

J. Daniel (Dan) Gezelter

Professor and Department Chair
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Education

1996-99	Postdoctoral Research Scientist, Columbia University Advisor: Bruce J. Berne
1995	Ph.D. in Chemistry, University of California at Berkeley Advisor: William H. Miller
1990	CPGS (Certificate of Postgraduate Study) in Chemistry, University of Cambridge Advisor: Ray Freeman, FRS
1989	B.S. in Chemistry & Philosophy, Duke University (<i>cum laude</i>) Advisors: Richard A. MacPhail and Donald B. Chestnut

Administrative Appointments

2025-present	Chair, Department of Chemistry and Biochemistry, University of Notre Dame
2023-25	Senior Associate Dean for Education and Undergraduate Programs, College of Science, University of Notre Dame
2020-23	Associate Dean for Undergraduate Studies, College of Science, University of Notre Dame
2015-20	Director of Undergraduate Studies, Department of Chemistry and Biochemistry, University of Notre Dame
2006-11	Director of Graduate Admissions, Department of Chemistry and Biochemistry, University of Notre Dame

Academic Appointments

2015-present	Professor, Department of Chemistry and Biochemistry, University of Notre Dame
2005-15	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 Accomplishments

Chair, Department of Chemistry and Biochemistry, University of Notre Dame (2025-present)

Leading a department of 77 faculty (40 tenure/tenure-track, 13 teaching, 11 research, 13 concurrent), 225 graduate students, 231 majors, 24 postdoctoral scholars, and 9 staff, with ~\$23M/year in research expenditures (10.3% of Notre Dame research awards, FY24-FY26) and a \$15.6 M annual operating budget. Over the past nine years, the department's graduate program ranking has risen from 59th to 43rd.

- Overseeing first- and second-year service instruction for 2,300-2,400 students annually, one of the largest undergraduate teaching operations at the University.
- Organizing a department-wide review of undergraduate grading practices and course policies on the use of generative AI, with new policies to be adopted in Fall 2026.
- Renewing departmental emphasis on creating a culture of safety in our research laboratories.

- Directing renovation of the nuclear magnetic resonance (NMR) facility.
- Leading departmental strategic planning on faculty hiring with three and five year scopes.
- Completed a successful department external academic review (2025-26).
- Recruited two new faculty; two faculty promoted to tenure.
- Launched two strategic senior hires, one in AI/machine learning and another in computational biophysics and pharmaceutical chemistry.

Senior Associate Dean for Education and Undergraduate Programs (2023-25)

Associate Dean for Undergraduate Studies (2020-23)

College of Science, University of Notre Dame

Chief undergraduate officer for a college of 1,900 undergraduates, 281 faculty, five departments, six centers, eighteen institutes, four interdisciplinary majors, and dual-degree programs with three other colleges. Responsible for curriculum, academic records and graduation certification, college-wide advising, course approval, teaching evaluation, undergraduate research, and teaching-laboratory facilities. Primary college liaison to the Registrar, ND Global's educational programs, and the Provost's committees on core curriculum, academic code and policy, and the honor code. Direct reports included the Assistant Dean for Advising, the Associate Dean for Advising and Academic Affairs, and the directors of the *Mary E. Galvin Science & Engineering Scholars* program, Undergraduate Research, Study Abroad, the Digital Visualization Theater, and the Neuroscience and Behavior program. Nine collegiate advisors reported through this position.

Student success and access

- Member of the Provost's Committee on *Promoting Success of Students from Lower-Resourced Backgrounds* led by Provost Emeritus Tom Burish. Its twelve recommendations produced a summer bridge program, expanded peer-facilitated study groups, increased financial aid, and restructured foundational coursework.
- Academic lead for the 'Huddles' pilot, which implemented and studied peer-facilitated study groups in General Chemistry.
- Introduced a required mathematics placement exam, a new pre-calculus course, and a re-leveling process for misplaced students.
- Supported Mathematics and Physics & Astronomy in redesigning their foundational courses.

Advising and Undergraduate Research

- Oversaw advising for all College of Science students, including the Center for Health Sciences Advising (79-85% medical school acceptance rate).
- Launched Student Research @ Notre Dame (STRAND), a matching program to widen access to undergraduate research.

Curriculum, policy, and accreditation

- Led the College of Science response to Higher Learning Commission and ABET accreditation reviews.
- Helped secure 6 new faculty lines and 4 teaching postdoctoral positions for the Neuroscience and Behavior major, and led benchmarking of its cross-college curriculum.
- During the pandemic, served on the Faculty Task Force for Instructional Continuity and the Advisory Committee on Academic Code and Policy. Helped implement hybrid and online instruction, credit/no-credit policy, expanded classroom use, and a new online winter term.

Advancement / development

- Worked with the Science Advisory Council and individual donors on fundraising, including the endowment of the Galvin Scholars Program (see below).

**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.
- Oversaw the expansion of the Galvin Scholars program to 320 students (80 / cohort).

Director of Undergraduate Studies

Department of Chemistry and Biochemistry, University of Notre Dame (2015-20)

- 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 (2006-11)

- 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.

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
2018-19	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

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 (two versions: AI/ML in Chemistry and Biochemistry & Science 2.0)

University Service (all at Notre Dame)

2025-26	Elected member, Five-Year Review Committee of the Provost
2024-present	Academic Council (and chair of the Undergraduate Studies Committee)
2024-present	Academic Lead, Student Research @ Notre Dame (<i>STRAND</i>) project
2024-25	Academic Lead, <i>Huddles</i> Peer-Facilitated Study Group pilot program
2023-24	ND-LEAD program
2022-23	Provost's committee on <i>Promoting Success of Students From Lower-Resourced Backgrounds</i>
2022-present	Advisory Board, Glynn Family Honors Program
2020-25	Core Curriculum Committee
2020-25	Advisory Committee on the Academic Code and Policies
2020-present	Deans and Chairs Committee, College of Science
2020-25	Chair, College Council, College of Science
2020-25	Goldwater Scholars Selection Committee
2020-21	Provost's Working Group on the Forms and Structures of a Notre Dame Education
2020-21	Learning Management System (LMS) Succession Committee
2020-21	Faculty Task Force on Instructional Continuity
2020-21	Strategic Plan Working Group, College of Science
2000-25	Member of seven faculty search committees (chair of two)
2020	Valedictorian Selection Committee
2020, 2003-4	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, 2011-12, 2004-5	Undergraduate Studies Committee, Department of Chemistry & Biochemistry
2018-21	Core Curriculum Subcommittee on Science and Technology
2018-20	Learning Management Guidance Council
2018-19	Faculty Fellow, Kaneb Center for Teaching Excellence
2012-15, 2006-7	Physical / Analytical Chemistry Group Coordinator
2011-12, 2009, 2007	University Committee on Academic Technologies (UCAT)
2006-11	Center for Research Computing Faculty Advisory Committee
2006-11, 1999-2000	Graduate Admissions Committee, Department of Chemistry & Biochemistry
2006-09	Search Committee for the Center for Research Computing (CRC) Director
2008-10	College of Science Computing Committee
2006	Committee on Appointments and Promotions, Department of Chemistry & Biochemistry
2006-present	Co-organizer of the Notre Dame Theoretical Chemistry "Super-Group,"
2001-02	Graduate Studies Committee, Department of Chemistry & Biochemistry
2000-05	Campus representative for the Churchill Scholarship
2000-present	Faculty advisor for (and member of) the Notre Dame Bagpipe Band
1999-2005	Committee on Technical Computing

Professional Service

2024	Workshop Organizer, <i>Structure and Dynamics of Ice Surfaces</i> , Telluride Science Research Center, Telluride, CO
2022-24	Symposium co-organizer, <i>Chemistry of Ice</i> , ACS National Meeting, Spring 2024
2020	Workshop Organizer, <i>Structure and Dynamics of Ice Surfaces</i> , Telluride Science Research Center, Telluride, CO
2019	Workshop Organizer, <i>Thermal Transport at the Nanoscale</i> , Telluride Science Research Center, Telluride, CO
2019	Conference Organizer, 51 st Midwest Theoretical Chemistry Conference
2016	Workshop Organizer, <i>Thermal Transport at the Nanoscale</i> , Telluride Science Research Center, Telluride, CO
2014	Invited Speaker and Panelist on Open Science at the <i>NIAID Bioinformatics and Computational Biosciences Festival</i>
2011	Conference Organizer, 43 rd Midwest Theoretical Chemistry Conference
2010	Speaker and Panelist at the NSF-sponsored workshop on <i>Archiving Experiments to Raise Scientific Standards</i>
2009	Speaker and Panelist at the Kauffman Innovation Roundtable on <i>Sharing Data and Code in Computational Science</i> at the Yale Information Society Project
2008	Speaker and Panelist at the <i>New Communication Channels for Biology</i> 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
2002-04	Grant reviewer and panelist for the National Institute of General Medical Sciences (NIGMS) at the NIH
1999-present	Reviewer for journals including the <i>Journal of Physical Chemistry</i> , <i>Journal of Chemical Physics</i> , <i>Journal of Chemical Theory and Computation</i> , <i>Chemical Physics Letters</i> , <i>Physical Review E</i> , <i>Journal of Cheminformatics</i> , and <i>Journal of Molecular Structure: THEOCHEM</i>

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 MCB-1817966, 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, 9/1/2000 - 8/31/2002, \$320,000
- J. Daniel Gezelter (PI), “New Faculty Award,” Camille and Henry Dreyfus Foundation, 2000, \$40,000
- J. Daniel Gezelter (PI), “The OpenScience Project,” Alfred P. Sloan Foundation, 1999, \$30,000 + \$2,700 in additional private donations

Publications

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Google Scholar: <https://scholar.google.com/citations?user=Q1HKYyYAAAAJ>

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

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2. Benjamin M. Harless[@] and J. Daniel Gezelter^{†*}, “Elucidating Trace Gas Interactions with Ice Surfaces using Molecular Dynamics,” *J. Phys. Chem. C* **130**(28), pp. 9932-9941 (2026). DOI: 10.1021/acs.jpcc.6c01908 , arXiv: 2608.14849
3. Benjamin M. Harless[@], Jasmine K. Sindelar[#], and J. Daniel Gezelter^{†*}, “Molecular Dynamics of Ice-Active Solutions at Ice-Water Interfaces,” *J. Chem. Phys.* **163**, 054116 (2025). DOI: 10.1063/5.0282695 , arXiv: 2508.03591
4. Sydney A. Shavali[@] and J. Daniel Gezelter^{†*}, “Thermal Transport Through CTAB- and MTAB-Functionalized Gold Interfaces using Molecular Dynamics Simulations,” *J. Chem. Inf. Model.*, **65**(2) pp. 811-824 (2025). DOI: 10.1021/acs.jcim.4c02195

5. 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).
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6. 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).
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7. Sydney A. Shavali[@] 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).
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8. 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).
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9. Sydney A. Shavali[@] 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
10. 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.jpcc.1c07127 , ChemRxiv: 10.33774/chemrxiv-2021-196zw
11. 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
12. Suzanne M. Neidhart[@] and J. Daniel Gezelter^{†*}, "Thermal Conductivity of Gold-Phenylethanethiol (Au₁₄₄PET₆₀) Nanoarrays: A Molecular Dynamics Study," *J. Phys. Chem. C* **124**(5), pp. 3389-3395 (2020).
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13. 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).
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14. Patrick B. Loudon[@] 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. 3686-3691 (2018).
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15. 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).
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16. Patrick B. Loudon[@] 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).
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17. 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
18. 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
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21. 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/acs.nano.5b01724
22. 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
23. 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
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29. 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)
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31. 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)
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32. 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)
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33. 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)
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34. 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)
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35. Xiuquan Sun[@] and J. Daniel Gezelter^{†*}, "Langevin Dynamics for Rigid Bodies of Arbitrary Shape," *J. Chem. Phys.* **128**, 234107 (2008)
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39. 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)
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41. 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)
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42. 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* **109** (35), pp.16695–16699 (2005)
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53. J. Daniel Gezelter^o and William H. Miller^{†*}, "Dynamics of the Photodissociation of Triplet Ketene," *J. Chem. Phys.* **104**, 3546 (1996)
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55. Simon W. North^o, David A. Blank^o, J. Daniel Gezelter^o, Cheryl A. Longfellow^o, and Yuan T. Lee^{†*}, "Evidence for Stepwise Dissociation Dynamics of Acetone at 248 nm and 193 nm," *J. Chem. Phys.* **102**, 4447 (1995)
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56. Thomas D. Sewell^o, Donald L. Thompson[†], J. Daniel Gezelter^o, and William H. Miller^{†*}, "Some problems of correcting the zero-point energy problem in classical trajectories," *Chem. Phys. Lett.* **193**, 512 (1992)
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57. J. Daniel Gezelter^o and Ray Freeman^{†*}, "Use of Neural Networks to Design Shaped Radio-Frequency Pulses," *J. Magn. Reson.* **90**, 397 (1990)
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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

Mentoring

Postdoctoral Research Associate (1)

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

Graduate Students (25 total)

1. Hemanta (Manu) Bhattacharai, Ph.D. (2021), now Assistant Professor of Physics at Goshen College
2. Zosia Bolde (2025-present)
3. Kyle Daily, M.S. (2006), now a chemistry teacher at the Milton Hershey School
4. Cody Drisko, Ph.D. (2025), now Scientific Software Engineer at Stellar Science
5. Anderson DaSilva Duraes, Ph.D. (2023), now a postdoctoral researcher at the University of Wisconsin
6. Christopher Fennell, Ph.D. (2007), now Associate Professor and Chair of Chemistry at Oklahoma State University
7. Veronica Freund (2022-present)
8. Benjamin Harless, Ph.D. (2025)
9. Shenyu Kuang, Ph.D. (2012), now a Research & Development Engineer at Synopsys
10. Chunlei Li, M.S. (2010), Ph.D. (2014), now a senior manager in AI Data Science at Meta
11. Teng Lin, Ph.D. (2006), now the SVP of Business Development at XtalPi, Inc.
12. Madan Lamichhane, Ph.D. (2016), now the Sr. Manager in the Retail Banking Analytics Team at FICO
13. Patrick Loudon, Ph.D. (2018), now the Manager for Data Science at Domino's
14. James Marr, Ph.D. (2014, co-advised by Zac Schultz), now a product manager at Leica Microsystems
15. Alex Mazanek, M.S. (2019)
16. Matthew Meineke, Ph.D. (2004), now a Clinical Radiation Physicist at the Ohio State University
17. Joseph Michalka, Ph.D. (2016)
18. Minh Nhat Pham (2023-present)
19. Suzanne Neidhart, Ph.D. (2019), now a Sr. R&D Scientist at the Kansas City National Security Campus
20. Sydney Shavali, Ph.D. (2024), now a Volatile Organic Compound Chemist at Intertek
21. Kelsey Stocker, Ph.D. (2014), now Associate Professor of Chemistry at Suffolk University
22. Xiuquan Sun, Ph.D. (2008)
23. Charles F. Vardeman II, Ph.D. (2009), now a Research Assistant Professor in Computer Science and Engineering at Notre Dame
24. Changsen Xu, M.S. (2001, co-advised by Sharon Hammes-Schiffer), now a software engineer
25. 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 Combust, 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 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), Postdoc (UCSF, 2022-25), now a Computational Biophysicist at NASA Ames Research Center
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 Cleveland/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)

Community Service

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|--------------|---|
| 2018-22 | 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 |