Rachael A. Mansbach, PhD

4606 Ave Draper ● Montreal, Quebec, CA ● +1 (515) 451-7375 ● re.mansbach@concordia.ca

Current Position

Assistant Professor of Physics August 2020-current
Concordia University
Principal Investigator of the Mansbach Lab

- Cutting-edge research at the intersection of computational biophysics and deep learning
- Drug design for novel therapeutic peptides and small molecules
- Polymer theory and molecular dynamics for studying small, disulfide-rich peptides

Education

Ph.D. | Physics August 2012 - August 2018
University of Illinois at Urbana-Champaign
Concentration: Computational Biophysics
Dissertation title: "Dimensionality Reduction and Multiscale Modeling for the Understanding of Protein Folding and Hierarchical Self-assembly"
GPA: 3.9/4.0

- Graduate research assistant employing machine learning and simulation for biomaterials design
- Graduate teaching assistant in PHYS 101, PHYS 212, and PHYS 213/214 and MSE 201, MSE 206, MSE 304, MSE 401, MSE 402, and MSE 406
- Received Graduate Teaching Certificate from the Center for Innovation in Teaching and Learning at University of Illinois at Urbana-Champaign
- Completed Computational Science and Engineering Graduate Certificate

B.A. | Physics August 2007 - June 2011
Swarthmore College, PA
Minor: Computer Science
Graduated with High Honors
GPA: 3.89/4.0

Research Experience

Director's Postdoctoral Fellow September 2018 - present
Theoretical Division, Los Alamos National Laboratory
Principal Investigator: Dr. S. Gnanakaran

- Performed emergency research including large-scale all-atom simulations of the full spike protein on the dynamics of D form and G form of the novel COVID-19 coronavirus
- Developed machine learning and statistical mechanical techniques for interpretable drug design and mentored an undergraduate student on this project
- Created theoretical biological models based on statistical physics techniques to understand aspects of Gram negative efflux pumps and kinase signaling systems
- Performed large-scale molecular dynamics simulations of small cysteine-rich proteins and characterized structure, thermodynamics and kinetics for design of novel analgesics
- Performed independent research into the modeling and simulation of intrinsically disordered proteins and mentored a graduate student on this project

- Conducted collaborative, interdisciplinary research in a diverse team of theoretical and experimental microbiologists, statisticians, mathematicians, and biophysicists

Graduate Research Assistant Spring 2014 - August 2018
Department of Materials Science and Engineering, UIUC
Advisor: Prof. Andrew L. Ferguson

- Performed independent research in understanding and design of self-assembling peptides for bio-electronic applications through simulations and data analysis
- Researched the application of nonlinear dimensionality reduction techniques to biomolecular systems
- Conducted strongly collaborative, interdisciplinary research in a diverse team composed of experimental chemical engineers, computational physicists and materials scientists
- Mentored an undergraduate student in the development of new coarse-grained peptide models

Graduate Research Assistant Spring 2013 – Fall 2013
Department of Physics, UIUC
Advisor: Prof. Nadya Mason

- Fabricated mesoscale structures to study low-temperature condensed matter phase transitions

Undergraduate Research Assistant Fall 2010
Department of Physics, Bryn Mawr College
Advisor: Prof. Eric Eaton

- Applied machine learning and spin-glass model to study of community detection in graphs

Undergraduate Research Assistant Summer 2010
Department of Physics, Swarthmore College/University of Pennsylvania
Advisors: Prof. Frank Moscatelli and Prof. Arjun Yodh

- Programmed LabView tools for study of diffuse optical tomography in medical imaging
- Designed and created new temperature controller for study of diffuse optical tomography

Science Undergraduate Laboratory Intern June 2009 - August 2009
Ames Laboratory
Advisor: Troy Benjegerdes

- Ported part of a power-benchmarking program from C++ to Python

Teaching Experience

Graduate Teaching Assistant
Department of Materials Science and Engineering, UIUC
Floating computational TA

- Designed curriculum changes to integrate computational modules into different courses
- Lectured, covered office hours, and graded homework assignments

MSE 201, 206, 304, 401, 402 and 406 Fall 2015-Spring 2016
Phases and Phase Relations
Mechanics for MatSE
Electronic Properties of Materials
Thermodynamics of Materials
Kinetic Processes in Materials
Thermo-mechanical Behavior of Materials

Graduate Teaching Assistant
Physics Department, UIUC
Discussion TA

- List of Teachers Ranked Excellent by Students (Fall 2012, Spring 2013, Fall 2013*, Spring 2014) (Mean score of $> 4.3/5$ on teaching evaluation forms) (* ranked as top 10% of instructors in terms of teaching effectiveness)

- Led discussion sections to cement concepts and teach problem-solving strategies
- Gave short lectures on physical concepts, graded quizzes, and proctored examinations

PHYS 212 Fall 2012, Summer 2014
University Physics: Electricity and Magnetism
Introductory electromagnetism for physics and engineering majors

PHYS 213/214 Fall 2013
University Physics: Quantum Physics/University Physics: Thermodynamics
Introductory quantum physics and thermodynamics for physics and engineering majors

PHYS 101 Spring 2013, Spring 2014
College Physics: Mechanics and Heat
Introductory classical mechanics and thermodynamics for non-majors

Graduate Teaching Certificate
Spring 2014
Center for Innovation in Teaching & Learning (CITL), UIUC
- Attended pre-semester teaching development program and six hours of teaching development workshops
- Discussed teaching practices with outside observer from CITL
- Analyzed and reflected on informal student feedback with mentor from CITL

Summer School for Integrated Computational Materials Education
June 15, 2015 – June 26, 2015
University of Michigan
- Attended two weeks of hands-on workshops on the use of computational modeling tools and their incorporation into the undergraduate materials science curriculum
- Areas covered were thermodynamics (using Thermo-Calc), DFT (using Quantum Espresso), mechanics (using OOF2), and kinetics (using Virtual Kinetics of Materials Laboratory)

Journal Articles and Conference Proceedings

17. **R.A. Mansbach**, Srirupa Chakraborty, Kien N. Nguyen, David C. Montefiori, Bette Korber, and S. Gnanakaran. "The SARS-CoV-2 Spike Variant D614G Favors an Open Conformational State." (Submitted, 2020).
16. Jitender Mehla, Giuliano Malloci, Cesar Lopez, Pedro D. Manrique, **R.A. Mansbach**, Ruslan Tsivkovski, Sally B. Grindstaff, Robert H. Cascella, Nicolas W. Hengartner, Liam Herndon, Alessio Atzori, Attilio V. Vargiu, Francesca Cardamone, Olga Lomovskaya, Paolo Ruggerone, S. Gnanakaran, Valentin V. Rybenkov and Helen I. Zgurskaya. "Discovery of predictive descriptors of efflux substrates, inhibitors and avoiders in Pseudomonas aeruginosa." Submitted, 2020.
15. **R.A. Mansbach**, Inga V. Leus, Jitender Mehla, Cesar A. Lopez, John K. Walker, Valentin Rybenkov, Helen I. Zgurskaya, Nicolas W. Hengartner, and S. Gnanakaran. "Machine Learning Algorithm Identifies an Antibiotic Vocabulary for Permeating Gram-Negative Bacteria" ArXiv preprint arXiv:1907.13459 (2020) [https://arxiv.org/abs/1907.13459] (Accepted, *J. Chem. Inf. Model.*)
14. **R.A. Mansbach**, Srirupa Chakraborty, Timothy Travers and S. Gnanakaran. "Graph-Directed Approach for Downselecting Toxins for Experimental Structure Determination.' *Mar. Drugs*. 18 5 256 (2020) https://www.mdpi.com/1660-3397/18/5/256 [https://www.biorxiv.org/content/10.1101/828129v1]
13. Kirill Shmilovich, **R.A. Mansbach**, Hythem Sidky, Olivia Dunne, Sayak Subhra Panda, John D. Tovar, and Andrew L. Ferguson. "Discovery of Self-Assembling π-Conjugated Peptides by Active Learning-Directed Coarse-Grained Molecular Simulation." *J. Phys. Chem. B*. 124 19 3873–3891 (2020) [https://pubs.acs.org/doi/full/10.1021/acs.jpcb.0c00708]
    (Selected as an ACS Editor's Choice, featured on the cover)
12. Timothy Travers, William Kanagy, **R.A. Mansbach**, Elton Jhamba, Cedric Cleyrat, Byron Goldstein, Diane S. Lidke, Bridget S. Wilson, and S. Gnanakaran. "Molecular aspects of multivalent engagement between Syk and FcϵRIγ." *Mol. Biol. Cell.* pp.mbc-E18 (2019). [https://www.molbiolcell.org/doi/abs/10.1091/mbc.E18-11-0722]
11. **R.A. Mansbach**, Timothy Travers, Benjamin H. McMahon, Jeanne M. Fair, and S. Gnanakaran. "Snails in Silico: A Review of Computational Studies on the Conopeptides." *Mar. Drugs*. 17 3 145 (2019) [https://www.mdpi.com/

1660-3397/17/3/145]
(One of the most cited articles of 2019 in Marine Drugs)

10. **R.A. Mansbach** and A.L. Ferguson. "Patchy Particle Model of the Hierarchical Self-Assembly of π-Conjugated Optoelectronic Peptides" *J. Phys. Chem. B*. 122 44 10219–10236 (2018) [http://dx.doi.org/10.1021/acs.jpcb.8b05781]
9. Z. Song, **R.A. Mansbach**, R. Baumgartner, K.-C. Shih, H. He, N. Zheng, X. Ba, Y. Huang, D. Mani, Y. Lin, M.-P. Nieh, A.L. Ferguson, L. Yin, and J. Cheng "Modulation of polypeptide conformation through donor-acceptor transformation of side-chain hydrogen bonding ligands" *Nat. Commun.* **92-8** 1-8 (2017) [http://dx.doi.org/10.1038/s41467-017-00079-5]
8. **R.A. Mansbach** and A.L. Ferguson. "Control of the hierarchical assembly of π-conjugated optoelectronic peptides by pH and flow." *Org. Biomol. Chem.* **15** 5484 – 5502 (2017) [http://dx.doi.org/10.1039/C7OB00923B]
(Invited submission for "Peptide Materials" special issue, featured on the cover)
(Featured in the 2017 Hot Articles in Organic and Biomolecular Chemistry Collection)
7. **R.A. Mansbach** and A.L. Ferguson. "Coarse-grained molecular simulation of the hierarchical self-assembly of π-conjugated optoelectronic peptides." *J. Phys. Chem. B* 121 7 1684–1706 (2017) [http://dx.doi.org/10.1021/acs.jpcb.6b10165]
6. **R.A. Mansbach**, A.L. Ferguson, K.A. Kilian, J. Krogstad, C. Leal, A. Schleife, D.R. Trinkle, M. West, and G.L. Herman. "Reforming an undergraduate materials science curriculum with computational modules." *J. Mater. Educ.* 38 3-4 161-174 (2016)
5. **R.A. Mansbach**, G.L. Herman, M. West, D.R. Trinkle, A.L. Ferguson, and A. Schleife. "Computational modules for the MatSE undergraduate curriculum." American Society for Engineering Education (ASEE) 123rd Annual Conference & Exposition, New Orleans, LA, June 26-29 2016
4. M. Xiong, M.W. Lee, **R.A. Mansbach**, Z. Song, Y. Bao, R.M. Peek Jr., C. Yao, L.-F. Chen, A.L. Ferguson, G.C.L. Wong, and J. Cheng. "Helical antimicrobial polypeptides with radial amphiphilicity." *Proc. Natl. Acad. Sci. USA* 112 43 13155-13160 (2015) [http://dx.doi.org/10.1073/pnas.1507893112]
3. **R.A. Mansbach** and A.L. Ferguson. "Machine learning of single-molecule free-energy surface and the impact of chemistry and environment upon structure and dynamics." *Journal of Chemical Physics* 142 105101 (2015) [http://dx.doi.org/10.1063/1.4914144]
(Ranked as one of the most read Biological Molecules and Networks articles of the year)
2. E. Eaton and **R.A. Mansbach**. "A spin-glass model for semi-supervised community detection." In *Proceedings of the Twenty-Sixth AAAI Conference on Artificial Intelligence (AAAI-12)*, pp. 900–906, AAAI Press, July 22–26 (2012)
1. **R.A. Mansbach**. "Power Measurement and Modulization in the Network Protocol Independent Performance Evaluator (NetPIPE)." *Journal of Young Investigators* 9 18 (2009)

Presentations

18. "
17. "Hunting fragments and theories: molecular dynamics and machine learning for therapeutics design." Theoretical Division Group Leaders' Meeting, LANL, July 28 2020. [Invited]
16. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." SickKids, Toronto, ON, CA, July 16 2019.
15. "Membranes and Machine Learning: Rational Design Methods for Antibiotics Targeting Gram Negative Bacteria". ASM Microbe, San Francisco, CA, June 20-24 2019. [Oral and poster]
14. "Membranes and Machine Learning." Biological Membranes, Santa Fe, NM, June 9-14 2019. *[Invited Talk]*
13. "Rational Molecular Design: Applications to Antibiotics and Conotoxins". T-6 Seminar Series, Los Alamos, NM, March 21 2019.
12. "Membranes and Machine Learning: Designing a Model of Antibiotic Activity to Bypass Gram Negative Membranes and Efflux Pumps". APS March Meeting, Boston, MA, March 4-8 2019
11. "Wires Within Wires: A Minimal Model for Computational Bioelectronic Peptide Design." Blue Waters Symposium, Sunriver, OR, June 4-7, 2018. [Oral and poster]
10. "Bio Bulbs." Loh Down on Science Communication Workshop, Urbana, IL, April 17-19, 2018. *[Top Ten Finalist]*
9. "A Coarse-grained Minimal Model for the Hierarchical Self-assembly of Biocompatible Optoelectronic Nanostructures." APS March Meeting, Los Angeles, CA, March 5-9, 2018.

8. “Multiscale molecular simulation for the study of a self-assembling optoelectronic peptide.” Edinburgh Thermodynamics Conference, Edinburgh, UK, September 6, 2017. *[Christopher J. Wormald Prize Speaker]*
7. “Computational and Theoretical Modeling of pH and Flow Effects on the Early-Stage Nonequilibrium Self-Assembly of Optoelectronic Peptides.” UIUC Computational Science and Engineering Annual Meeting, Urbana, IL, April 26, 2017.
6. “Computational and theoretical modeling of pH and flow effects on the early-stage non-equilibrium self-assembly of optoelectronic peptides.” APS March Meeting, New Orleans, LA, March 13-17 2017
5. “Computational Modules for the MatSE Undergraduate Curriculum.” ASEE Annual Conference and Exposition, New Orleans, LA, June 26-29 2016 [Poster]
4. “Simulation and Numerical Modeling of an Optoelectronic Peptide.” APS March Meeting, Baltimore, MD, March 14-18 2016
3. “Machine learning of single molecule free energy landscapes.” APS March Meeting, San Antonio, TX, March 2-6 2015
2. “Molecular simulation and machine learning in self-assembly, folding, and virology.” UIUC Materials Science Graduate Recruiting Weekend, Urbana, IL, February 28 2015 [Poster]

Honors and Awards

- Los Alamos Director’s Fellowship, Los Alamos National Lab — 2018–current
- NIST NRC Research Associate Program Fellowship (Declined) — 2018
- Campus nominee to apply for Schmidt Science Fellowship — 2017
- Christopher J. Wormald Prize, Edinburgh Thermodynamics Conference — 2017
- Blue Waters Graduate Fellow, Blue Waters Foundation — 2017–2018
- Computational Science and Engineering (CSE) Fellow, UIUC — 2016–2017
- Building Future Faculty Program Fellow, NCSU — March 29–Apr 2, 2016
- Mavis Future Faculty Fellow, UIUC — 2015-2016
- American Physical Society (APS) Forum on Graduate Student Affairs Travel Award for Excellence in Graduate Research — 2015
- UIUC Dept. of Physics Graduate Travel Award — 2015
- UIUC Dept. of Physics Excellence in Teaching Award — 2013 (Fall)
- UIUC Dept. of Physics Excellence in Teaching Award — 2013 (Spring)
- National Science Foundation (NSF) Fellowship Honorable Mention — 2012
- Goldwater Fellowship Honorable Mention — 2010
- Department of Energy (DOE) Science and Energy Research Challenge finalist — 2009
- Swarthmore Department of Mathematics Morris Monsky Prize — 2008

Professional Affiliations

- Biophysical Society of Canada — 2020–present
- American Society for Microbiology — 2019–present
- American Chemical Society — 2019–present
- Tau Beta Pi — 2015–present
- Society of Women Engineers — 2014–present
- American Physical Society — 2014–present
- Phi Beta Kappa — 2011–present
- Sigma Xi — 2010–present

Journal Referee

- Marine Drugs — 2020
  - Guest Editor for Special Issue “Virtual Screening of Marine Natural Products”
- PLOS ONE — 2017

Extracurricular Activities and Service

- Chaos theory and chemical equations, 2020 Virtual Summer Physics Camp for Girls, LANL — June 16, 2020
- Informal Diversity Consultant to Division Head, T6 Division, LANL — Spring 2019–present
- Poster Judge, Summer Student Symposium, LANL — Aug 6, 2019
- Computing for Impact, 2019 Summer Physics Camp for Girls, LANL — June 12, 2019
- Member of Serving Communities Subcommittee of the Strategic Planning Committee, APS — 2018
- Member-at-large, Forum on Graduate Student Affairs Committee, APS — 2016–2019
- Member of Physics Diversity Journal Club, UIUC — 2017–2018
- Founding Member and Co-Chair of Physics Grad Student Diversity Committee, UIUC — 2016–2018
- GLAM Camp: Girls Learning About Materials for 10th-12th graders, UIUC — 2016, 2018
  - Jessica Anne Krogstad; Nicole E Johnson-Glauch; Kaitlin Tyler; **R.A. Mansbach**; Andrew Ferguson (2018), "Understanding Fracture Behavior in Materials Using Cheese," https://nanohub.org/resources/28588.
- Illinois GPS: Physics graduate students mentoring undergraduates, UIUC — 2015–2018
- NanoSTRuCT: Providing K-12 students with exposure to engineering — 2015
- High School Science Day: introducing female high schoolers to physics, UIUC — 2013
- Tech-nights: recruiting middle-school girls to STEM fields, Carnegie Mellon — 2011

Key Skills

- Strong expertise in machine learning/artificial intelligence and applications to biophysical problems
- Strong expertise in multiscale model development and force-field design for molecular dynamics simulations
- Strong expertise in nonlinear dimensionality reduction techniques, especially the diffusion map, and free energy landscape calculations
- Proficient with multiple molecular simulation softwares, including Gromacs, HOOMD, and LAMMPS
- Proficient with coding, especially in Python and Matlab, moderately proficient in C++
- Strong communication skills honed over years of collaborative interdisciplinary research
- Experience mentoring graduate and undergraduate students from different backgrounds
- Ability to listen to other ideas and to communicate my own, especially developed during my time liaising with six different professors to develop and deploy computational modules in the undergraduate curriculum and during preparation for my recent nine-author paper as part of a large NIH grant

References

Postdoctoral Supervisor:

S. Gnanakaran, Ph.D.
Staff Scientist, Theoretical Biology and Biophysics
Los Alamos National Lab
Mailstop K710, P.O. Box 1663
Los Alamos, NM 87545

Tel: (505)-665-1923
Email: gnana@lanl.gov

Doctoral Advisor:

Andrew L. Ferguson
Associate Professor of Molecular Engineering
The University of Chicago
Pritzker School of Molecular Engineering

5640 South Ellis Ave
Chicago, IL 60637

Tel: (773) 702-5950
Email: andrewferguson@uchicago.edu

Thesis Committee Chair:

Nigel Goldenfeld
Professor of Physics
University of Illinois at Urbana-Champaign
3113 Engineering Sciences Building
1101 W Springfield Ave
Urbana, IL 61801

Tel: (217) 333-8027
Email: nigel@illinois.edu

Thesis Committee Member:

Nadya Mason
Associate Professor of Physics
University of Illinois at Urbana-Champaign
1017 Seitz Materials Research Lab
104 South Goodwin Ave
Urbana, IL 61801

Tel: (217) 244-9114
Email: nadya@illinois.edu

Teaching Supervisor:

S Lance Cooper
Professor of Physics
University of Illinois at Urbana-Champaign
227B Loomis Laboratory
1110 West Green Street
Urbana, IL 61801

Tel: (217) 333-2589
Email: slcooper@illinois.edu

Others available upon request