# Rachael (Ré) A. Mansbach, PhD

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## Current Position

**Assistant Professor of Physics** August 2020-current
Concordia University
***CRC Chair Tier II in Computational Biophysics***
*Junior Co-Director, Centre for Research in Molecular Modeling*
*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
- Multiscale modeling for understanding of protein aggregation and disease progression in the brain

## 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*

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

## Student and Postdoctoral Supervision

**Current Postdoctoral Scholars**

- Samith Rathnayake May 2023–current
  - *Project lead: Active learning and multi-scale modeling of antimicrobial peptide design*

**Current Students**

- Shreyas Gowrishankar, BSc Jan 2024–current
  - *Phys 497 Independent Project: Dimensionality Reduction for Multi-scale Simulation*
- Jasmine Boyd, BSc Jan 2024–current
  - *Independent project: Simulation and analysis of a novel $\beta$ sheet-forming antimicrobial peptide*
- Indra Guzman Morena, BSc Jan 2024–current
  - *Independent project: Autoencoders and the Representation of the Ising Model*
- Jyler Menard, PhD Jan 2023–current
  - *Thesis Project: Generative Deep Learning in Biomolecular Contexts*
- Adam Graves, PhD Jan 2023–current (co-supervised with Prof. Yiming Xiao)
  - *Thesis Project: Design of Active Learning Platform for Antimicrobial Peptide Search Spaces*
- Lindsay Wright, MSc Aug 2022–current (co-supervised with Prof. Claudine Gauthier)
  - *Thesis Project: Deep Learning for Generative Modelling of Brain Medical Imaging*

- Natalya Watson, PhD — Aug 2020–current
  - *Thesis Project: Free Energy Landscapes for Design of Disulfide-Rich Peptides*
- Vrinda Nair, PhD — Jan 2021–current
  - *Thesis Project: Virtual Screening of RNA-targeting antibiotics*
- Mohammadreza Niknam Hamidabad, PhD — Jan 2022–current
  - *Thesis Project: Multi-scale modeling and Active Learning for Design of $\beta$-sheet-forming Antimicrobial Peptides*

**Previous Students**

- Ho Yen Chi Nguyen, BSc — Aug 2023–Dec 2023
  - *Phys 289 Independent Project: Machine Learning Prediction of Docking Results for RNA-targeting Small Molecules*
- Martina Mai, MSc — Aug 2021–Aug 2023 (co-supervised with Prof. Valter Zazubovitz)
  - *Thesis Project: Molecular Dynamics Simulations to Identify Two-Level Systems in Protein-Pigment Complexes*
- Tisha Dash, BSc — May 2023–current
  - *Mitacs Globalink Intern: Membrane-peptide simulations for assessing the mechanisms of action of a beta-sheet-forming antimicrobial peptide*
- Sophia Padvaiskas, BSc — May 2023–current
  - *PHYS 389 Project: Mutual information for diverse system dimensionality reduction*
- Samuel Renaud, MSc — May 2021–May 2023
  - *Thesis Project: Design of Continuous and Interpretable Latent-space-based Deep Learning Models for Antimicrobial Peptide Design*
  - Currently a systems engineer at MDA
- Rami Zemouri, BSc — Jan 2023–May 2023
  - *Independent Research Project: Comparison of Dimensionality Reduction Methods for Multi-System Analysis*
- Taïda An, CEGEP Student — Jan 2023–May 2023
  - *Project for Independent Research Course, John Abbott College: Simulations of Hydrophobic and Hydrophilic $\mu$-Conotoxins*
- Saim Bokhari, BSc — Jan 2023–May 2023
  - *Phys Specialization Thesis: Data Structuring on Simulations of Photonic Crystal Ring Resonators*
- David Mikota, BSc — May 2022–Aug 2022
  - *Co-op Project: Structural Prediction Tool for Analysis of Latent Spaces for Antimicrobial Peptide Design*
- Muhammad Sabih Armaghan, BSc — May 2022–Aug 2022
  - *Individual Research Project: Use of Persistent Homology for Deep Neural Network Design*
- Gregory Holloway, BSc — Summer 2022 (co-supervised with Prof. Pablo Bianucci)
  - *NSERC USRA: Machine Learning on Electronic Band Structures of Symmetric Rings*
- Patrick McClay, BSc — Aug 2021–May 2022
  - *Honours Thesis (Graduated with an A+): Molecular Dynamics Investigation of $\alpha$-Conotoxins with Disconnected Disulfides*
- Samuel Renaud, BSc — Aug 2020–May 2021
  - *Honours Thesis (Graduated with an A+): De Novo 3D Antimicrobial Peptide Design with Variational Autoencoders*
- Lindsay Wright, BSc — May 2021–Aug 2021
  - *Honours Thesis (Graduated with an A+): The Many Conformations of GL13K: Charged Coils to Neutral $\beta$-Structure*
- Liam Herndon, BSc (co-supervised) — Summer 2019
  - *Project: Identifying Features Responsible for Antibiotic Activity*
  - Designed and created a poster and presentation for the annual LANL Summer Student Symmposium that was selected to be one of the LANL Intern Presentation Lightning Talks, which resulted in an invitation to discuss a market research project and a commendation from the LANL Director's Office.
- Richard Justin Lindsay, PhD (co-supervised) — Aug 2018–Aug 2020
  - *Project: Computational Methodologies for Intrinsically Disordered Proteins*
- Kirill Shmilovich, PhD (co-supervised) — Summer 2018
  - *Project: Discovery of Self-Assembling $\pi$-Conjugated Peptides by Active Learning-Directed Coarse-Grained*

*Molecular Simulation*

## Previous Research Experience

**Director's Postdoctoral Fellow** September 2018 - September 2020
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

## Assistant Professor

Physics Dept, Concordia

**Computational Methods in Physics with Python (Phys 440/Phys 679)** Fall 2021, Fall 2022, Fall 2023, Fall 2024

- Redesigned course for a focus on molecular dynamics and machine learning in Python
- Created wholly new infrastructure including curriculum, slides, assignments, and Jupyter notebooks
- Created project-based focus for student engagement
- Synthesized slides with Jupyter notebooks and prepared prerecorded lectures for missing classes or, if necessary, online delivery

**Methods of Theoretical Physics II (Phys 335)** Winter 2021, Winter 2022, Winter 2023

- Modified course for fully virtual delivery during the COVID-19 pandemic
- Taught the course during the transition from online to in-person, with corresponding need to pivot mid-semester
- Added active learning component
- Recorded lectures, wrote new homework problems, wrote and administered final exams
- Supervised one TA

**Workshops Attended**

- Winterfest 10: Blended Learning Panel Dec 3, 2021, Concordia Center for Teaching and Learning
  - learned tips and tricks for asynchronous learning and ways to complement in-person time with online time
- Indigenous Education in Canada Dec 3, 2021, Pîkiskwêtân, Indigenous Learning Series
  - Learned about the history of colonization in education in Canada and how it is ongoing
- Practical Strategies on Decolonizing Eurocentric 'Normative Discourse' in Curriculum and Pedagogical Practices Sep 23, 2021, Concordia Center for Teaching and Learning
  - Ways to write an inclusive curriculum
  - Sparked thoughts and discussion on the difficulty of doing this in the sciences
  - Pointed me to reading materials to begin educating myself on decolonization in STEM
- How to Combat Zoom Fatigue Jan 28, 2021, Concordia Center for Teaching and Learning
  - Suggestions for improving a classroom experience to avoid zoom fatigue
  - Implemented small points from this workshop, including a stretch break, which I've started bringing back to in-person classroom as well

## 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

24. Mohammadreza Niknam Hamidabad, Lindsay Wright, Natalya A. Watson, and **R. A. Mansbach**. "Molecular Dynamics Simulations Reveal Details of the Early Stages of Aggregation of a Synthetic Antimicrobial Peptide." (Accepted, *ChemBioChem*, 2024). *(Invited submission)*
23. Martina Mai, Valter Zazubovits, and **R.A. Mansbach**. "Identification of residues involved in optical shifts in the water-soluble chlorophyll-a binding protein through molecular dynamics simulations." (XXXX, XXX, XXX-XXX, *J. Phys. Chem. B*, 2024) [https://doi.org/10.1021/acs.jpcb.3c06889].
22. **R.A. Mansbach**, Lara A. Patel, Natalya A. Watson, Jessica Z. Kubicek-Sutherland, and S. Gnanakaran. "Inferring pathways of oxidative folding from pre-folding free energy landscapes of disulfide-rich toxins." ( *J. Phys. Chem. B*, 2023, 127, 8, 1689–1703) [https://doi.org/10.1021/acs.jpcb.2c07124]
21. Samuel Renaud and **R.A. Mansbach**. "Latent Spaces for Antimicrobial Peptide Design." *Digital Discovery.* 2, 441–458 (2023) *(Invited submission for deep learning on antibiotic design)*
20. Pedro D. Manrique, Srirupa Chakraborty, Rory Henderson, Robert J. Edwards, **R.A. Mansbach**, Kien Nguyen, Victoria Stalls, Carrie Saunders, Katayoun Mansouri, Priyamvada Acharya, Bette Korber, and S. Gnanakaran. "Network analysis uncovers the communication structure of SARS-CoV-2 spike protein identifying sites for immunogen design." *iScience.* 26, 1. (2023) [https://doi.org/10.1016/j.isci.2022.105855]
19. Kien Nguyen, Srirupa Chakraborty, **R.A. Mansbach**, Bette Korber, and S. Gnanakaran. "Exploring the role of glycans in the interaction of SARS-CoV-2 RBD and human receptor ACE2." *Viruses.* 13, 5. 927 (2021).
18. Richard. J. Lindsay, **R.A. Mansbach**, S. Gnanakaran, and Tongye Shen. "Effects of pH on an IDP conformational ensemble explored by molecular dynamics simulation." *Biophysical Chemistry*. 271, 1 (2021).
17. **R.A. Mansbach**, Srirupa Chakraborty, Kien Nguyen, David C. Montefiori, Bette Korber, and S. Gnanakaran. "The SARS-CoV-2 Spike Variant D614G Favors an Open Conformational State." *Sci. Adv.* 7, 16. eabf3671. (2021).
16. Jitender Mehla, Giuliano Malloci, **R.A. Mansbach**, Cesar Lopez, Ruslan Tsivkovski, Keith Haynes, Inga V. Leus, Sally B. Grindstaff, Robert H. Cascella, Napoleon D'Cunha, Liam Herndon, Nicolas W. Hengartner, Enrico Margiotta, Alessio Atzori, Attilio V. Vargiu, Pedro D. Manrique, John K. Walker, Olga Lomovskaya, Paolo Ruggerone, S. Gnanakaran, Valentin V. Rybenkov and Helen I. Zgurskaya. "Predictive rules of efflux inhibition and avoidance in Pseudomonas aeruginosa." *mBio*. 12, 1 (2021).
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" *J. Chem. Inf. Model.* 60 6 2838–2847 (2020). [https://pubs.acs.org/doi/abs/10.1021/acs.jcim.0c00352]

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
13. Kirill Shmilovich, **R.A. Mansbach**, Hythem Sidky, Olivia Dunne, Sayak Subhra Panda, John D. Tovar, and Andrew L. Ferguson. "Discovery of Self-Assembling $\pi$-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. 'Combinatorial diversity of Syk recruitment driven by its multivalent engagement with Fc$\epsilon$RI$\gamma$." *Mol. Biol. Cell.* 30, 17, 2331–2347 (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 $\pi$-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 $\pi$-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 $\pi$-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)

## Papers in Preparation

2. Samith Rathnayake, Mohammadreza Niknam Hamidabad, Natalya A. Watson, and **R.A. Mansbach**. "Unveiling

the Dynamics of GL13K Peptide Folding and Membrane Engagement: A Molecular Dynamics Simulation Study." (In preparation, 2024)

1. Samith Rathnayake, Jyler Menard, Adam Graves, Mohammadreza Niknam Hamidabad, and **R.A. Mansbach**. "How much difference does initial structure really make? Benchmarking Alphafold2 on experimental and simulation data of short peptides." (In preparation, 2024)

## Other Written Contributions

- Vrinda Nair and **R.A. Mansbach**. "The fight against antibiotic resistance is growing more urgent, but artificial intelligence can help." The Conversation, Feb 9, 2023. [https://theconversation.com/the-fight-against-antibiotic-resistance-is-growing-more-urgent-but-artificial-intelligence-can-help-198709]
- **R. A. Mansbach**. "A Notebook Full of Colors." Biophysical Society of Canada e-news article, August 4, 2022.

## Student Presentations

10. Natalya A. Watson*, Rami Zemouri*, Mohammadreza Niknam Hamidabad*, and **R.A. Mansbach**. "Toxic Energy : Using MD to Fine-Tune Energy Surfaces for Cone Snail Venom." Centre for Research in Molecular Modeling Annual Symposium, Concordia University, May 29, 2023 [Poster presentation].
9. Mohammadreza Niknam Hamidabad*, Natalya A. Watson*, Lindsay Wright*, and **R.A. Mansbach**. "Aggregation of a Synthetic Beta-sheet-forming Antimicrobial Peptide." Centre for Research in Molecular Modeling Annual Symposium, Concordia University, May 29, 2023 [Poster presentation].
8. Natalya A. Watson*, Rami Zemouri*, Mohammadreza Niknam Hamidabad*, and **R.A. Mansbach**. "Toxic Energy : Using MD to Fine-Tune Energy Surfaces for Cone Snail Venom." Biophysical Society of Canada Annual Meeting, Calgary, May 2023 [Poster presentation].
7. Lindsay N. Wright*, Stéfanie A. Tremblay, Zacharie Potvin-Jutras, Ali REzaei, Safa Sanami, Dalia Sabra, Agathe Godet, Amélie Mainville-Berthiaume, Roni Zaks, Zineb Rouabah, Josep Iglesies-Grau, Anil Nigam, Mathieu Gayda, Louis Bherer, Claudine Gauthier, and **R.A. Mansbach**. "Deep learning-enabled graphical network data augmentation and function analysis of brain imaging." Biophysical Society of Canada Annual Meeting, Calgary, May 2023 [Poster presentation].
6. Martina Mai*, **R.A. Mansbach**, and Valter Zazubovits. "Molecular Dynamics Simulations of Pigment-Protein Complexes : Identifying STructural Features Responsible for Spectral Dynamics." Biophysical Society of Canada Annual Meeting, Calgary, May 2023 [Poster presentation].
5. Mohammadreza Niknam Hamidabad*, Natalya A. Watson*, Lindsay Wright*, and **R.A. Mansbach**. "Aggregation of a Synthetic Beta-sheet-forming Antimicrobial Peptide." Biophysical Society of Canada Annual Meeting, Calgary, May 2023 [Poster presentation].
4. Vrinda Nair*, **R.A. Mansbach**, and Nicolas Moitessier. "Machine Learning Methods for Design of RNA-targeting Small-molecule Antibiotics." Biophysical Society of Canada Annual Meeting, Calgary, May 2023 [Poster presentation].
3. Samuel Renaud* and **R.A. Mansbach**. "AMPLE: Antimicrobial Peptide Latent Space Exploration." Centre for Research in Molecular Modelling (CERMM) Symposium, Concordia University, May 12, 2022.
2. Natalya Watson* and **R.A. Mansbach**. "Comparison of $\alpha$-conotoxin free energy landscapes via simulation and dimensionality reduction." APS March Meeting, Chicago, IL, March 14, 2022.
1. Samuel Renaud* and **R.A. Mansbach**. "Multi-Model Analysis of De novo Antimicrobial Peptide Design Via Variational Autoencoder Latent Sampling." APS March Meeting, Chicago, IL, March 14, 2022.

## Selected Student Awards

- Lindsay Wright
  - Canada Graduate Scholarship MSc, NSERC, 2023
  - Master's Training Scholarship, FRQNT, 2023
- Jyler Menard
  - Canada Graduate Scholarship Doctoral Program, NSERC, 2023
- Vrinda Nair

- Concordia Applied AI Institute Fellowship, 2023
- Vrinda Nair, Concordia Conference and Exposition Award, 2023
- Vrinda Nair, Concordia University Public Scholar Award, 2022

## Presentations

45. "$\beta$eing AMPle: In silico study of the early stages of aggregation of $\beta$ sheet forming peptide GL13K." Contributed Talk, APS March Meeting, March 6, 2024.
44. "Nothing is a Straight Line: Solving Non-linear Biophysical Problems (Including Life)." Colloquium Talk, Queen's University, Jan. 12, 2024. *Invited Talk*
43. "Nothing is a Straight Line: Solving Non-linear Biophysical Problems (Including Life)." Seminar Talk, Polytechnique Montréal, Dec. 7, 2023. *Invited Talk*
42. "AMPle Data: Understanding of Spaces and Starting Points for Antimicrobial Peptide Design." Seminar Talk, Université de Montréal, Nov. 9, 2023. *Invited Talk*
41. "Unstable Equilibrium: One physicist's journey through research and life." Enriched Science Colloquium Talk, Dawson College, Montreal, QC, Sept. 29, 2023. *Invited Talk*
40. "AMPle Data: Aggregation of a Synthetic Beta-Sheet Forming Antimicrobial Peptide." Canadian Chemistry Conference and Exhibition, Vancouver, BC, June 2023. *Invited Talk*
39. "AMPle Data: Understanding of Spaces and Starting Points for Antimicrobial Peptide Design." Biophysical Society of Canada, Calgary, AB, May 2023. *Invited Talk.*
38. "Learning non-linearity: artificial and natural intelligence applied to non-linear biophysical problems (including life)." BOLD Science Conference, Concordia University, May 3, 2023. *Keynote Address*
37. "Design of $\beta$-sheet forming antimicrobial peptides using deep learning and molecular dynamics simulations." APS March Meeting, 2023. [Virtual Meeting component]
36. "Living History: Reiy Mansbach." Living Histories series [https://iyerbiswas.com/outreach/livinghistories/]. Virtual Talk, Jan 18, 2023. *Invited Talk* [https://www.youtube.com/watch?v=71hzqZNAPW4]
35. "Nothing is a straight line: Solving non-linear biophysical problems (including life.)" Colloquium Talk, University of Toronto Mississauga, Nov 30, 2022. *Invited Talk*.
34. "Multi-scale modeling and machine learning for understanding of complex biophysical problems." PROTEO Webinaire, Nov 18, 2022. *Invited Talk*
33. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." 2nd Annual Symposium of BiophysQ, Université de Montréal, Oct 6, 2022. *Invited Talk*
32. "Biophysical Design for Therapeutic Applications." Concordia University Research in Conversation Series, Sept 19, 2022. *Invited Discussion*
31. "Exploration and Design of Latent Search Spaces for Antimicrobial Peptides." Therapeutics $\times$ LGBTQ2IA+ Symposium, McGill University, August 5, 2022.
30. "'Design and Analysis of Search Spaces for Active Learning of Biomolecular Targets." First Computational Energy and Materials Design Infrastructure Seminar Series, INRS, July 2022. *Invited Talk*
29. "Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." CAP Congress, Hamilton, ON, June 2022. *Invited Talk*
28. "Unified free energy landscapes of $\mu$-conotoxins reveal prefolding predictors of folding pathway classification." Biophysical Society of Canada, Ottawa, ON, May 2022.
27. "Unified free energy landscapes of $\mu$-conotoxins reveal prefolding predictors of folding pathway classification." Centre for Research in Molecular Modelling (CERMM) Symposium, Concordia University, May 12, 2022. [Co-organizer]
26. "Unified free energy landscapes of $\mu$-conotoxins reveal prefolding predictors of folding pathway classification." APS March Meeting, March 14, 2022. [Virtual talk.]
25. "Unstable Equilibrium: One physicist's journey through research and life." McGill University, Oct 18, 2021. *Invited Talk*
24. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." McGill University, Sept 17, 2021. *Invited Talk.*
23. "The SARS-CoV-2 Spike Variant D614G Favors an Open Conformational State." Virtual Symposium on Theoretical and Computational Chemistry in Canada, July 21, 2021.
22. "The SARS-CoV-2 Spike Variant D614G Favors an Open Conformational State." Canadian Biophysical Society

Meeting, May 26, 2021.

21. "Venomous Landscapes and Viral Trajectories: Evaluation of Free Energy Surfaces for Disulfide-Rich Peptide Design and a Side Story about the SARS-CoV2 Spike Protein." QBIOC Seminar Series, Apr 27, 2021.*[Invited Talk.]*
20. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." Simon Fraser University, Apr 7, 2021. *Invited Talk.* [Virtual format]
19. "Science in the Time of Corona: Free Energy Landscapes of $\mu$ Conotoxins and Symmetry and Asymmetry in the SARS-CoV2 Spike." APS March Meeting, March 18, 2021. *Invited Talk.* [Virtual meeting format]
18. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Physical Modeling and Machine Learning." Dawson College, March 5, 2021. *Invited Talk.* [Virtual format]
17. "THE SARS-COV-2 SPIKE VARIANT D614G FAVORS AN OPEN CONFORMATIONAL STATE." Biophysical Society Meeting, Feb 26, 2021. [Virtual Poster]
16. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Physical Modeling and Machine Learning." Concordia University Physics Colloquium Series, Concordia University, Sept 9, 2020. *[Invited Talk.]*
15. "Hunting fragments and theories: molecular dynamics and machine learning for therapeutics design." Theoretical Division Group Leaders' Meeting, LANL, July 28 2020. *[Invited Talk.]*
14. "Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning." SickKids, Toronto, ON, CA, July 16 2019. *[Invited Talk.]*
13. "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]
12. "Membranes and Machine Learning." Biological Membranes, Santa Fe, NM, June 9-14 2019. *[Invited Talk]*
11. "Rational Molecular Design: Applications to Antibiotics and Conotoxins". T-6 Seminar Series, Los Alamos, NM, March 21 2019.
10. "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
9. "Wires Within Wires: A Minimal Model for Computational Bioelectronic Peptide Design." Blue Waters Symposium, Sunriver, OR, June 4-7, 2018. [Oral and poster]
8. "Bio Bulbs." Loh Down on Science Communication Workshop, Urbana, IL, April 17-19, 2018. *[Top Ten Finalist]*
7. "A Coarse-grained Minimal Model for the Hierarchical Self-assembly of Biocompatible Optoelectronic Nanostructures." APS March Meeting, Los Angeles, CA, March 5-9, 2018.
6. "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]*
5. "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.
4. "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
3. "Computational Modules for the MatSE Undergraduate Curriculum." ASEE Annual Conference and Exposition, New Orleans, LA, June 26-29 2016 [Poster]
2. "Simulation and Numerical Modeling of an Optoelectronic Peptide." APS March Meeting, Baltimore, MD, March 14-18 2016
1. "Machine learning of single molecule free energy landscapes." APS March Meeting, San Antonio, TX, March 2-6 2015
0. "Molecular simulation and machine learning in self-assembly, folding, and virology." UIUC Materials Science Graduate Recruiting Weekend, Urbana, IL, February 28 2015 [Poster]

## Grants and Funding

### Awarded

1. Simulations and Deep Learning for Multi-scale Biophysical Problems, Fast-track Application for Resources for Research Groups, Principal Applicant, 2024
    - **Funder**: Digital Research Alliance of Canada

    - **Total Funding**: 6,756 CAD
2. In silico modeling of the dynamical assembly of cysteine-rich glycopeptides, Alliance International Catalyst Grant, Principal Applicant, 2023
    - **Funder**: NSERC
    - **Total Funding**: 25,000 CAD
3. The Sub-measurable is Not Unreal: Modeling and Communication of the Effect of COVID-19 on the Brain, New Frontiers in Research Fund Exploration, Principal Applicant, 2023-2025
    - **Funder**: NFRF-E (SSHRC)
    - **Total Funding**: 200,000 CAD
4. Simulations and Deep Learning for Multi-scale Biophysical Problems, Resources for Research Groups, Principal Applicant, 2023
    - **Funder**: Digital Research Alliance of Canada
    - **Total Funding**: 26,844 CAD
5. Explainable Artificial Intelligence for Design of Antimicrobial Peptides, AI2 Funding Program, Principal Applicant, 2023-2025
    - **Funder**: Concordia AI Institute
    - **Total Funding**: 15,000 CAD
6. Deep Learning Methods for Design of RNA-targeting Small-Molecule Antibiotics, Principal Applicant, 2022
    - **Funder**: Mitacs
    - **Total Funding**: 30,000 CAD
7. Canada Research Chair Tier 2 in Computational Biophysics, Principal Applicant, 2021–2026
    - **Funder**: Natural Sciences and Engineering Research Council of Canada (NSERC), Canada Research Chairs Program
    - **Total Funding**: 600,000 CAD
8. A Physics-Based Approach to Artifical Intelligence for Understanding of Biophysical Search Spaces, Principal Applicant, 2021–2026
    - **Funder**: NSERC Discovery Grants Program
    - **Total Funding**: 195,000 CAD
9. John R. Evans Leaders Fund, Principal Applicant, 2021
    - **Funder:** Canadian Foundation for Innovation
    - **Total Funding**: 150,000 CAD
10. Horizon Postdoctoral Funding, Principal Applicant, 2022–2023
    - **Funder:** Concordia University
    - **Total Funding:** 60,000 CAD

## Completed

1. Director's Postdoctoral Fellowship, Principal Applicant, 2018–2020
    - **Funder:** Los Alamos National Laboratory
    - **Total Funding:** 198,721 USD
2. Blue Waters Graduate Fellowship, Principal Applicant, 2017–2018
    - **Funder:** Blue Waters Foundation
    - **Total Funding:** 67,137 USD
3. Computational Science and Engineering Fellowship, Principal Applicant, 2016–2017
    - **Funder:** University of Illinois at Urbana-Champaign
    - **Total Funding:** 16,985 USD

## Declined

1. NIST NRC Research Associate Program Fellowship, Principal Applicant
    - **Funder:** National Institute of Standards and Technology
    - **Total Funding:** 190,967 USD

## Pending

- Energy Landscapes in Pigment-Protein Complexes: Identifying the Structural Features Responsible for Spectral Dynamics via Multi-scale Simulations and Optical Spectroscopy, Co-Investigator, Team Grant, FRQNT, 2024
- Sloan Research Fellowship, Alfred P. Sloane Foundation, 2024

## Did Not Receive

- Cottrell Scholar Award, Research Corporation for Science Advancement, 2024
- Consortium universitaire en biophysique du Québec. Co-Applicant, Regroupements stratégiques en émergence, FRQNT, 2023
- Molecular Dynamics Simulations of Energy Landscapes in Pigment-Protein Complexes: Identifying the Structural Features Responsible for Spectral Dynamics, Co-Applicant, OVPRGS Seed Funding, Concordia University, 2023
- Active Learning Optimization of the Properties of Beta-Sheet-Forming Antimicrobial Peptides, Principal Applicant, Funds for New Researchers, FRQNT, 2023
- Sloan Research Fellowship, Alfred P. Sloane Foundation, 2023
- Artificial Intelligence, Modelling, and Simulation for Multi-scale Activities, Research, and Training (AIM SMART) for Materials Design, Co-applicant, NSERC CREATE, 2022
  - Although not the primary applicant, I was the primary mover behind this grant. I was not the primary applicant because we could not have two primary applicants.
- Active Learning Optimization of the Properties of Beta-Sheet-Forming Antimicrobial Peptides, Principal Applicant, Funds for New Researchers, FRQNT, 2022
- Transformative, Innovative, and Game-Changing Research on AI & Society, Science, and Emerging Disruptive Technology, Co-applicant, New Frontiers in Research Fund Transformation, NSERC, 2022
- How COVID-19 Enters the Brain: A Computational Modelling, Imaging, and Public Multimedia Communication Framework, Co-applicant, New Frontiers in Research Fund Exploration, NSERC, 2022
- Deep Learning for Design of Combinatorial Search Spaces for Hybrid Antibiotic Design, Principal Applicant, Research Grants & Challenges, Merck KGaA, 2021
- AIM SMART: Artificial Intelligence, Modeling, and Simulation for Multidisciplinary Activities, Research, and Training, Principal Applicant, NSERC CREATE, 2021
- Multiscale Model of Brain Vasculature, Principal Applicant, Discovery Horizons Grant, NSERC, 2021
- Molecular Dynamics Simulations of Energy Landscapes in Pigment-Protein Complexes: Identifying the Structural Features Responsible for Spectral Dynamics, Co-Applicant, Concordia OVPRGS Seed Grant, 2021

## Honors and Awards

- Outstanding Reviewer for Molecular Systems Design & Engineering 2023
- Dean's Award for Excellence in Research, Concordia University 2022
- Canada Research Chair, Tier II 2021–present
- Los Alamos Director's Fellowship, Los Alamos National Lab 2018–2020
- 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

- Canadian Association of Physicists 2022–present

- 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

- Recognized as an Outstanding reviewer of Molecule Systems Design & Engineering 2023
- Molecular Systems Design & Engineering 2023 (four articles)
- Computer Methods in Biomechanics and Biomedical Engineering 2023
- Biophysical Journal 2023
- RSC Advances 2022
- Microbiology Spectrum 2021
- Marine Drugs 2020
  - Guest Editor for Special Issue “Virtual Screening of Marine Natural Products”
- PLOS ONE 2017

## Extracurricular Activities and Service

- Member of Departmental EDI Committee 2023–current
- Co-organizer of Women & LGBTQ+ Physics Teas, Concordia University Department of Physics, 2023–current
- Member of Organizing Committee for Biophysical Society of Canada Annual Meeting, 2023–2024
- Conversation on Generative AI, Policy Horizons Canada, Canadian Government Aug 14, 2023
- Technology Evaluator, Scientific Venture Program March 13, 2023
- Guest Lecturer, University of Ottawa, Biochemistry (BCH8102) March 7, 2023
- Reviewer for NSF proposal Winter 2023, Fall 2023/Winter 2024
- Reviewer for Mitacs proposal Feb 2023
- Reviewer for Compute Canada Resource Allocation Competitions Fall 2022–Winter 2023
  - Reviewed multiple applicant documents and assessed them
  - Participated in full-committee meeting, Jan 18, 2023
- Member of the APS DBIO Engagement Committee Summer 2022–Summer 2023
  - Attended committee meeting
  - Helped plan virtual events
  - Moderated virtual panel on mental health in biological physics, Jan 26, 2023
- Poster Judge, Canadian Association of Physicists, CAP Annual Congress June 6, 2022
- Poster Judge, Biophysical Society of Canada, BSC Annual Meeting May 25, 2022
- Poster Judge, Garnet Key Society, Concordia May 9, 2022
- Reviewer for Compute Canada Resource Allocation Competitions Fall 2021–Winter 2022
  - Reviewed multiple applicant documents and assessed them
  - Participated in full-committee meeting, Jan 12, 2022
- Junior Co-Director, Centre for Research in Molecular Modeling (CERMM), Concordia Aug 2021 – Jan 2024
  - Wrote full renewal document for six years
  - Wrote interim renewal document
  - Hired administrative assistant, oversaw major transition
  - Worked to reinvent the Centre through new mission statements, new members, new meetings
  - Co-organized 2022 CERMM Symposium, the first in-person since the pandemic
- Presentation Judge, Virtual Symposium on Theoretical and Computational Chemistry in Canada July 19-25, 2021
- Member of CRC Hiring Committee, Concordia Fall 2021–Winter 2022
  - Attended weekly meetings

  - Reviewed candidate dossiers
  - Discussed best hiring practices and assessed candidates
- Member of Curriculum and Awards Committee, Concordia — Fall 2020 – current
  - Attended quarterly meetings
  - Reviewed and ranked USRA and CUSRA applications
  - Reviewed student performance and helped identify award recipients
- Chair of Colloquium Committee, Concordia — Fall 2021–Winter 2024
  - Identified potential speakers
  - Called committee meetings
  - Organized speakers
  - Oversaw pivoting from in-person to online in Winter 2022
- Moderator of DBIO LGBTQ+ networking session at APS March Meeting 2021 — March 16, 2021
- Invited speaker at Dawson College Enriched Science Colloquium — March 5, 2021
- Host for McGill mini-coding competition, Concordia — Nov 7-8 2020
- Member of Curriculum and Awards Committee, Concordia — Fall 2020-Spring 2022
- Member of Colloquium Committee, Concordia — Fall 2020
- 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

## Committee Memberships

**Supervisory Committees**

- Emilio Espejo (Misra) – Phys 497 Student, Concordia University
- Carolane Bergeron (Helfield) – PHYS 496 Student, Concordia University
- Stephanie Beram (Frank) – PHYS 496 Student, Concordia University
- Zoe Brisson-Tsavoussis (Frank) – PHYS 497 Student, Concordia University
- Lucas Etienne (Zazubovitz) – PHYS 497 Student, Concordia University
- Briget Hamilton (Gauthier) – PHYS 497 Student, Concordia University
- Mehdi Shamekhi (Peslherbe) – PhD Student, Concordia University
- Arezoo Jahanpour (Erol) – MSc Student, Concordia University
- Navjote Kooner (Erol) – MSc Student, Concordia University
- Golshad Ghojoghi (Erol) – PhD Student, Concordia University
- Hamed Ghazikhani (Butler) – PhD Student, Concordia University

**Thesis Examination Committees**

- Zahra Alinia (Peslherbe) – CHEM 896 Student, Concordia University
- Sina Pourebrahimi (Peslherbe and De Visscher) – PhD Student, Concordia University
- Fang Liang (Peslherbe and De Visscher) – PhD Student, Concordia University
- William Copp (Wilds) – PhD Student, Concordia University (Defense Chair)
- Zarish Abbas (Arvanitogiannis) – PhD Student, Concordia University

- F. Ifthiha Mohideen (Kwan) – PhD Student, Concordia University (Defense Chair)

## 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

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**Others available upon request**