the Nanoscale*, Telluride Science Research Center, Telluride, CO
2014	Invited Speaker and Panelist on Open Science at the *NIAID Bioinformatics and Computational Biosciences Festival*
2011	Conference Organizer, 43rd Midwest Theoretical Chemistry Conference
2010	Speaker and Panelist at the NSF-sponsored workshop on *Archiving Experiments to Raise Scientific Standards*
2009	Speaker and Panelist at the Kauffman Innovation Roundtable on *Sharing Data and Code in Computational Science* at the Yale Information Society Project
2008	Speaker and Panelist at the *New Communication Channels for Biology* workshop sponsored by the California Institute for Telecommunication and Information Technology (CalIT2)
2002 – present	NSF Grant review panels (and ad hoc reviewer) - CHE, OCI, CDS&E programs
2002 – 2004	Grant reviewer and panelist for the National Institute of General Medical Sciences (NIGMS) at the NIH
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*

Community Service

2018 – 2022	Science Olympiad (ChemLab) Coach - John Adams High School, South Bend, IN
2012	Presenter for the Center for Research Computing (CRC) Summer Scholars program
2010	Chemistry Presenter for College Mentors for Kids
2009	Chemistry Presenter for Ms. Wizard Day
2000 – present	Board member (and officer) for three non-profit organizations in the greater South Bend community.

Peer-Reviewed Journal Articles

Key: # = undergraduate, @ = graduate student, % = post-doc, † = faculty, * = corresponding authors

1. Benjamin M. Harless@, Jasmine K. Sindelar#, and J. Daniel Gezelter†*, "Molecular Dynamics of Ice-Active Solutions at Ice-Water Interfaces," submitted to *J. Chem. Phys.* (2025).

2. Sydney A. Shavalier@ and J. Daniel Gezelter†*, "Thermal Transport Through CTAB- and MTAB-Functionalized Gold Interfaces using Molecular Dynamics Simulations," *Journal of Chemical Information and Modeling*, **65**(2) pp. 811-824 (2025).
DOI: 10.1021/acs.jcim.4c02195

3. Cody R. Drisko@, Hemanta Bhattarai†, Christopher J. Fennell†, Kelsey M. Stocker†, Charles F. Vardeman II†, and J. Daniel Gezelter†*, "OpenMD: A parallel molecular dynamics engine for complex systems and interfaces," *Journal of Open Source Software*, **9**(102), 7004. (2024).
DOI: 10.21105/joss.07004

4. Cody R. Drisko[@] and J. Daniel Gezelter[†*], "A Reverse Non-Equilibrium Molecular Dynamics (RNEMD) Algorithm for Coupled Mass and Heat Transport in Mixtures," *J. Chem. Theory Comput.* **20**(12), pp. 4986-4997 (2024).
DOI: 10.1021/acs.jctc.4c00182 , arXiv: 2408.02621

5. Sydney A. Shavalier[@] and J. Daniel Gezelter[†*], "Heat Transfer in Gold Interfaces Capped with Thiolated Polyethylene Glycol: A Molecular Dynamics Study," *J. Phys. Chem. B* **127**(47), pp. 10215–10225 (2023).
DOI: 10.1021/acs.jpcb.3c05238 , arXiv: 2312.05689

6. Anderson D. S. Duraes[@] and J. Daniel Gezelter[†*], "A theory of pitch for the hydrodynamic properties of molecules, helices, and achiral swimmers at low Reynolds number," *J. Chem. Phys.* **159**, 134105 (2023).
DOI: 10.1063/5.0152546 , arXiv: 2310.03712

7. Sydney A. Shavalier[@] and J. Daniel Gezelter[†*], "Thermal Transport in Citrate-Capped Gold Nanostructures using a Polarizable Force Field," *J. Phys. Chem. C*, **126**(30), pp. 12742-12754 (2022).
DOI: 10.1021/acs.jpcc.2c01333, ChemRxiv: 10.26434/chemrxiv-2022-7xp7g
correction: 10.1021/acs.jpcc.4c03188

8. Anderson D. S. Duraes[@] and J. Daniel Gezelter[†*], "Separation of Enantiomers through Local Vorticity: A Screw Model Mechanism," *J. Phys. Chem. B*, **125**(42), pp. 11709–11716 (2021).
DOI: 10.1021/acs.jpcb.1c07127 , ChemRxiv: 10.33774/chemrxiv-2021-196zw

9. Hemanta Bhattarai[@], Kathie E. Newman[†], and J. Daniel Gezelter[†*], "The Role of Polarizability in the Interfacial Thermal Conductance at the Gold-Water Interface," *J. Chem. Phys.* **153**, 204703 (2020).
DOI: 10.1063/5.0027847

10. Suzanne M. Neidhart[@] and J. Daniel Gezelter[†*], "Thermal Conductivity of Gold-Phenylethanethiol ($Au_{144}PET_{60}$) Nanoarrays: A Molecular Dynamics Study," *J. Phys. Chem. C* **124**(5), pp. 3389-3395 (2020).
DOI: 10.1021/acs.jpcc.9b10895

11. Hemanta Bhattarai[@], Kathie E. Newman[†], and J. Daniel Gezelter[†*], "Polarizable Potentials For Metals: The Density Readjusting Embedded Atom Method (DR-EAM)," *Phys. Rev. B* **99**, 094106 (2019).
DOI: 10.1103/PhysRevB.99.094106, arXiv:1904.00263

12. Patrick B. Louden[@] and J. Daniel Gezelter[†*], "Why is Ice Slippery? Simulations of Shear Viscosity of the Quasi-Liquid Layer on Ice," *J. Phys. Chem. Lett.* **9**, pp. 2686-3691 (2018).
DOI: 10.1021/acs.jpclett.8b01339

13. Suzanne M. Neidhart[@] and J. Daniel Gezelter[†*],"Thermal Transport is Influenced by Nanoparticle Morphology: A Molecular Dynamics Study," *J. Phys. Chem. C*, **122**(2), pp. 1430-1436, (2018).
DOI: 10.1021/acs.jpcc.7b12362

14. Patrick B. Louden[@] and J. Daniel Gezelter[†*], "Friction at Ice-I_h / Water interfaces is governed by solid / liquid hydrogen-bonding" *J. Phys. Chem. C* **121**(48), pp. 26764–26776 (2017).
DOI: 10.1021/acs.jpcc.7b07169, arXiv: 1501.01056

15. 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

16. 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

17. 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

18. 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

19. 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

20. 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

21. 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

22. 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).

23. 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)

24. 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

25. 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

26. 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

27. 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

28. 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

29. 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

30. 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

31. 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

32. 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

33. 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

34. 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

35. 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

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

37. 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

38. 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

39. 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

40. 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

41. 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

42. 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

43. 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

44. 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

45. 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

46. 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

47. 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

48. 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

49. 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

50. 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

51. 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

52. 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

53. 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

54. 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

55. 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

Invited Presentations

2025 "Molecular Dynamics of Ice-Active Solutions at Ice-Water Interfaces," Chemical Dynamics in Complex Environments (Chem-DICE), Telluride Science Research Center, Telluride, CO

2024 "Structural & Dynamic Changes at ice / water interfaces in contact with small molecule cryoprotectants," Workshop on Structure and Dynamics of Ice Surfaces, Telluride Science Research Center, Telluride, CO

2024 "Structural & Dynamic Changes at ice / water interfaces in contact with small molecule cryoprotectants," ACS National Meeting, New Orleans, LA

2023 "Molecular Pitch Matrices," Chemical Dynamics in Complex Environments (Chem-DICE), Telluride Science Research Center, Telluride, CO

2022 "Thermal Transport in Citrate-Capped Gold Interfaces using a Polarizable Force Field," Workshop on Thermal Transport at the Nanoscale, Telluride Science Research Center, Telluride, CO

2022 "Why is ice slippery? Simulations of solid-liquid friction and the shear viscosity of the quasi-liquid layer on ice," Workshop on Structure and Dynamics of Ice Surfaces, Telluride Science Research Center, Telluride, CO

2022 "Separation of Enantiomers Using Vortex Flow," Chemical Engineering Seminar Series, University of Illinois, Chicago

2021 "Why is ice slippery? Simulations of solid-liquid friction and the shear viscosity of the quasi-liquid layer on ice," Workshop on Cryopreservation, Telluride Science Research Center, Telluride, CO

2021 "Separation of Enantiomers Using Vortex Flow," Chemical Dynamics in Complex Environments (Chem-DICE), Telluride Science Research Center, Telluride, CO

2019 "Why is ice slippery? Simulations of solid-liquid friction and the shear viscosity of the quasi-liquid layer on ice," ACS National Meeting, San Diego, CA

2019 "Polarization Effects in Interfacial Thermal Transport at Metal Surfaces," Thermal Transport at the Nanoscale workshop, Telluride Science Research Center, Telluride, CO

2019 "Modeling Polarization and Charge Transfer at Metal Surfaces," Chemical Dynamics in Complex Environments (Chem-DICE) meeting, Telluride Science Research Center, Telluride, CO

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-Ih 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
2014 "Thermal transport at metal nanoparticle interfaces: ligand and curvature effects," University of Nevada, Reno, NV
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, University of California, San Diego, 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, Notre Dame, IN
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, Notre Dame, IN
2005 "(The Math Underlying) Computer Simulations of Water Phase Transitions," Applied Math Seminar, Department of Mathematics, University of Notre Dame, Notre Dame, IN
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 Modeling 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

External Research Support

- J. Daniel Gezelter (PI), "CDS&E: Development of methods for molecular simulation of enantiomeric separation and metal-oxide formation," NSF CHE-1954648, 8/1/2020 - 7/31/2023, $486,433
- Holly Goodson (PI) and J. Daniel Gezelter (key participant), "Developing a multi-scale understanding of microtubule dynamic instability," NSF CHE-180406, 7/15/2018 – 6/30/2022, $987,675 (0.25 months / year as other key participant)
- J. Daniel Gezelter (PI), "CDS&E: Method Development for Coupled Charge and Thermal Transport in Molecular Simulations, NSF CHE-1663773, 8/1/2017 - 7/31/2020 + 1 year no-cost extension, $450,000
- J. Daniel Gezelter (PI), "Real space electrostatics and non-equilibrium molecular dynamics for nanoscale transport," NSF CHE-1362211, 7/1/2014 - 6/30/2018, $447,121

- J. Daniel Gezelter (PI), "Computational Methods for Simulating Metal Nanoparticle-solvent interfaces," NSF CHE-0848243, 8/15/2009 - 7/31/2014, $400,000
- J. Daniel Gezelter (PI), "CAREER: Dynamics of Model Biological Membranes and Glass Formation in Liquid Metals," NSF CHE-0134881, 6/19/2003 - 6/18/2008, $465,000
- Olaf Wiest (PI), Laszlo Barabasi (co-PI), Ed Maginn (co-PI), Mark Stadtherr (co-PI), and J. Daniel Gezelter (co-PI), "Acquisition of a High Performance Computing System," NSF DMR-0079647, $320,000
- J. Daniel Gezelter (PI), "New Faculty Award," Camille and Henry Dreyfus Foundation, $40,000
- J. Daniel Gezelter (PI), "The OpenScience Project," Alfred P. Sloan Foundation, $30,000 + $2,700 in additional private donations

Mentoring

Postdoctoral Research Associate (1)

1. Jayashree Saha (1999-2001), now a Professor of Physics at Calcutta University

Graduate Students (24 total)

1. Hemanta (Manu) Bhattarai, Ph.D. (2021), now Assistant Professor of Physics at Goshen College
2. Kyle Daily, M.S. (2006), now a chemistry teacher at the Milton Hershey School
3. Cody Drisko, Ph.D. (2025), now Scientific Software Engineer at Stellar Science
4. Anderson DaSilva Duraes, Ph.D. (2023), now a postdoctoral researcher at Dartmouth College
5. Christopher Fennell, Ph.D. (2007), now Associate Professor and Acting Chair of Chemistry at Oklahoma State University
6. Veronica Freund (2022 – present)
7. Benjamin Harless (2021 – present)
8. Shenyu Kuang, Ph.D. (2012), now a Research & Development Engineer at Synopsys
9. Chunlei Li, M.S. (2010), Ph.D. (2014), now a senior manager in AI Data Science at Meta
10. Teng Lin, Ph.D. (2006), now the SVP of Business Development at XtalPi, Inc.
11. Madan Lamichhane, Ph.D. (2016), now the Sr. Manager in the Retail Banking Analytics Team at FICO
12. Patrick Louden, Ph.D. (2018), now the Manager for Data Science at Domino's
13. James Marr, Ph.D. (2014, co-advised by Zac Schultz), now a product manager at Leica Microsystems
14. Alex Mazanek, M.S. (2019)
15. Matthew Meineke, Ph.D. (2004), now a Clinical Radiation Physicist at the Ohio State University
16. Joseph Michalka, Ph.D. (2016)
17. Nhat Pham Minh (2023 – present)
18. Suzanne Neidhart, Ph.D. (2019), now a Sr. R&D Scientist at the Kansas City National Security Campus
19. Sydney Shavalier, Ph.D. (2024), now a Volatile Organic Compound Chemist at Intertek
20. Kelsey Stocker, Ph.D. (2014), now Associate Professor of Chemistry at Suffolk University
21. Xiuquan Sun, Ph.D. (2008)
22. Charles F. Vardeman II, Ph.D. (2009), now a Research Assistant Professor in Computer Science and Engineering at Notre Dame
23. Changsen Xu, M.S. (2001, co-advised by Sharon Hammes-Schiffer), now a software engineer
24. Yang Zheng, M.S. (2005)

Undergraduate Students (22 total)

1. Levi Cherek, B.S. (2025), now in the PhD program at the University of Chicago
2. Heather Chiarello, B.S. (2013), D.M.D (University of Pennsylvania, 2019)
3. Dan Combest, REU student, B.S. (2004), Ph.D. (WUSTL, 2012), now Staff CFD Engineer at Rivian
4. Patrick Conforti, B.S. (2003), Ph.D. (Penn State, 2008), now a Senior Scientist at Spectral Sciences
5. Peter DeCarlo, B.S. (2001), Ph.D. (University of Colorado, Boulder, 2007), now Associate Professor of Environmental Health and Engineering at Johns Hopkins
6. Kenneth Fletcher, REU student, B.S. (Andrews University, 2008) M.S. (University of Michigan, 2011)
7. Skyler Hamilton, B.S. (2022)
8. Erik Helgesen, B.S. (2012)
9. Soren Holm, B.S. (2018), Ph.D. (Stanford, 2024)
10. Patrick Holvey, B.S. (2010), J.D. (NYU, 2015), now an Attorney for the U.S. Department of Justice
11. Andrew Latham, B.S. (2017), Ph.D. (MIT, 2022), now a Postdoctoral scholar at UCSF
12. Patrick McIntyre, B.S. (2013), D.D.S (Indiana University, 2018)
13. Nicholas Milikich, B.S. (2020), M.S. (2021), now Lead Data Scientist at Bain
14. Jennifer (Morton) O'Mahony, B.S. (2008), M.S. (University of Pittsburgh, 2014), now an Industrial Engineer at Cleaveland/Price
15. Thomas Parsons, B.S. (2016), now Senior Data Scientist at Amazon Robotics
16. Chelsea Popoola, B.S. (2022), M.E. (Dartmouth, 2023), now Embedded Software Developer at GE HealthCare
17. Christie (Puglis) Francia, B.S. (2008), O.D. (Southern College of Optometry, 2012)
18. Reem Shanab, B.S. (2024)
19. Jasmine Sindelar, B.S. (2022), now in medical school at Rosalind Franklin
20. Megan Sprague, B.S. (2003), now Adjunct Instructor of Chemistry at Heartland Community College
21. Jenna Stevens, B.S. (2007)
22. Victoria Tatarynova, B.S. (2025)

Teaching

Teaching at the University of Notre Dame has included large service courses, special sections of service courses designed for student success programs, required courses for majors, science electives, and graduate courses. All have been taught multiple times. Data on course instructor feedback (CIF) surveys available upon request.

1. General Chemistry I for the Galvin Scholars - includes an extra 2 credit problem solving class
2. General Chemistry I (in both 1-2-1 and 2-2 models)
3. General Chemistry II (in a 2-2 model)
4. Mathematical Methods for the Chemical Sciences
5. Physical Chemistry I (Quantum Mechanics and Spectroscopy)
6. Physical Chemistry II (Statistical Mechanics, Thermodynamics, and Kinetics)
7. Physical Chemistry for Chemical Engineers
8. Chemistry of Fermentation and Distillation
9. Statistical Mechanics I
10. Statistical Mechanics II
11. Quantum Mechanics I
12. Computational Chemistry
13. Chemistry Seminar