Grant Murray Rotskoff rotskoff@stanford.edu statmech.stanford.edu

Education and Appointments

Assistant Professor of Chemistry (2020–) **Stanford University.**
Institute for Computational and Mathematical Engineering
Member, Bio-X
Member, Biophysics Program

James S. McDonnell Fellow (2017–2020) **Courant Institute of Mathematical Sciences, NYU.**
Research advisor: Prof. Eric Vanden-Eijnden

Ph.D. in Biophysics (2013–2017) **University of California, Berkeley.**
Research advisors: Prof. Phillip Geissler and Dr. Gavin Crooks.
Thesis: The Statistical Dynamics of Nonequilibrium Control

S.B. in Mathematics (2009–2013) **University of Chicago.**
Departmental and general honors.
Research advisors: Prof. Greg Voth, Prof. Sean Crosson, and Prof. Benoît Roux.

High School (2006–2009) **Illinois Mathematics and Science Academy.**

Awards, Honors, and Grants

2025 National Science Foundation CAREER Award: *Accelerating Conformational Sampling of Biomolecules with Transferable Generative Models*

2024 Research Corporation and the Beckman Foundation: *Automated workflows to assess physical constraints in neural networks for molecular property prediction*

2024 Scialog Fellow: *Automating Chemical Laboratories*

2024 France-Stanford Center for Interdisciplinary Studies Collaborative Grant (w/ Marylou Gabrié) *Accelerating physics-based models with generative neural networks*

2023 Wellcome Leap, Quantum for Bio Grant (PI)

2022–2027 Department of Energy Early Career Research Program

2022 Google Research Scholar Award

2020–2023 Terman Faculty Fellow

2017–2020 James S. McDonnell Foundation Postdoctoral Fellowship in Complex Systems Science

2015 Outstanding Graduate Student Instructor Award, UC Berkeley

2013–2017 National Science Foundation Graduate Research Fellow

2009–2013 University Scholar (Merit-based Academic Scholarship), University of Chicago

Invited Seminars and Colloquia

Upcoming

Frontiers in Probabilistic Inference: Sampling Meets Learning, Apr. 2025 International Conference on Learning Representations, Singapore.

Data Science Seminar, Mar. 2025 Yale University, New Haven, CT.

Applied Physics Seminar, Mar. 2025 Yale University, New Haven, CT.

NSF Workshop on AI+Science, Mar. 2025 MIT, Boston, MA.

Biophysical Society Annual Meeting: Theory and Computation Subgroup Invited Speaker, Feb. 2025 Los Angeles, CA.

Past

Chemistry Seminar, Nov. 2024 Johns Hopkins University, Baltimore, MD.

Chalmers AI Research Center Workshop for Structured Learning, Oct. 2024 Göteberg, Sweden.

Six Lectures for the School on Mathematical Physics, Sep. 2024 Ravello, Italy.

ACS Fall Meeting, Aug. 2024 Enhanced sampling methods for the study of chemical reactions and conformational transitions. Denver, CO.

Workshop on Condensed Phase Dynamics, Jul. 2024 Telluride Science Research Center, Telluride, CO.

American Conference on Theoretical Chemistry, Jun. 2024 Rising Talent Session, University of North Carolina, Chapel Hill.

AI+Science Workshop, Jun. 2024 Simons Institute, Berkeley, CA.

CVRI Department Seminar, Jun. 2024 University of California, San Francisco, CA.

2nd SIMPLAIX Workshop on Machine Learning for Multiscale Molecular Modeling, May 2024 Heidelberg, Germany.

Learning Collective Variables and Coarse Grained Models, Apr. 2024 University of Chicago, Chicago, IL.

Machine learning meets many-body physics, Apr. 2024 University of Nottingham, UK.

Biological Data Science Seminar, Apr. 2024 Stanford University, Stanford, CA.

Machine Learning for Molecules and Materials, Mar. 2024 University of Chicago, Chicago, IL.

APS March Meeting, Mar. 2024 Minneapolis, MN.

Frontiers in AI in Theoretical Chemistry, Nov. 2023 Caltech, Pasadena, CA.

Challenges and opportunities in non-equilibrium soft matter, Sep 2023 Món Sant Benet, Spain.

Frontiers in ion channels and nanopores, Sep. 2023 Sapienza, Università di Roma.

Theory seminar, Sep 2023 Laboratoire Matière et Systèmes Complexes, Université Paris Diderot.

Probabilistic sampling for physics: finding needles in a field of high-dimensional haystacks, Sep. 2023 Institut Pascal, Université Paris-Saclay.

AI+Science Summer School Instructor, Jul. 2023 University of Chicago, Chicago, IL.

Machine Learning and Informatics for Chemistry and Materials, Jun. 2023 Telluride Science Research Center, Telluride, CO.

Self-assembly and organization in non-equilibrium systems, Jun. 2023 Telluride Science Research Center, Telluride, CO.

MolSSI workshop on Machine Learning for Molecular Sciences, Jun. 2023 University of Maryland, College Park, MD.

Structure Design and Emerging Phenomena in Nanoparticle Assemblies: What's next?, Apr. 2023 Kavli Institute for Theoretical Physics, Santa Barbara, CA.

Nanoparticle Assemblies: A New Form of Matter with Classical Structure and Quantum Function, Mar. 2023 Kavli Institute for Theoretical Physics, Santa Barbara, CA.

Rare Events: Analysis, Numerics, Applications, Feb. 2023 Brin Center, University of Maryland.

The Lennard-Jones Centre Discussion Group, Nov. 2022 Cambridge University, UK.

Sampling, Diffusions, and Transport, Nov. 2022 Flatiron Institute, New York, NY.

Materials Science and Engineering Colloquium, Nov. 2022 Stanford University, Stanford, CA.

Seoul National University - Stanford Joint Symposium, Nov. 2022 Seoul, South Korea.

Machine Learning Meets Statistical Mechanics: Success and Future Challenges in Biosimulations, Oct. 2022 CECAM-IT-SIMUL, Sorrento, Italy.

Workshop on Condensed Phase Dynamics, Jul. 2022 Telluride Science Research Center, Telluride, CO.

Workshop on Machine Learning for Scientific Discovery, Jun. 2022 National Science Foundation, Washington, D.C.

Mathematics of Complex Data, Jun. 2022 Royal Institute of Technology, Stockholm, Sweden.

Sampling Methods and Inverse Problems, Jun. 2022 Duke University, Durham, NC.

Third Workshop on Stochastic Thermodynamics, Jun. 2022 University of Tokyo, Tokyo, Japan.

James Franck Institute Emerging Frontiers Seminar, Apr. 2022 University of Chicago, Chicago, IL.

SIAM Uncertainty Quantification, Apr. 2022 Atlanta, GA.

Math Colloquium, Apr. 2022 Rutgers University, Camden, NJ.

Applied Math Seminar, Mar. 2022 Stanford University, Stanford, CA.

Theoretical Chemistry Seminar, Dec. 2021 Purdue University, West Lafayette, IN.

Eran Karmon Memorial Lecture, Nov. 2021 University of California, Berkeley, CA.

Mean-Field Approaches in Machine Learning and Statistics, Oct. 2021 Institute for Mathematical and Statistical Innovation, University of Chicago, Chicago, IL.

Physics Seminar, Sep. 2021 Université du Luxembourg.

On Future Synergies for Stochastic and Learning Algorithms, Sep. 2021 CIRM, Marseille, France.

Accelerating the Understanding of Rare Events, Sep. 2021 Lorentz Center, Leiden, Netherlands.

SIAM Dynamical Systems, May 2021 Portland, OR.

Greater Boston Theoretical Chemistry Seminar, Mar. 2021 MIT / Harvard / Boston University.

Machine Learning Physical Sciences NEXUS, Feb. 2021 University of California, Irvine, CA.

Applied Mathematics Seminar, Feb. 2021 University of California, Santa Cruz, CA.

Deep Learning Theory Summer School, May. 2020 Shanghai Jiao Tong University, Shanghai, China.

Theoretical Chemistry Seminar, May 2020 University of California, Berkeley, CA.

Physics Seminar, May. 2020 Rockefeller University, New York, NY.

Applied Mathematics Seminar, Feb. 2020 Courant Institute, New York, NY.

Kavli Institute for Theoretical Physics: Cellular Energetics, Dec. 2019 Santa Barbara, CA.

AIM Deep Learning and PDE, Oct. 2019 San Jose, CA.

International Conference on Machine Learning (ICML), Jun. 2019 Long Beach, CA. (*accepted paper*)

Dynamical Systems and Computation, Jun. 2019 Mo'orea, French Polynesia.

Interdisciplinary Challenges in Non-equilibrium Physics, Apr. 2019 Edinburgh, UK.

Applied Math Colloquium, Apr. 2019 Rensselaer Polytechnic Institute , Troy, New York.

Statistical Physics Seminar, Mar. 2019 University of Maryland, College Park.

Applied Math Colloquium, Feb. 2019 Northwestern University, Evanston, Illinois.

Applied Math Seminar, Feb. 2019 Brown University, Providence, Rhode Island.

Special Chemistry Seminar, Jan. 2019 Cornell University, Ithaca, New York.

Theoretical Chemistry Seminar, Jan. 2019 Stanford University, Stanford, California.

Workshop Machine Learning & Physics, Nov. 2018 CUNY Graduate Center, New York.

SIAM Materials Meeting, Jul. 2018 Portland, Oregon.

Theory Seminar, Jun. 2018 University of Paris, Diderot.

APS March Meeting, 2017 New Orleans. Finalist for the GSNP student speaker award.

Learning and Nonequilibrium Working Group, 2016 Berkeley, California. Seminar.

Statistical Mechanics Seminar, 2015 Berkeley, California.

The Chemistry and Physics of Liquids, GRC, 2015 Holderness, New Hampshire. Poster.

Simulation with thermodynamic-like gradients, CECAM, 2015 Zaragoza, Spain.

Service and Teaching Activities

Stanford University Teaching

- Chem 91: Introduction to Chemical Research (Winter 2023)
- Chem 175: Statistical Mechanics (Winter 2021)
- Chem 175/273: Advanced Physical Chemistry (Winter 2022, Winter 2023, Winter 2024)
- Chem 263: Machine Learning for Chemical and Dynamical Data (Autumn 2021, Autumn 2023, Autumn 2024)

Conference / Workshop Organization

- APS March Meeting Focus Session: "Generative models and machine learning in chemical physics" (Mar 16-21, 2025; Anaheim, CA, USA)
- CECAM Workshop: Generative Models for Classical and Quantum Matter (Dec 3-6. 2024; Lausanne, Switzerland)
- AAAI Tutorial: Recent Advances in Physics Informed Neural Networks (Feb 20th, 2024; Vancouver, CA)
- Phillip L. Geissler Memorial Symposium (Jan 13, 2023; Berkeley, CA.)
- CECAM Workshop: Machine Learning Augmented Sampling (May 11-13, 2021; Lausanne, Switzerland)

Service and Outreach

- Stanford Summer Research Program Amgen Scholars Mentor (2024)
- Theoretical Chemistry Preview Day co-organizer (2020, 2021, 2022)
- DARE: Diversifying Academia, Recruiting Excellence mentor (2022-2023)
- Chemistry Department Equity and Inclusion Committee (2020-)
- Chemistry Department Graduate Admissions Committee (2020-)

PhD Students Mentored

- Shriram Chennakesavalu, Chemistry (2020–2024) → Research Scientist at Prescient Design.
- Andy Mitchell, Chemistry (2020–)
- Emmit Pert, Chemistry (2020–)
- Xiang Sherry Li, Chemistry (2021–)
- Nicholas Juntunen, Chemistry (2022–)
- Yinuo Ren, Computational and Mathematical Engineering (2022–)
- Steven Dunne, Biophysics (2023–)
- Abigail Park, Chemistry (2023–)
- Sebastian Ibararran, Chemistry (2023–)

Postdoctoral Scholars Mentored

- Jiawei Yan (2020–2022) → Machine Learning Scientist at Roche.
- Clay Batton (2022–)
- Sreekanth K. Manikandan (2022–2024) → Wallenberg Fellow at Chalmers.
- Jérémie Klinger (2023–)

Reviewing Physical Review Letters, Proceedings of the National Academy of Sciences, Nature Communications, Journal of Chemical Physics, Journal of Computational and Theoretical Chemistry, Journal of Machine Learning Research, Transactions on Machine Learning Research, Physical Review E, Biophysical Journal, Journal of Statistical Mechanics, Journal of Computational Physics, Europhysics Letters, Journal of Physics A: Mathematical and Theoretical, Physica A, Neurocomputing, Neural Information Processing Systems (NeurIPS 2019, 2020, 2021, 2023), International Conference on Machine Learning (ICML 2020 *top reviewer*, 2021), International Conference on Learning Representations (ICLR 2021, 2022), Mathematical and Scientific Machine Learning (MSML 2021, 2022), SIAM Journal on Mathematical Analysis, SIAM Journal on Uncertainty Quantification, Communications on Pure and Applied Mathematics

Research Facilitator, Marine Biological Laboratory at Woods Hole, Summer 2019

- Oversaw theory research rotations for the Physical Biology of the Cell summer school alongside Jasna Brujic.

Undergraduates Mentored

- Ramin Khajeh (2015–2016)
- Isaac Applebaum (2020–2023)
- David J. Toomer (2021–2023)
- Jasper Shogren-Knaak (2021–2024)
- Alondra Diez (Summer 2024)
- Dmitrii Skvortsov (2024–)

UC Berkeley, Graduate Student Instructor

- Spring 2016, Introduction to Computational Chemistry, Prof. Phillip Geissler.
- Autumn 2014, Graduate Statistical Mechanics, Prof. David Chandler.

The Compass Project, Fall 2014

- Mentoring for URM Berkeley chemistry and physics students.

The Compass Project, Summer 2014

- Designed and taught a two-week summer program about spectroscopy for incoming Berkeley freshmen from under-represented minority groups with an interest in studying physics.

Submitted Preprints

[52] Emmit K. Pert, Clay H. Batton, Sherry Li, Steven Dunne, and Grant M. Rotskoff. Scaling field-theoretic simulation for multi-component mixtures with neural operators. 2024.

[51] Javan Tahir, Surya Ganguli, and Grant M. Rotskoff. Features are fate: a theory of transfer learning in high-dimensional regression. ca. 2024. eprint: 2410.08194.

[49] Nicolas PD Sawaya, Daan Camps, Norm M. Tubman, Grant M. Rotskoff, and Ryan LaRose. Non-Clifford Diagonalization for Measurement Shot Reduction in Quantum Expectation Value Estimation. 2024.

[48] Luke Causer, Grant M. Rotskoff, and Juan P. Garrahan. Discrete generative diffusion models without stochastic differential equations: a tensor network approach arXiv:2407.11133. 2024.

[47] Abid Khan, Prateek Vaish, Yaoqi Pang, Nikhil Kowshik, Michael S. Chen, Clay H. Batton, Grant M. Rotskoff, J. Wayne Mullinax, Bryan K. Clark, Brenda M. Rubenstein, and Norm M. Tubman. Quantum Hardware-Enabled Molecular Dynamics via Transfer Learning. 2024.

[45] Shriram Chennakesavalu, Frank Hu, Sebastian Ibarraran, and Grant M. Rotskoff. Energy Rank Alignment: Using Preference Optimization to Search Chemical Space at Scale. *Submitted.* 2024.

Peer-Reviewed Publications

[50] Yinuo Ren, Haoxuan Chen, Grant M. Rotskoff, and Lexing Ying. How Discrete and Continuous Diffusion Meet: Comprehensive Analysis of Discrete Diffusion Models via a Stochastic Integral Framework. 2024. eprint: 2410.03601.

[46] Jérémie Klinger and Grant M. Rotskoff. Computing Nonequilibrium Responses with Score-Shifted Stochastic Differential Equations. 2024.

[44] Jérémie Klinger and Grant M. Rotskoff. Universal Energy-Speed-Accuracy Trade-Offs in Driven Nonequilibrium Systems. *Accepted at Phys. Rev. E.* 2024.

[43] Frank Hu, Michael S. Chen, Grant M. Rotskoff, Matthew W. Kanan, and Thomas E. Markland. Accurate and Efficient Structure Elucidation from Routine One-Dimensional NMR Spectra Using Multitask Machine Learning. *ACS Central Science* 10:11. 2024.

[42] Haoxuan Chen, Yinuo Ren, Lexing Ying, and Grant M. Rotskoff. Accelerating Diffusion Models with Parallel Sampling: Inference at Sub-Linear Time Complexity.

[41] Andrew R. Mitchell and Grant M. Rotskoff. Committor Guided Estimates of Molecular Transition Rates. *Journal of Chemical Theory and Computation*. 2024.

[40] Emmit K. Pert, Paul J. Hurst, Robert M. Waymouth, and Grant M. Rotskoff. Coacervation drives morphological diversity of mRNA encapsulating nanoparticles. 2024. arXiv: 2410.00406.

[39] Shiqi Chen, Emmanuel Valenton, Grant M. Rotskoff, Andrew L. Ferguson, Stuart A. Rice, and Norbert F. Scherer. Power Dissipation and Entropy Production Rate of High-Dimensional Optical Matter Systems. *Physical Review E* 110:4. 2024.

[38] Carlos L. Bassani, Greg van Anders, Uri Banin, Dmitry Baranov, Qian Chen, Marjolein Dijkstra, Michael S. Dimitriyev, Efi Efrati, Jordi Faraudo, Oleg Gang, Nicola Gaston, Ramin Golestanian, G. Ivan Guerrero-Garcia, Michael Gruenwald, Amir Haji-Akbari, Maria Ibáñez, Matthias Karg, Tobias Kraus, Byeongdu Lee, Reid C. Van Lehn, Robert J. Macfarlane, Bortolo M. Mognetti, Arash Nikoubashman, Saeed Osat, Oleg V. Prezhdo, Grant M. Rotskoff, Leonor Saiz, An-Chang Shi, Sara Skrabalak, Ivan I. Smalyukh, Mario Tagliazucchi, Dmitri V. Talapin, Alexei V. Tkachenko, Sergei Tretiak, David Vaknin, Asaph Widmer-Cooper, Gerard C. L. Wong, Xingchen Ye, Shan Zhou, Eran Rabani, Michael Engel, and Alex Travesset. Nanocrystal Assemblies: Current Advances and Open Problems. *ACS Nano*. 2024.

[37] Clay H. Batton and Grant M. Rotskoff. Microscopic Origin of Tunable Assembly Forces in Chiral Active Environments. *Soft Matter* 20:20. 2024.

[36] Grant M. Rotskoff. Sampling Thermodynamic Ensembles of Molecular Systems with Generative Neural Networks: Will Integrating Physics-Based Models Close the Generalization Gap? *Current Opinion in Solid State and Materials Science* 30. 2024.

[35] Shriram Chennakesavalu and Grant M. Rotskoff. Data-Efficient Generation of Protein Conformational Ensembles with Backbone-to-Side-Chain Transformers. *The Journal of Physical Chemistry B*. 2024.

[34] Shriram Chennakesavalu, Sreekanth K. Manikandan, Frank Hu, and Grant M. Rotskoff. Adaptive Nonequilibrium Design of Actin-Based Metamaterials: Fundamental and Practical Limits of Control. *Proceedings of the National Academy of Sciences* 121:8. 2024.

[33] Kangxin Liu, Grant M. Rotskoff, Eric Vanden-Eijnden, and Glen M. Hocky. Computing Equilibrium Free Energies through a Nonequilibrium Quench. *The Journal of Chemical Physics* 160:3. 2024.

[32] Yinuo Ren, Yiping Lu, Lexing Ying, and Grant M. Rotskoff. Statistical Spatially Inhomogeneous Diffusion Inference. *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024, February 20-27, 2024, Vancouver, Canada.*

[31] Gregory R. Bowman, Stephen J. Cox, Christoph Dellago, Kateri H. DuBay, Joel D. Eaves, Daniel A. Fletcher, Layne B. Frechette, Michael Grünwald, Katherine Klymko, JiYeon Ku, Ahmad Omar, Eran Rabani, David R. Reichman, Julia R. Rogers, Andreana M. Rosnik, Grant M. Rotskoff, Anna R. Schneider, Nadine Schwierz, David A. Sivak, Suriyanarayanan Vaikuntanathan, Stephen Whitelam, and Asaph Widmer-Cooper. Remembering the Work of Phillip L. Geissler: A Coda to His Scientific Trajectory. *Annual Review of Physical Chemistry* 74:1. 2023.

[30] Shriram Chennakesavalu and Grant M. Rotskoff. Unified, Geometric Framework for Nonequilibrium Protocol Optimization. *Physical Review Letters* 130:10. 2023.

[29] Shriram Chennakesavalu, David J. Toomer, and Grant M. Rotskoff. Ensuring Thermodynamic Consistency with Invertible Coarse-Graining. *The Journal of Chemical Physics (Editor's Choice 2023)* 158:12. 2023.

[28] Grant Rotskoff and Eric Vanden-Eijnden. Trainability and Accuracy of Artificial Neural Networks: An Interacting Particle System Approach. *Communications on Pure and Applied Mathematics* 75:9. 2022.

[27] Jiawei Yan and Grant M. Rotskoff. Physics-informed graph neural networks enhance scalability of variational nonequilibrium optimal control. *The Journal of Chemical Physics* 157:7. 2022.

[26] Jiawei Yan, Hugo Touchette, and Grant M. Rotskoff. Learning Nonequilibrium Control Forces to Characterize Dynamical Phase Transitions. *Physical Review E* 105:2. 2022.

[25] Marylou Gabrié, Grant M. Rotskoff, and Eric Vanden-Eijnden. Adaptive Monte Carlo Augmented with Normalizing Flows. *Proc. Natl. Acad. Sci. U.S.A.* 119:10. 2022.

[24] Grant M. Rotskoff, Andrew R. Mitchell, and Eric Vanden-Eijnden. Active Importance Sampling for Variational Objectives Dominated by Rare Events: Consequences for Optimization and Generalization. *Mathematical and Scientific Machine Learning, 16-19 August 2021, Virtual Conference / Lausanne, Switzerland.*

[23] Shriram Chennakesavalu and Grant M Rotskoff. Cooperative Multi-Agent Reinforcement Learning for High-Dimensional Nonequilibrium Control. *Fourth Workshop on Machine Learning and the Physical Sciences (NeurIPS 2021).*

[22] Shriram Chennakesavalu and Grant M. Rotskoff. Probing the Theoretical and Computational Limits of Dissipative Design. *J. Chem. Phys.* 155:19. 2021.

[21] Marylou Gabrié, Grant M. Rotskoff, and Eric Vanden-Eijnden. Efficient Bayesian Sampling Using Normalizing Flows to Assist Markov Chain Monte Carlo Methods. *ICML Workshop on Invertible Neural Networks, Normalizing Flows, and Explicit Likelihood Models ICML 2021.*

[20] Zhengdao Chen, Grant M. Rotskoff, Joan Bruna, and Eric Vanden-Eijnden. A Dynamical Central Limit Theorem for Shallow Neural Networks. *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, Virtual.*

[19] Carles Domingo-Enrich, Samy Jelassi, Arthur Mensch, Grant M. Rotskoff, and Joan Bruna. A Mean-Field Analysis of Two-Player Zero-Sum Games. *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, Virtual.*

[18] Grant M. Rotskoff and Eric Vanden-Eijnden. Dynamical Computation of the Density of States and Bayes Factors Using Nonequilibrium Importance Sampling. *Phys. Rev. Lett.* 122:15. 2019.

[17] Grant M. Rotskoff, Samy Jelassi, Joan Bruna, and Eric Vanden-Eijnden. Neuron Birth-Death Dynamics Accelerates Gradient Descent and Converges Asymptotically. *Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA.*

[16] Matthew R. Hauwiller, Layne B. Frechette, Matthew R. Jones, Justin C. Ondry, Grant M. Rotskoff, Phillip Geissler, and A. Paul Alivisatos. Unraveling Kinetically-Driven Mechanisms of Gold Nanocrystal Shape Transformations Using Graphene Liquid Cell Electron Microscopy. *Nano Lett.* 18:9. 2018.

[15] Grant M. Rotskoff and Eric Vanden-Eijnden. Parameters as Interacting Particles: Long Time Convergence and Asymptotic Error Scaling of Neural Networks. *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada.*

[14] Grant M Rotskoff and Phillip L Geissler. Robust Nonequilibrium Pathways to Microcompartment Assembly. *Proc. Natl. Acad. Sci. U.S.A* 112. 2018.

[13] Todd R Gingrich, Grant M Rotskoff, and Jordan M Horowitz. Inferring Dissipation from Current Fluctuations. *J. Phys. A: Math. Theor.* 50:18. 2017.

[12] Grant M. Rotskoff, Gavin E. Crooks, and Eric Vanden-Eijnden. Geometric approach to optimal nonequilibrium control: Minimizing dissipation in nanomagnetic spin systems. *Physical Review E* 95:1. 2017.

[11] Grant M Rotskoff. Mapping Current Fluctuations of Stochastic Pumps to Nonequilibrium Steady States. *Phys. Rev. E* 95:3-1. 2017.

[10] Gabriele Cesare Sosso, Sebastiano Caravati, Grant Rotskoff, Suriyanarayan Vaikuntanathan, and Ali Hassanali. On the Role of Nonspherical Cavities in Short Length-Scale Density Fluctuations in Water. *J. Phys. Chem. A* 121:1. 2017.

[9] Todd R Gingrich, Grant M Rotskoff, Gavin E Crooks, and Phillip L Geissler. Near-Optimal Protocols in Complex Nonequilibrium Transformations. *Proc. Natl. Acad. Sci. U.S.A.* 113:37. 2016.

[8] Suriyanarayanan Vaikuntanathan, Grant Rotskoff, Alexander Hudson, and Phillip L Geissler. Necessity of Capillary Modes in a Minimal Model of Nanoscale Hydrophobic Solvation. *Proc. Natl. Acad. Sci. U.S.A.* 113:16. 2016.

[7] Xingchen Ye, Matthew R Jones, Layne B Frechette, Qian Chen, Alexander S Powers, Peter Ercius, Gabriel Dunn, Grant M Rotskoff, Son C Nguyen, Vivekananda P Adiga, Alex Zettl, Eran Rabani, Phillip L Geissler, and A Paul Alivisatos. Single-Particle Mapping of Nonequilibrium Nanocrystal Transformations. *Science* 354:6314. 2016.

[6] Grant M Rotskoff and Gavin E Crooks. Optimal Control in Nonequilibrium Systems: Dynamic Riemannian Geometry of the Ising Model. *Phys. Rev. E* 92:6. 2015.

[5] Jonathan W Willett, Julien Herrou, Ariane Briegel, Grant Rotskoff, and Sean Crosson. Structural Asymmetry in a Conserved Signaling System That Regulates Division, Replication, and Virulence of an Intracellular Pathogen. *Proc. Natl. Acad. Sci. U.S.A.* 112:28. 2015.

[4] Sander Pronk, Iman Pouya, Magnus Lundborg, Grant Rotskoff, Björn Wesén, Peter M Kasson, and Erik Lindahl. Molecular Simulation Workflows as Parallel Algorithms: The Execution Engine of Copernicus, a Distributed High-Performance Computing Platform. *J. Chem. Theory Comput.* 11:6. 2015.

[3] Todd R Gingrich, Grant M Rotskoff, Suriyanarayanan Vaikuntanathan, and Phillip L Geissler. Efficiency and Large Deviations in Time-Asymmetric Stochastic Heat Engines. *New J. Phys.* 16:10. 2014.

[2] James F Dama, Grant Rotskoff, Michele Parrinello, and Gregory A Voth. Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. *J. Chem. Theory Comput.* 10:9. 2014.

[1] Julien Herrou, Grant Rotskoff, Yun Luo, Benoît Roux, and Sean Crosson. Structural Basis of a Protein Partner Switch That Regulates the General Stress Response of α-Proteobacteria. *Proc. Natl. Acad. Sci. U.S.A.* 109:21. 2012.