# Todd R. Gingrich

#### Assistant Professor · Department of Chemistry

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## Professional Appointments

2018–present Assistant Professor of Chemistry, Northwestern University
 2015–2018 Physics of Living Systems Fellow, Massachusetts Institute of Technology

## Education \_\_\_\_\_

University of California, Berkeley Рн.D. IN Снемізтку • Advisor: Prof. Phillip L. Geissler • Thesis: Two Paths Diverged: Exploring Trajectories, Protocols, and Dynamic Phases	Berkeley, CA 2010–2015
<ul> <li>University College, Oxford University</li> <li>M.Sc. (By Research) IN PHYSICAL AND THEORETICAL CHEMISTRY</li> <li>Advisor: Prof. Mark Wilson</li> <li>Thesis: Simulating Surface Charge Effects in Carbon Nanotube Templated Ionic Crystal Growth</li> </ul>	Oxford, UK 2008–2010
California Institute of Technology B.S. wiтн Honors in Cнемізтку • Advisor: Prof. Nathan S. Lewis	Pasadena, CA 2004–2008

# Major Research Interests \_\_\_\_\_

Statistical mechanics, stochastic thermodynamics, chemical kinetics, molecular motors, tensor networks, molecular simulations, and theoretical biophysics.

# Awards and Honors \_\_\_\_\_

New Horizons Solvay Lecture in Chemistry, International Solvay Institutes	2025
Camille Dreyfus Teacher-Scholar Award, Camille and Henry Dreyfus Foundation	2024
Weinberg College of Arts & Sciences Distinguished Teaching Award, Northwestern University	2023
NSF Faculty Career Development (CAREER) Award, National Science Foundation	2023
Sloan Research Fellow, Sloan Foundation	2023
Searle Fellows Program, Searle Center for Advancing Learning and Teaching	2019-2020
APS Oppenheim Award, American Physical Society	2019
Physics of Living Systems Fellowship, Massachusetts Institute of Technology	2015
Outstanding Graduate Student Instructor, University of California, Berkeley	2013
Dan Lucas Book Prize, College of Chemistry, University of California, Berkeley	2011
Richard P. Schuster Chemistry Prize, California Institute of Technology	2008
Fannie and John Hertz Foundation Graduate Fellowship, Fannie and John Hertz Foundation	2008
National Science Foundation Graduate Research Fellowship, National Science Foundation	2008
Rhodes Scholarship, Rhodes Trust	2008
Robert L. Noland Leadership Award, California Institute of Technology	2007
Amgen Scholars Summer Research Fellowship, Amgen Foundation	2007
Upper Class Merit Award, California Institute of Technology	2005-2008
Robert C. Byrd Honors Scholarship, U.S. Department of Education	2004-2008

# Publications.

(TRG as corresponding author in bold; Gingrich group members underlined)

#### Preprints

Strand, N.E.; Nicholson, S.B.; Vroylandt, H.; **Gingrich, T.R.** "From high-dimensional committors to reactive insight." arXiv:2406.01452, 2024.

Penocchio, E.; <u>Gu, G.</u>; Albaugh, A.; **Gingrich, T.R.** "Power strokes in molecular motors: predictive, irrelevant, or somewhere in between?" ChemRXiv:10.26434/chemrxiv-2024-rjbdc, 2024.

Tan, T.H.; Watson, G.A.; Chao, Y.-C.; Li, J.; Gingrich, T.R.; Horowitz, J.M.; Fakhri, N. "Scale-dependent irreversibility in living matter." arXiv:2107.05701, 2021.

#### Published

Northwestern Faculty Career

- 31. <u>Albaugh, A.; Fu, R.-S.; Gu, G.</u>; **Gingrich, T.R.** "Limits on the Precision of Catenane Motors: Insights from Thermodynamics and Molecular Dynamics Simulations." *J. Chem. Theory Comput.*, 2024, *20*, 1-6. [DOI:10.1021/acs.jctc.3c01201]
- 30. Nicholson, S.B.; **Gingrich, T.R.** "Quantifying Rare Events in Stochastic Reaction-Diffusion Dynamics Using Tensor Networks." *Phys. Rev. X*, 2023, *13*, 041006. [DOI:10.1103/PhysRevX.13.041006]
- 29. Albaugh, A.; Gu, G.; **Gingrich, T.R.** "Sterically driven current reversal in a molecular motor model." *Proc. Natl. Acad. Sci. USA*, 2023, *120*(33), e2210500120. [DOI:10.1073/pnas.2210500120]
- 28. Binks, L.; Borsley, S.; Gingrich, T.R.; Leigh, D.A.; Penocchio, E.; Roberts, B.W. "The role of kinetic asymmetry and power strokes in an information ratchet." *Chem*, 2023, *9*, 1-16. [DOI:10.1016/j.chempr.2023.05.035]
- 27. Fu, R.-S.; **Gingrich, T.R.** "Thermodynamic uncertainty relation for Langevin dynamics by scaling time." *Phys. Rev. E*, 2022, *106*, 024128. [DOI:10.1103/PhysRevE.106.024128]
- 26. <u>Strand, N.E.</u>; <u>Vroylandt, H.</u>; **Gingrich, T.R.** "Computing time-periodic steady-state currents via the time evolution of tensor network states." *J. Chem. Phys.*, 2022, *157*, 054104. [DOI:10.1063/5.0099741]
- 25. Gingrich, T.R. "Measuring how effectively light drives a molecular pump." *Nat. Nanotechnol.*, 2022, *17*, 675. [DOI:10.1038/s41565-022-01152-x] (News & Views)
- 24. <u>Strand, N.E.</u>; Vroylandt, H.; **Gingrich, T.R.** "Using tensor network states for multi-particle Brownian ratchets." *J. Chem. Phys.*, 2022, *156*, 221103. [DOI:10.1063/5.0097332] (Editor's Pick)
- 23. Albaugh, A.; **Gingrich, T.R.** "Simulating a Chemically Fueled Molecular Motor with Nonequilibrium Molecular Dynamics." *Nat. Comm.*, 2022, *13*, 2204. [DOI:10.1038/s41467-022-29393-3]
- 22. Albaugh, A.; **Gingrich, T.R.** "Estimating Reciprocal Partition Functions to Enable Design Space Sampling." *J. Chem. Phys.*, 2020, *153*, 204102. [DOI:10.1063/5.0025358]
- 21. Strand, N.E.; Fu, R.-S.; **Gingrich, T.R.** "Current inversion in a periodically driven two-dimensional Brownian ratchet." *Phys. Rev. E*, 2020, *102*, 012141. [DOI:PhysRevE.102.012141] **(Editor's Suggestion)**
- 20. Owen, J.A.; Gingrich, T.R.; Horowitz, J.M. "Universal thermodynamic bounds on nonequilibrium response with biochemical applications." *Phys. Rev. X*, 2020, *10*, 011066. [DOI:10.1103/PhysRevX.10.011066]
- 19. Vroylandt, H.; Proesmans, K.; **Gingrich, T.R.** "Isometric Uncertainty Relations." *J. Stat. Phys.*, 2020, *178*, 1039-1053. [DOI:10.1007/s10955-020-02484-5]
- 18. Horowitz, J.M.; **Gingrich, T.R.** "Thermodynamic uncertainty relations constrain nonequilibrium fluctuations." *Nat. Phys.*, 2020, *15*, 1. [DOI:10.1038/s41567-019-0702-6]

17. Li, J.; Horowitz, J.M.; **Gingrich, T.R.**; Fakhri, N. "Quantifying dissipation using fluctuating currents." *Nat. Comm.*, 2019, *10*, 1666. [DOI:10.1038/s41467-019-09631-x]

Independent Postdoctoral Fellowship

- 16. **Gingrich, T.R.**; Horowitz, J.M. "Fundamental Bounds on First Passage Time Fluctuations for Currents." *Phys. Rev. Lett.*, 2017, *11*9, 170601. [DOI:PhysRevLett.119.170601]
- 15. Bisker, G.; Polettini, M.; Gingrich, T.R.; Horowitz, J.M.; "Hierarchical Bounds on Entropy Production Inferred from Partial Information." *J. Stat. Mech.: Theory Exp.*, 2017, 093210. [DOI:10.1088/1742-5468/aa8c0d]
- 14. Horowitz, J.M.; **Gingrich, T.R.** "Proof of the Finite-Time Thermodynamic Uncertainty Relation for Steady-State Currents." *Phys. Rev. E*, 2017, *96*, 020103(R). [DOI:10.1103/PhysRevE.96.020103] **(Editor's Suggestion)**
- 13. Zakine, R.; Solon, A.; Gingrich, T.R.; van Wijland, F. "Stochastic Stirling engine operating in contact with active baths." *Entropy*, 2017, *19(5)*, 193. [DOI:10.3390/e19050193]
- 12. Gingrich, T.R.; Rotskoff, G.M.; Horowitz, J.M. "Inferring dissipation from current fluctuations." *J. Phys. A*, 2017, *50*, 184004. [DOI:10.1088/1751-8121/aa672f]
- 11. **Gingrich, T.R.**; Horowitz, J.M.; Perunov, N.; England, J.L. "Dissipation bounds all steady-state current fluctuations." *Phys. Rev. Lett.*, 2016, *116*, 120601. [DOI:PhysRevLett.116.120601]

#### Mentored Research

- 10. **Gingrich, T.R.**; Rotskoff, G.M; Crooks, G.E.; Geissler, P.L. "Near-optimal protocols in complex nonequilibrium transformations." *Proc. Natl. Acad. Sci. USA*, 2016, *113*(37), 10263.[DOI:10.1073/pnas.1606273113]
- 9. Gingrich, T.R.; Geissler, P.L. "Preserving correlations between trajectories for efficient path sampling." *J. Chem. Phys.*, 2015, *142*(23), 234104. [DOI:10.1063/1.4922343] (Editor's Choice)
- Gingrich, T.R.; Rotskoff, G.M.; Vaikuntanathan, S.; Geissler, P.L. "Efficiency and large deviations in time-asymmetric stochastic heat engines." *New J. Phys.*, 2014, *16(10)*, 102003. [DOI:10.1088/1367-2630/16/10/102003] (Fast Track Communication)
- 7. Gingrich, T.R.; Vaikuntanathan, S.; Geissler, P.L. "Heterogeniety-induced large deviations in activity and (in some cases) entropy production." *Phys. Rev. E*, 2014, *90*, 042123. [DOI:10.1103/PhysRevE.90.042123]
- 6. Vaikuntanathan, S.; Gingrich, T.R.; Geissler, P.L. "Dynamic phase transitions in simple driven kinetic networks." *Phys. Rev. E*, 2014, *89*, 062108. [DOI:10.1103/PhysRevE.89.062108]
- 5. Gingrich, T.R.; Wilson, M. "The control of inorganic nanotube morphology using an applied potential." *J. Phys. Condens. Matter*, 2011, *23(13)*, 135306. [DOI:10.1088/0953-8984/23/13/135306]
- 4. Gingrich, T.R.; Wilson, M. "On the Ewald summation of Gaussian charges for the simulation of metallic surfaces." *Chem. Phys. Lett.*, 2010, *500(1)*, 178. [DOI:10.1016/j.cplett.2010.10.010]
- Katz, J.E.; Gingrich, T.R.; Santori, E.A.; Lewis, N.S. "Combinatorial synthesis and high-throughput photopotential and photocurrent screening of mixed-metal oxides for photoelectrochemical water splitting." *Energy Environ. Sci.*, 2009, 2(1), 103. [DOI:10.1039/B812177J]
- 2. Thallapally, P.K.; Dobrzanska, L.; Gingrich, T.R.; Wirsig, T.B.; Barbour, L.J.; Atwood, J.L. "Acetylene absorption and binding in a nonporous crystal lattice." *Agnew. Chem.*, 2006, *45*(*39*), 6506. [DOI:10.1002/anie.200601391]
- 1. Gingrich, T.R.; Smith, G.P. "Hydroxyapatite chromatography of phage-display virions." *BioTechniques*, 2005, *39(6)*, 879. [DOI:10.2144/000112032]

#### PATENTS

N.S. Lewis, J.E. Katz, T.R. Gingrich. "High-throughput screening and device for photocatalysts." Issued 9/8/2015, US Patent No. 9,126,175.

# Research Support\_\_\_\_\_

Present		
<b>Computer Simulation of Molecular Motors Far from Equilibrium</b> Gordon and Betty Moore Foundation, PI, \$1,963,820	December 1, 2021-February 1, 2026	
CAREER: Reaction-Diffusion Kinetics with Tensor Networks NSF CHE, PI, \$650,000	September 1, 2023–August 31, 2028	
Sloan Research Fellowship Sloan Foundation, \$75,000	September 15, 2023–September 14, 2025	
From Microscopic Motors to Macroscopic Work Northwestern IIN Seed Grant, Seed Investigator, \$100,000	September 15, 2023–September 14, 2024	
Self-Propellant Nanoparticle@MOF Catalysts for Chemical Warfare Agent Detoxification DTRA, co-PI with Omar Farha, \$2,500,000 (\$240,000 for TRG)	March 2024-March 2029	
Computational Tools for Stochastic, Far-From-Equilibrium Chemical Kinetics Camille Dreyfus Teacher-Scholar Award, \$100,000	June 2024-June 2029	
Completed		
EAGER: ADAPT: Optimizing chemical reaction networks with AI NSF CHE, PI, \$300,000	September 1, 2021–August 31, 2023	
Steering the dynamics of nanomachines Northwestern IIN Seed Grant, Seed Investigator, \$100,000	February 1, 2021–July 31, 2022	
Invited Lectures		
Scheduled		
New Horizons Solvay Lecture in Chemistry, Belgium	2025	
Telluride Workshop on Condensed Phase Dynamics. Telluride. CO	2023	
Dissipative Processes in Molecular Systems Workshop, Padova, Italy	July 2024	
	June 2024	
DELIVERED		
Nonequilibrium Dynamics, Information Processing, and Aging of Living Cells W Graduate Center, CUNY, New York, NY	orkshop, ITS @ The May 2024	
University of Michigan Chemistry, Ann Arbor, MI	April 2024	
University of Michigan Complex Systems, Ann Arbor, MI	April 2024	
University of Chicago, Department of Chemistry, Chicago, IL	March 2024	
Stanford University, Department of Chemistry, Palo Alto, CA	March 2024	
New York University, Department of Chemistry, New York, NY	March 2024	
Rice University Center for Theoretical Biophysics, Houston, TX	February 2024	
Northwestern (Mugneter Summer of Chemistry, New Brunswick, NJ	December 2023	
Suggestion II	August 2023	
Evaluation, IL		
Iniversity of North Carolina, Department of Chemistry, Chapel Hill, NC	June 2023	
Informal Statistical Physics Seminar University of Maryland College Park MD	April 2023	
Rare Events: Analysis Numerics and Annlications Brin Mathematics Descared (	April 2023	
Maryland, College Park, MD	February 2023	
Northwestern University, Department of Physics, Evanston, IL	January 2023	
Berkeley Statistical Mechanics Meeting, Berkeley, CA	January 2023	

Telluride Workshop on Condensed Phase Dynamics, Telluride, CO	July 2022
Midwest Theoretical Chemistry Conference, Columbus, OH	June 2022
Workshop on Stochastic Thermodynamics II, Sante Fe Institute, Sante Fe, NM (Virtual)	May 2021
University of Colorado at Boulder, Department of Chemistry, Boulder, CO (Virtual)	March 2021
Oxford University, Theoretical Chemistry Group, Oxford, England (Virtual)	February 2021
Telluride Workshop on Condensed Phase Dynamics, Virtual	July 2020
Illinois State University, Department of Physics, Normal, IL	February 2020
Oppenheim Prize Talk, APS March Meeting, Boston, MA	March 2019
Lawrence Berkeley National Lab/UC Berkeley Soft Matter Seminar, Berkeley, CA	January 2019
Why Measure Entropy Production?, Princeton Center for Theoretical Science, Princeton, NJ	November 2018
Stochastic Thermodynamics: Experiment and Theory, Max Planck Institute for the Physics of	September 2018
Complex Systems, Dresden, Germany	
Telluride Workshop on Condensed Phase Dynamics, Telluride, CO	July 2018
CCI Solar Fuels Workshop, Ventura, CA	July 2018
Large deviation theory in statistical physics: Recent advances and future challenges, Indian Center	September 2017
for Theoretical Sciences (ICTS), Bangalore, India	
Igert Summer Institute, Brandeis University, Waltham, MA	lune 2017
Berkeley Statistical Mechanics/Machine Learning Meeting, Berkeley, CA	January 2017
New York University, Department of Chemistry, New York, NY	December 2016
Stanford University, Department of Chemistry, Palo Alto, CA	December 2016
Columbia University, Department of Chemistry, New York, NY	November 2016
University of California at Santa Barbara, Department of Chemistry, Santa Barbara, CA	November 2016
Northwestern University, Department of Chemistry, Evanston, IL	October 2016
Boston University, Condensed Matter Theory/Biophysics, Boston, MA	March 2016
JCP Editor's Choice Session, APS March Meeting, Baltimore, MD	March 2016
Modeling and Inference from Single Molecules to Cells, MBI Workshop, Columbus, OH	February 2016
Large Deviation Theory in Principle and in Practice, Princeton Center for Theoretical Science, Princeton, NJ	November 2015
Chemistry & Physics of Liquids Gordon Research Conference, Poster Prize Short Talk, Holderness, NH	August 2015
Workshop on Statistical Mechanics and Computation of Large Deviation Rate Functions, Ecole Normale Superieure, Lyon, France	June 2015
Princeton University, Princeton Biophysics Symposium, Princeton, NJ	December 2014
Workshop on Large Deviations in Statistical Physics, National Institute for Theoretical Physics	July 2014
(NITheP), Stellenbosch, South Africa	
Teaching Experience	
CHEM 171: Advanced General Inorganic Chemistry (New Curriculum Development)	
· Course Rating: 5.09/6.00; Instructor Rating: 5.66/6.00; 186 Students	Fall 2023
· Course Rating: 4.64/6.00; Instructor Rating: 5.26/6.00; 175 Students	Fall 2022
CHEM 348: Physical Chemistry for ISP (New Curriculum Development)	
· Course Rating: 5.40/6.00; Instructor Rating: 6.00/6.00; 11 Students	Spring 2022
Course Rating: 5.30/6.00; Instructor Rating: 5.90/6.00; 12 Students	Spring 2021
Course Rating: 5.43/6.00; Instructor Rating: 6.00/6.00; 11 Students	Spring 2020
· Course Rating: 5.63/6.00; Instructor Rating: 5.88/6.00; 8 Students	Spring 2020
CHEM 444: Elementary Statistical Mechanics (New Curriculum Development)	
· Course Rating: 5.24/6.00; Instructor Rating: 5.65/6.00; 22 Students	Fall 2023
· Course Rating: 5.27/6.00; Instructor Rating: 5.57/6.00; 20 Students	Fall 2022
· Course Rating: 5.67/6.00; Instructor Rating: 5.67/6.00; 9 Students	Fall 2020

<ul> <li>Course Rating: 5.67/6.00; Instructor Rating: 6.00/6.00; 14 Students</li> <li>Course Rating: 5.50/6.00; Instructor Rating: 5.58/6.00; 13 Students</li> </ul>	Fall 2019 Fall 2018
Advising/Supervision	
Graduate Students (2 Completed PhDs, 4 in Progress)	
John Zima, PhD Student	2024-
Cathryn (Kate) Murphy, PhD Student	2024
Jonah Greenberg, PhD Student	2019-
Geyao Gu, PhD Student	2019-
Nils Strand, PhD, Now a Postdoc at UChicago with Aaron Dinner and Yuehaw Koon	2018-2023
Rueih-Sheng (Ray) Fu, PhD	2018-2023
Postdoctoral Scholars (2 Completed, 4 in Progress)	
John Strahan, Postdoctoral Scholar	2024-
Kathleen Krist, Postdoctoral Scholar	2023-
Emanuele Penocchio, Postdoctoral Scholar	2023-
Schuyler (Sky) Nicholson, Postdoctoral Scholar and Research Associate	2020-
Alex Albaugh, Postdoctoral Scholar, Now Assistant Professor of Chemical Engineering & Materials Science, Wayne State University	2018-2023
Hadrien Vroylandt, Postdoctoral Fellow, Now a Postdoctoral Researcher at CERMICS, École des Ponts ParisTech	2018-2020
UNDERGRADUATE RESEARCH STUDENTS Drew Alvarez, WCAS Summer Undergraduate Research Award and McCormick Summer Undergraduate Research Award	2023-
Isabelle Goodrow, Cornell University Summer Experience Grant	Summer 2023
Ashini Shah, Undergraduate Researcher	2022-2024
<b>Niles Babin</b> , International Institue of Nanotechnology REU <b>Akhil Kalghatgi</b> , ISP 398 student	Summer 2022 2021
Service	
External	
Editorial Board Member, Physical Review E	2022-2024
<b>Co-organizer and Statistical Mechanics Instructor</b> , Telluride School on Theoretical Chemistry, Telluride Science Research Center	2021, 2023
Selection Committee Member, ACS Junior/Senior Theory Award	2022
Selection Committee Member, APS Oppenheim Award	2020
Selection Committee Member, Rhodes Scholarship, District 15 (USA)	2013-15
University Service	
Associate Director, Integrated Science Program (ISP), Northwestern University	2023-
Residential College Fellow, Slivka Residential College, Northwestern University	2023-
Committee Member, Integrated Science Program (ISP) Committee, Northwestern University	2022-
Department Service	
Committee Member, Graduate Curriculum Committee	2023-
Chair, Assistant Professor of Instruction Search Committee, Successful Double Hire	2022-2023
Committee Member, General Chemistry Committee	2021-
Committee Member, Graduate Admissions Committee	2018-