LAYNE B. FRECHETTE

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Brandeis University, 415 South Street Waltham, MA 02453

EDUCATION

University of California, Berkeley (UC Berkeley) *August 2015 - May 2020*
Ph.D., Physical Chemistry

Brown University *September 2011 - May 2015*
Sc.B., Chemical Physics, *magna cum laude*

RESEARCH EXPERIENCE

Brandeis University Department of Physics *July 2022 - Present*
Advisors: Michael Hagan and Aparna Baskaran

- Use theory and simulation to study active matter and self-assembly

NIDDK, NIH Laboratory of Chemical Physics *August 2020 - May 2022*
Advisor: Robert B. Best

- Developed and used models of protein residue coevolution to attempt to identify and design fold-switching proteins
- Created Boltzmann machine code to learn Potts models for families of protein sequences and protein folding trajectories

UC Berkeley Department of Chemistry *October 2015 - July 2020*
Advisor: Phillip L. Geissler
Thesis: "Chemical Transformations of Nanocrystals: Theory and Molecular Simulation"
Project 1: Understanding nonequilibrium shape transformations of etched nanocrystals

- Developed kinetic Monte Carlo simulations to uncover the atomic details of nonequilibrium shape transformations of nanocrystals undergoing chemical etching
- Worked closely with experimental and theoretical collaborators to connect model results with observations from liquid-cell transmission electron microscopy experiments

Project 2: Modeling cation exchange reactions with an elastic lattice model

- Developed Monte Carlo simulations and analytical theory to model lattice mismatch and study its impact on cation exchange reactions
- Created a novel graphical construction to describe elastic phase coexistence
- Determined the microscopic origin of mean-field behavior observed in spin-crossover compounds
- Used kinetic Monte Carlo simulations to reveal how elastic forces create nonequilibrium patterns in model nanocrystals

Brown University Department of Chemistry *September 2013 - May 2015*
Advisor: Richard M. Stratt
Honors Thesis: "Geodesic pathways through the potential energy landscape of liquid crystal formers"

- Implemented and used molecular dynamics simulations and geodesic theory to study dynamics of liquid-crystal-forming molecules

- Developed mean-field and path-integral theories for molecular motion in liquid crystal phases
- Found evidence for dynamical frustration in nematic liquid crystals

Brown University Department of Physics *February 2012 - August 2013*
Advisor: Derek M. Stein
Development of electrospray ionization mass spectrometry for DNA sequencing

- Helped interpret mass spectra of biomolecule fragments
- Used transmission electron microscopy to image glass nanopores
- Systematically characterized the onset of electrospray of sodium iodide in formamide as a function of nanopore diameter

PUBLICATIONS

* Denotes equal contributions.

1. D. Wang,* L.B. Frechette,* and R.B. Best. "On the role of native contact cooperativity in protein folding." Submitted.
2. A. Sciortino, H. Faizi, S. Uplap, L. Frechette, M.S.E. Peterson, P. Vlahovska, A. Baskaran, M.F. Hagan, and A. Bausch. "Active membrane deformations of a minimal synthetic cell." *bioRxiv*, doi:10.1101/2023.12.18.571643 (2023).
3. G.R. Bowman, S.J. Cox, C. Dellago, K.H. DuBay, J.D. Eaves, D.A. Fletcher, L.B. Frechette, M. Grünwald, K. Klymko, J. Ku, A.K. Omar, E. Rabani, D.R. Reichman, J.R. Rogers, A.M. Rosnik, G.M. Rotskoff, A.R. Schneider, N. Schwierz, D.A. Sivak, S.n Vaikuntanathan, S. Whitelam, and A. Widmer-Cooper. "Remembering the Work of Phillip L. Geissler: A Coda to His Scientific Trajectory." *Annu. Rev. Phys. Chem.*, **74**, 1-27 (2023).
4. J.C. Ondry, L.B. Frechette, P.L. Geissler, and A.P. Alivisatos. "Trade-offs between translational and orientational order in 2D superlattices of polygonal nanocrystals with differing edge count." *Nano Lett.*, **22**, 389-395 (2021).
5. L.B. Frechette, C. Dellago, and P.L. Geissler. "Elastic forces drive nonequilibrium pattern formation in a model of nanocrystal ion exchange." *Proc. Natl. Acad. Sci. U.S.A.*, **118**, e2114551118 (2021).
6. L.B. Frechette, C. Dellago, and P.L. Geissler. "Origin of mean-field behavior in an elastic Ising model," *Phys. Rev. B* **102**, 024102 (2020).
7. L.B. Frechette, C. Dellago, and P.L. Geissler. "Consequences of lattice mismatch for phase equilibrium in heterostructured solids," *Phys. Rev. Lett.* **123**, 135701 (2019).
8. M.R. Hauwiller, L.B. Frechette, M.R. Jones, J.C. Ondry, G.M. Rotskoff, P. Geissler, and A.P. Alivisatos. "Unraveling kinetically-driven mechanisms of gold nanocrystal shape transformations using graphene liquid cell electron microscopy," *Nano Lett.* **18**, 5731-5737 (2018).
9. X. Ye, M.R. Jones, L.B. Frechette, Q. Chen, A.S. Powers, P. Ericus, G. Dunn, G.M. Rotskoff, S.C. Nguyen, V.P. Adiga, A. Zettl, E. Rabani, P.L. Geissler, A.P. Alivisatos, "Single-particle mapping of nonequilibrium nanocrystal transformations," *Science* **354**, 874-877 (2016).
10. L. Frechette and R.M. Stratt, "The inherent dynamics of isotropic- and nematic-phase liquid crystals," *J. Chem. Phys.* **144**, 234505 (2016).
11. L. Frechette, D. Jacobson, and R.M. Stratt, "Erratum: "The inherent dynamics of a molecular liquid: Geodesic pathways through the potential energy landscape of a liquid of linear molecules" [J. Chem. Phys. 140, 174503 (2014)]," *J. Chem. Phys.* **141**, 209902 (2014).

FELLOWSHIP & AWARDS

- Berkeley Statistical Mechanics Meeting Poster Prize, 2019
- Erwin Schrödinger Institute Junior Research Fellowship, 2018
- Outstanding Graduate Student Instructor Award, UC Berkeley, 2017 – 2018
- Clapp Prize for Outstanding Undergraduate Thesis, Brown Department of Chemistry, 2015
- Karen T. Romer Undergraduate Teaching and Research Award, Brown University, 2014

TEACHING EXPERIENCE

Adjunct Instructor, Montgomery College

- CHEM 131D: Principles of Chemistry I Discussion, Fall 2021
- CHEM 131L: Principles of Chemistry I Laboratory, Fall 2021

Graduate Student Instructor, UC Berkeley

- CHEM 220A: Thermodynamics and Statistical Mechanics, Fall 2017
- CHEM 120B: Physical Chemistry, Fall 2016
- CHEM 3AL: Organic Chemistry Laboratory, Fall 2015

Undergraduate Teaching Assistant, Brown University

- PHYS 1600: Computational Physics, Spring 2015
- CHEM 330: Equilibrium, Rate, and Structure, Fall 2013.

Tutor, Brown University Science Center

- Introductory mechanics and electricity and magnetism, Spring 2014 – Spring 2015

Certifications

- Certificate of Training, 'Scientists Teaching Science', National Institutes of Health, 2020
- UC Berkeley Certificate in Teaching and Learning in Higher Education, 2020

SKILLS

Programming: C/C++, Python, Bash, MATLAB, LaTeX
Software: Mathematica, LAMMPS, HOOMD-blue, VMD

ORAL PRESENTATIONS

- "Mean-field critical behavior and dynamics of a model lattice-mismatched solid," Northern California Theoretical Chemistry Meeting, Contributed Talk, May 19, 2019
- "Modulated order and unconventional coexistence in a model of lattice-mismatched solids," APS March Meeting, Contributed Talk, March 6, 2019
- "Exploring the phase behavior of an elastic Ising model for cation exchange," Pitzer Center Theoretical Chemistry Seminar, April 4, 2018
- "The inherent dynamics of liquid crystal formers," Berkeley Statistical Mechanics Seminar, April 1, 2016

POSTER PRESENTATIONS

- "Inverstigating fold-switching proteins with coevolutionary models," NIDDK Scientific Conference (Virtual), April 2, 2021.

- "Evoluionary models of fold-switching proteins," Annual Meeting of the Biophysical Society (Virtual), February 23-24, 2021.
- "Elastic phase behavior significantly biases the kinetics of model ion-exchange reactions," Berkeley Statistical Mechanics Meeting, January 11, 2019
- "Exploring the phase behavior of an elastic Ising model for cation exchange," West Coast Theoretical Chemistry Symposium, March 28, 2018
- "The statistical mechanics of ion exchange in nanocrystals," Berkeley Statistical Mechanics Meeting, January 12, 2018
- "A simple model for cation exchange in nanocrystals," Chemistry and Physics of Liquids Gordon Research Conference, August 8, 2017
- "Nonequilibrium shape transformations of etched nanocrystals," Berkeley Statistical Mechanics Meeting, January 13, 2017

PROFESSIONAL SERVICE

- Served as a reviewer for *Nano Letters*

OUTREACH

- Helped foster a supportive peer network for incoming chemistry graduate students through the pilot CHEMentor program
- Taught a two-hour course on computational chemistry to high school students through the Berkeley Splash program