

## Paul S. Nerenberg

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### Education

Ph.D. in Physics, *Massachusetts Institute of Technology (MIT)*, February 2010.

Thesis title: “The Mechanism of Collagenolysis: A Substrate-centric View”, advisor: Prof. Collin Stultz.

B.S. in Physics with University and Department honors, *Johns Hopkins University (JHU)*, May 2004.

### Academic Positions

Kravis Associate Professor, Kravis Dept. of Integrated Sciences, *Claremont McKenna College (CMC)*, 07/2023 – present.

Associate Professor, Dept. of Physics & Astronomy and Dept. of Biological Sciences, *California State University, Los Angeles (Cal State LA)*, 08/2021 – 06/2023.

Assistant Professor, Dept. of Physics & Astronomy and Dept. of Biological Sciences, *Cal State LA*, 03/2016 – 08/2021.

Research Assistant Professor, Div. of Geological and Planetary Sciences, *California Institute of Technology*, 07/2014 – 03/2016.

Visiting Assistant Professor, W.M. Keck Science Department, *Claremont McKenna, Pitzer, and Scripps Colleges*, 08/2011 – 06/2014.

### Research Experience

Postdoctoral scholar with Prof. Teresa Head-Gordon, California Institute of Quantitative Biosciences (QB3), *University of California, Berkeley*, 03/2010 – 07/2011.

Graduate research assistant with Prof. Collin Stultz, Dept. of Electrical Engineering and Computer Science and Harvard-MIT Division of Health Sciences and Technology, *MIT*, 09/2006 – 01/2010.

REU student with Prof. Jim Houck (deceased), Dept. of Astronomy, *Cornell University*, 06/2003 – 08/2003.

Undergraduate research assistant with Prof. Cila Herman (retired), Dept. of Mechanical Engineering, *JHU*, 09/2002 – 06/2003.

### Teaching Experience

As faculty at *CMC*:

- SCI 10L: Codes of Life (Spring 2024, Fall 2024)

See website for prior teaching experience in the W.M. Keck Science Department during 2011-14 and Cal State LA during 2016-23.

## Publications

% Undergraduate student author.

# MS student author.

\* Both authors contributed equally to this work.

1. Rishch A, Rebel A, **Nerenberg PS**, and Forouzesh N. Calculation of Protein-Ligand Binding Entropies using a Rule-based Molecular Fingerprint. *Biophysical Journal* 2024; 123:2839-2848.
2. Lee BU, Papoutsis BM, Wong NY, Piacentini J, Kearney C, Huggins NA%, Cruz N%, Ng TT%, Hao KH, Kramer JS, Fenlon EE, **Nerenberg PS**, Phillips-Piro CM, and Brewer SH. Unraveling Complex Local Protein Environments with 4-Cyano-L-phenylalanine. *Journal of Physical Chemistry B* 2022; 126:8957-8969.
3. Stoppelman JP, Ng TT%, **Nerenberg PS**, and Wang L-P. Development and Validation of AMBER-FB15-compatible Force Field Parameters for Phosphorylated Amino Acids. *Journal of Physical Chemistry B* 2021; 125:11927-11942.
4. Leal JA\*, Estrada-Tober ZM\*, Wade F#, Mendiola AJP, Meza A, Mendoza M, **Nerenberg PS**, Zurita-Lopez CI. Phosphoserine Inhibits Neighboring Arginine Methylation in the RKS Motif of Histone H3. *Archives of Biochemistry and Biophysics* 2021; 698: 108716.
5. McDonald AR, Nash JA, **Nerenberg PS**, Ball KA, Sode O, Foley JJ, Windus TL, and Crawford TD. Building Capacity for Undergraduate Education and Training in Computational Molecular Science: A Collaboration between the MERCURY Consortium and the Molecular Sciences Software Institute. *International Journal of Quantum Chemistry* 2020; 120:e26359.
6. Menezes GB, **Nerenberg PS**, Li N, and Allen EL. Results of an Intro to Mechanics Course Designed to Support Student Success in Physics I and Foundational Engineering Courses. *ASEE Virtual Conference* 2020. [Peer-reviewed conference paper.]
7. Schauerl M, **Nerenberg PS**, Jang H, Wang L-P, Bayly CI, Mobley DL, and Gilson MK. Non-bonded Force Field Model with Advanced Restrained Electrostatic Potential Charges (RESP2). *Nature Communications Chemistry* 2020; 3:44.
8. Zhou A%, Schauerl M, and **Nerenberg PS**. Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. *Journal of Chemical Information and Modeling* 2020; 60:249-258.
9. Qiu Y, **Nerenberg PS**, Head-Gordon T, and Wang L-P. Systematic Optimization of Water Models Using Liquid/Vapor Surface Tension Data. *Journal of Physical Chemistry B* 2019; 123:7061-7073.
10. **Nerenberg PS** and Head-Gordon T. New developments in biomolecular force fields. *Current Opinion in Structural Biology* 2018; 49:129-138.
11. Li N, Menezes GB, Allen EL, and **Nerenberg PS**. First-Year Experience (FYrE@ECST): Intro to Physics Course (WIP). *The Collaborative Network for Engineering and Computing Diversity Conference (CoNECD)*, Crystal City, VA, 2018. [Peer-reviewed conference paper.]
12. Yedvabny E, **Nerenberg PS**, So C%, and Head-Gordon T. The Disordered Structural Ensembles of Vasopressin and Oxytocin and Their Mutants. *Journal of Physical Chemistry B* 2015; 119:896-905.
13. Chapman DE%\*, Steck JK%\*, and **Nerenberg PS**. Optimizing Protein-Protein van der Waals Interactions for the AMBER ff9x/ff12 Force Field. *Journal of Chemical Theory and Computation* 2014; 10:273-281.
14. Liguori N, **Nerenberg PS**, and Head-Gordon T. Embedding A $\beta$ 42 in Heterogeneous Membranes Depends on Cholesterol Asymmetries. *Biophysical Journal* 2013; 105:899-910.
15. **Nerenberg PS**, Jo B%, So C%, Tripathy A%, and Head-Gordon T. Optimizing Solute-Water van der Waals Interactions To Reproduce Solvation Free Energies. *Journal of Physical Chemistry B* 2012; 116:4524-4534.
16. Ball KA, Phillips AH, **Nerenberg PS**, Fawzi NL, Wemmer DE, and Head-Gordon T. Homogeneous and Heterogeneous Tertiary Structure Ensembles of Amyloid- $\beta$  Peptides. *Biochemistry* 2011; 50:7612-7628.
17. **Nerenberg PS** and Head-Gordon T. Optimizing Protein-Solvent Force Fields to Reproduce Intrinsic Conformational Preferences of Model Peptides. *Journal of Chemical Theory and Computation* 2011; 7:1220-1230.
18. Chen MM, Bartlett AI, **Nerenberg PS**, Friel CT, Hackenberger CPR, Stultz CM, Radford SE, and Imperiali B. The effects of N-linked glycosylation on protein folding kinetics and thermodynamics: a combined

experimental and computational analysis. *Proceedings of the National Academy of Sciences* 2010; 107:22528-22533.

19. Salsas-Escat R\*, **Nerenberg PS\***, and Stultz CM. Cleavage site specificity and conformational selection in type I collagen degradation. *Biochemistry* 2010; 49:4147-4158.
20. Gurry T, **Nerenberg PS**, and Stultz CM. The contribution of interchain salt bridges to triple-helical stability in collagen. *Biophysical Journal* 2010; 98:2634-2643.
21. Phillips CM, **Nerenberg PS**, Drennan CL, and Stultz CM. The Physical Basis of Metal Binding Specificity in *E. coli* NikR. *Journal of the American Chemical Society* 2009; 131:10220-10228.
22. **Nerenberg PS** and Stultz CM. Differential Unfolding of  $\alpha 1$  and  $\alpha 2$  Chains in Type I Collagen and Collagenolysis. *Journal of Molecular Biology* 2008; 382:246-256.
23. **Nerenberg PS**, Salsas-Escat R, Stultz CM. Do collagenases unwind triple-helical collagen prior to peptide bond hydrolysis? Reinterpreting experimental observations with mathematical models. *Proteins* 2008; 70:1154-1161.
24. **Nerenberg PS**, Salsas-Escat R, Stultz CM. Collagen – A Necessary Accomplice in the Metastatic Process. *Cancer Genomics and Proteomics* 2007; 4:319-328.

## Federal Grant Funding

**NSF MRI Consortium: Track 1 Acquisition of a High-Performance Computing Cluster for Interdisciplinary Research at the Claremont Colleges.** (PI, award #2408259, \$918K, 09/2024-08/2027.) Research grant to acquire a heterogeneous HPC cluster for faculty and student research spanning the natural sciences, mathematics, and economics at both Claremont McKenna College and Harvey Mudd College.

**NSF PREC Track 1: Cal State LA-MoISSI PREC Pathway to Diversity Program.** (Co-PI, award #2216858, \$886K, 08/2022-06/2023.) Research and training grant to increase the number of students from underrepresented groups in chemistry and related fields. Activities include mentoring students in molecular simulation research, using machine learning (ML) to parameterize next-generation force fields, and co-leading an annual hands-on workshop on molecular simulation and ML methods for early-stage undergraduate students.

**NASA MIRO: Data Intensive Research and Education Center in Science, Technology, Engineering and Mathematics (DIRECT-STEM).** (Co-PI, award #NNX15AQ06A, \$5.0M, 08/2015-09/2021.) Research and training grant to increase the number of students from underrepresented groups pursuing future careers in STEM. Activities included mentoring students in molecular simulation research and co-leading the pre-trainee program, a series of hands-on Saturday workshops for students from all disciplines about scientific computing, data science, and applied mathematics.

**NSF IUSE: First Year Experience for Engineering, Computer Science & Technology (FYrE).** (Co-PI, award #1727054, \$465K, 08/2017-07/2021.) Undergraduate science education grant to improve outcomes for Cal State LA engineering majors. Activities included physics/engineering education research, the development and implementation of a pre-physics course for first-time freshmen, and development of introductory physics curriculum and course structure.

**NSF SI2-CHE: Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces.** (PI, award #1453123 (formerly 1265660), \$57K, 05/2013 – 04/2016.) A joint US/UK effort of 12 PIs funded by the NSF and EPSRC to develop software infrastructure and polarizable force fields for MD simulations. Activities included force field development, grand challenge modeling, and leading an annual hands-on workshop in biomolecular simulation methods for undergraduate and early-stage graduate students.

## Mentoring Experience

% Senior thesis student.

- Cal State LA undergraduates (2016-2023): Jesse Garcia Castillo, Nicole Cruz, Cindy Garcia, Nia Huggins, Judith Landau, Kevin Mai, Charles Metzler-Winslow%, Muan Meurer%, Tracey Ng, Vinh Ngo, Anson Noland%, Yecenia Peraza, Jessica Romero, Luke Villarama%, Lucas Velasquez, Alex Zhou%
- Cal State LA MS students (2016-2023): Kevin Abbott, Valerie Arriero, Anthony Contrado, Gabriel Lucero, Jonah Otto, Maisha Rahman, Erin Uhlfelder, Frederick Wade, Danielle Wilkerson
- Claremont McKenna (CMC), Pitzer, and Scripps College undergraduates (2011-14): Dail Chapman% (Scripps), Roxanne Fries% (CMC), Stella Hoft% (Pitzer), Kiley Lawrence% (Scripps), Crystal Lim (CMC), Georgia Macy% (Scripps), Jonathan Steck% (CMC), Patrick Shultz (CMC), David Wych (CMC)
- UC Berkeley undergraduates (2010-11): Brian Jo, Clare So, Ajay Tripathy
- Visiting students at UC Berkeley (2010-11): Nicoletta Liguori (Roma Tre University MS), Lin Mao (Zhejiang Univ. undergrad.)

## Academic and University Service (past five years)

- Member, Committee on Academic Computing, 2024-present.
- Member, Field Investigative Subcommittee, 2024.
- Co-Advisor, 3+2 Combined Program with Engineering Partner Schools, 2024-present.
- Member, Faculty Search Committees, Kravis Dept. of Integrated Sciences, 2023-24 (3) and 2024-25 (3).
- Associate Department Chair, Dept. of Physics & Astronomy, 2022-23.
- Faculty Co-Director, Cal State LA High Performance Computing Center, 2022-23.
- Department Undergraduate and Graduate Student Advisor, Dept. of Physics & Astronomy, 2020-23.
- Chair, Instructional Affairs Committee, Dept. of Physics & Astronomy, 2019-21 and 2022-23.
- College Representative and Chair (2018-19), University Education Policy Committee, 2017-23.
- Member, Faculty Search Committee, Dept. of Physics & Astronomy, 2021-22 and 2022-23.
- Member, Faculty Search Committee, Dept. of Biological Sciences, 2021-22.
- Research colloquium coordinator, Dept. of Physics & Astronomy, Cal State LA, Spring 2021.
- Judge, Cal State LA Symposium on Research, Scholarship, and Creative Activity, 2020.
- Lead organizer of NSF MoISSI-funded workshop held in conjunction with the MERCURY conference for undergraduates in computational chemistry, 2017-19 and 2021-22.
- Reviewer for *Gene*, *Journal of Chemical Information and Modeling*, *Journal of Chemical Theory and Computation*, *Journal of Physical Chemistry B*, *Journal of Physical Chemistry Letters*, and *PLoS ONE*.
- Reviewer for NSF programs in CHE (CTMC), 2021-24, and IUSE (EHR), 2022.
- Member, MERCURY Consortium for Undergraduate Computational Chemistry, 2019-present.

## Recent Conferences, Workshops, and Colloquia (past five years)

*Colloquium* Dept. of Physics and Astronomy, CSU Northridge; Sept. 11, 2024.

*Colloquium* Dept. of Physics and Astronomy, Pomona College; April 16, 2024.

*Colloquium* Chemistry Theory Groups' Seminar, UC Davis; May 18, 2022.

*Presentation* Spring 2022 American Chemical Society National Meeting (San Diego, CA); Mar. 20-24, 2022.

*Colloquium* Dept. of Physics, Cal Poly Pomona; Nov. 3, 2020.

*Poster* 64<sup>th</sup> Annual Meeting of The Biophysical Society (San Diego, CA); Feb. 15-19, 2020.

*Presentation* Fall 2019 American Chemical Society National Meeting (San Diego, CA); Aug. 25-29, 2019.

*Presentation* NSF MoISSI Workshop: Software for Advanced Potential Energy Surfaces (Berkeley, CA); Aug. 1-2, 2019.

*Participant* AAC&U Teaching to Increase Diversity and Equity in STEM (TIDES) Institute (Los Angeles, CA); June 11-14, 2019.

*Colloquium* Dept. of Physics, CSU Fullerton; Apr. 26, 2019.

*Participant* Open Force Field Consortium Workshop, UC San Diego; Jan. 7-8, 2019.

## **Awards and Honors**

- Buechner Teaching Prize, Department of Physics, *MIT*, 2008.
- Graduate Student Life Grant, *MIT*, 2006 and 2007.
- Donald E. Kerr Memorial Medal, Department of Physics and Astronomy, *JHU*, 2004.
- Phi Beta Kappa Society, 2004.
- Sigma Pi Sigma Society, 2003.
- Provost's Undergraduate Research Award, *JHU*, 2003.