Brenda M. Rubenstein, Ph.D.

Vernon K. Krieble Professor of Chemistry and Director of Data Science
Brown University

Website: rubenstein.group, Email: brenda_rubenstein@brown.edu

(Last Updated August 2025)

RESEARCH INTERESTS

I am a computational/theoretical chemist interested in three broad areas: 1) developing new quantum and statistical mechanics techniques for modeling strongly correlated molecules and quantum materials in the post-DFT era [Electronic Structure]; 2) designing new alternative (molecular, quantum, and cellular) computing techniques and algorithms [Alternative Computing]; and 3) using biophysical and statistical methods to predict the evolution of proteins, and by extension, drugs that can target them [Biophysics]. To date, my group has developed a wide variety of new, more accurate and efficient quantum Monte Carlo methods; demonstrated how simple organic molecules can be used to store information and compute; and designed physics- and ML-based computational tools for rapidly predicting the structures and resultant phenotypes of proteins of relevance to medicine and basic science. Other past and recurring research interests include problems in computational biology, neuroscience, data science, information theory, computational linear algebra, stochastics, and condensed matter physics. We frequently collaborate with experimentalists and industry to realize our theories regarding quantum materials, biophysics, and alternative computing strategies.

APPOINTMENTS

Brown University, Providence, RI — *Vernon K. Krieble Professor of Chemistry, Professor of Physics*

December 2024 - Present, Director of the Brown Data Science Institute
June 2024 - Present, Therapeutic Sciences Graduate Trainer
June 2024 - Present, Member, Legorreta Cancer Center
January 2022 - July 2025, Associate Professor of Chemistry and Physics with Tenure
August 2021 - Present, Center for Computational Molecular Biology (CCMB) Graduate Trainer
June 2020 - Present, Molecular and Cell Biology Graduate Trainer, NIH T32 Trainer
July 2020 - December 2021, Joukowsky Family Assistant Professor of Chemistry
July 2016 - June 2020, Assistant Professor of Chemistry

University of Twente, Enschede, Netherlands — *Senior Fulbright Scholar*

February 2024 - June 2024

Led research efforts in the Computational Chemical Physics (head: Prof. Claudia Filippi) and Molecules and Materials (collaborator: Albert Wong) Groups and taught a graduate-level Electronic Structure Theory course while promoting cultural exchange.

Lawrence Livermore National Laboratory, Livermore, CA — *Lawrence Distinguished Postdoctoral Fellow*

September 2013 - April 2016

Primary Staff Collaborators: Dr. Miguel Morales-Silva, Dr. Annie Kersting, Dr. Steve Libby, Dr. Berni Alder, Dr. Jonathan Dubois, and Dr. Vince Lordi

Los Alamos National Laboratory, Los Alamos, NM — *Visiting Research Scientist in the Center for Nonlinear Studies*

June 2009 - August 2009

EDUCATION

Columbia University, New York, NY — *PhD in Chemical Physics (GPA: 4.01/4.0)*

September 2008 - July 2013

Advisor: Prof. David Reichman
Thesis: *Novel Quantum Monte Carlo Techniques for Bosons and Fermions*

University of Cambridge, Cambridge, UK — *MPhil in Theoretical Chemistry (w/ First Class Honors)*

October 2007 - August 2008

Advisors: Prof. Mark Miller, Prof. Daan Frenkel
Thesis: *Protein Folding and Binding Amidst Entropy Sources*

Brown University, Providence, RI — *ScB in Chemical Physics, AB in Applied Math (w/ High Honors, GPA: 3.86/4.0)*

August 2003 - May 2007

Thesis Advisor: Prof. Richard Stratt
Thesis: *Complex Structure, Complex Dynamics: The Dynamics of Liquid Crystals in the Nematic Phase*
Summer Research Advisors: Prof. Laura Kaufman (Columbia), Dr. Shibo Zhang (New York Blood Center Virology)

PUBLICATIONS

Note: **Denotes Rubenstein Main Contributor (i.e., Wrote Paper and/or Contributed Main Ideas); [#]Denotes PI; [$]Denotes Rubenstein Graduate Student or Postdoc; [+]Denotes Rubenstein Undergraduate*

Refereed Journal Articles

Since Independent Career Began

1. [$]Bidart, A., [$]Vaish, P., [$]Kabengele, T., [$]Pang, Y., Liu, Y., and *[#]**B.M. Rubenstein.** Quantum Computing Beyond Ground State Electronic Structure: A Review of Progress Toward Quantum Chemistry Out of the Ground State. *Accepted for Annual Reviews of Physical Chemistry* (2025). [Electronic Structure]

2. [$]Lopez, A., Melton, C.A., Ahn, J., *[#]**Rubenstein, B.M.,** and Krogel, J. Identifying Band Inversions in Topological Materials Using Diffusion Monte Carlo. *J. Chem. Theory Comput.* (2025).

arXiv:2412.14388. [Electronic Structure]

3. Wines, D., Ahn, J., Benali, A., Kent, P.R.C., Krogel, J.T., Kwon, Y., Mitas, L., Reboredo, F.A., **Rubenstein, B.M**., Saritas, K., Shin, H., Stitch, I., and C. Ataca. Towards Improved Property Prediction of Low-Dimensional Materials Using Many-Body Quantum Monte Carlo Methods. *Advanced Physics Reviews* (2025). *arXiv:2406.02753.* [Electronic Structure]

4. [$]Monteiro da Silva, G., [+]Lam, K., Dalgarno, D., and [*#]**B.M. Rubenstein.** Compound Mutations in Abl1 Kinase Cause Inhibitor Resistance by Shifting DFG Flip Mechanisms and Relative State Populations. *eLife* (2025). *arXiv:2405.14968.* [Biophysics]

5. Gabruk, M., Luszczynski, M., Safran, K., Ogrodzinska, W., **Rubenstein, B.M**., and G. Monteiro da Silva. Mobility of Four Isostructural Regions Drives Isoform-Specific Properties of Plant LPOR. *Journal of Biological Chemistry,* **301** (3), 108261 (2025). *bioRxiv:2024.10.21.619389v1.* [Biophysics]

6. Wolpert, D., Korbel, J., Lynn, C., Tasnim, F., Grochow, J., Kardes, G., Aimone, J., Balasubramanian, V., de Giuli, E., Doty, D., Freitas, N., Marsili, M., Ouldridge, T.E., Richa, A., Riechers, P., Roldan, E., **Rubenstein, B.M**., Toroczkai, Z., and J. Paradiso. Is Stochastic Thermodynamics the Key to Understanding the Energy Costs of Computation? *Accepted at PNAS* (2024). arXiv:2311.17166. [Alternative Computing] **Cover Article**

7. [$]Iyer, G., [+]Whelpley, N., Tiihonen, J., Krogel, J.T., Kent, P.R.C., and [*#]**B.M. Rubenstein**. Force-Free Identification of Minimum-Energy Pathways and Transition States for Stochastic Electronic Structure Theories. *J. Chem. Theor. Comput.,* **20** (17): 7416-7429 (2024). arXiv:2402.13189. [Electronic Structure]

8. [$]Iyer, G. and [*#]**B.M. Rubenstein**. Atomistic Descriptor Optimization Using Complementary Euclidean and Geodesic Distance Information. *Molecular Physics*. e2381617 (2024). arXiv:2403.18090. [Electronic Structure]

9. [$]Shen, T., Barghati, H., Del Maestro, A., and *[#]**B.M. Rubenstein.** Disentangling the Physics of the Attractive Hubbard Model via the Accessible and Symmetry-Resolved Entanglement Entropies. *Phys. Rev. B,* **109**, 195119 (2024). *arXiv:2312.11746*. [Electronic Structure]

10. [$]Landinez-Borda, E., Berard, K.O., Lopez, A., and *[#]**B.M. Rubenstein.** Gaussian Processes for Finite-Size Extrapolation of Many-Body Simulations. *Faraday Discussions (Advanced Article).* (2024). *arXiv:2112.10334*. [Electronic Structure]

11. Sahoo, S.J., Xu, Q., Lei, X., [$]Staros, D., [$]Iyer, G., **Rubenstein, B.M.,** Suryanarayana, P., and A.J. Medford. Self-consistent Convolutional Density Functional Approximations: Formulation and Application to Adsorption at Metal Surfaces. *Chem. Phys. Chem.,* e202300688 (2024).

arXiv:2308.05310. [Electronic Structure] **Cover Article**

12. [$]Monteiro da Silva, G., Cui, J., Dalgarno, D., Lisi, G., and *[#]**B.M. Rubenstein.** High-Throughput Prediction of Protein Conformational Distributions with Subsampled AlphaFold2. *Nature Communications,* **15**, 2464 (2024)*. BioRxiv:10.1101/2023.07.25.550545v2.* [Biophysics] **See Related Press**

13. [$]Nader, D. and *[#]**B.M. Rubenstein.** VMC Optimization of Ultra-Compact, Explicitly-Correlated Wave Functions of the Li Isoelectronic Sequence in Its Lowest 1s2s2p Quartet State. *Chem. Phys. Lett.,* **838**, 141091 (2024). *arXiv:2310.00916*. [Electronic Structure]

14. Gumus, S., Biechele-Speziale, D., Manz, K., Pennell, K., *[#]**Rubenstein, B.M.**, and J. Rosenstein. Repurposing Waste Chemicals for Sustainable and Durable Molecular Storage. *ACS Omega*, 9(18), 19904 (2024). [Alternative Computing]

15. [$]Staros, D., Ganesh, P., and *[#]**B.M. Rubenstein.** A First-Principles Study of Bilayer 1T'-WTe2/CrI3: A Candidate Topological Spin Filter. *npj Spintronics,* **2**, 4 (2024). *arXiv:2308.06415.* [Electronic Structure]

16. DiScala, M.F., [$]Staros, D., de la Torre, A., [$]Lopez, A., Wong, D., Schulz, C., Barkowiak, M., Bisogni, V., Pelliciari, J., **Rubenstein, B.M.,** and K. Plumb. Elucidating the Role of Dimensionality on the Electronic Structure of the Van der Waals Antiferromagnet $NiPS_3$. *Adv. Phys. Res.*, 2300096 (2024). *arXiv:2302.07910*. [Electronic Structure]

17. Shen, M., [$]Afshar, A., Sinai, N., Guan, H., Harris, C., **Rubenstein, B.M.,** and S. Sun. Tuning Pd Catalytic Selectivity on Intermetallic B2-CuPd@Pd Core/Shell Structures for High-Performance Polymer Synthesis. *ACS Nano,* **18(1):** 178-185 (2024). [Electronic Structure]

18. Baiz, C.R., Berger, R.F., Donald, K.J., de Paula, J.C., Fried, S.D., [#]**Rubenstein, B.M.,** Stokes, G.Y., Takematsu, K., and C. Londergan. Lowering Activation Barriers to Success in Physical Chemistry (LABSIP): A Community Project. *J. Phys. Chem. A,* **128(1)**: 3-9 (2024). [Education]

19. [$]Shen, T., Barghati, H., [$]Yu, J., Del Maestro, A., and *[#]**B.M. Rubenstein.** A Stable, Recursive Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble: Applications to Thermometry and the Hubbard Model. *Phys. Rev. E*: **107**, 055302 (2023). *arXiv:2212.08654*. [Electronic Structure]

20. Agiza, A., Oakley, K., Rosenstein, J., **Rubenstein**, **B.M.,** Kim, E., Riedel, M., and S. Reda.Digital Circuits and Neural Networks Based on Acid-Base Chemistry Implemented Using Robotic Fluid Handling. *Nature Communications,* **14:** 496 (2023). [Alternative Computing]

21. [$]Huang, C. and *[#]**B.M. Rubenstein.** Machine Learning Diffusion Monte Carlo Forces. *J. Phys. Chem. A,* 127(1): 339-355 (2022). *arXiv:2211.07103*. [Electronic Structure]

22. Li, S., Patel, J. S., Crabtree, A., [$]Yang, H., **Rubenstein**, **B.M.,** Lund-Andersen, P., Ytreberg, F. M., and P.A. Rowley. Defining the HIV Capsid Binding Site of Nucleoporin 153. *mSphere,* **7(5)**: e00310-22 (2022). *bioRXiv:2022.05.06.490988v1*. [Biophysics]

23. [$]Iyer, G. and *[#]**B.M. Rubenstein.** Finite-Size Error Cancellation in Diffusion Monte Carlo Calculations of Surface Chemistry. *J. Phys. Chem A*, **126(28)**, 4636-4646 (2022). *arXiv:2206.00729*. [Electronic Structure]

24. [$]Monteiro da Silva, G., [$]Yang, J., [$]Leang, B., [$]Huang, J., Weinreich, D., and *[#]**B.M. Rubenstein.** Covalent Docking and Molecular Dynamics Simulations Reveal the Specificity-Shifting Mutations Ala237Arg and Ala237Lys in TEM β-Lactamase. *PLoS Comput. Biol.* **18(6)**: e1009944 (2022). *bioRXiv: 10.1101/2022.04.29.490038v1*. [Biophysics]

25. Tang, W.-S., [$]Monteiro da Silva, G., Kirveshlahti, H., [$]Skeens, E., [$]Feng, B., Sudijono, T., Yang, K., Mukherjee, S., *[#]**Rubenstein, B.M**., and L. Crawford (Dual Corresponding Authors). A Topological Data Analytic Approach for Discovering Biophysical Signatures in Protein Dynamics. *PLoS Comput Biol.* **18(5)**: e1010045 (2022). *bioRXiv:10.1101/2021.07.28.454240*. [Biophysics]

26. [$]Foulon, B., Ray, K., Kim, C., [$]Liu, Y., *[#]**Rubenstein**, **B.M.**, and V. Lordi (Dual Corresponding Authors). 1/w Electric-Field Noise in Surface Ion Traps from Correlated Adsorbate Dynamics. *Phys. Rev. A,* **105**, 013107 (2022). *arXiv:2107.01177*. [Alternative Computing]

27. Lai, J., [$]Yang, J., Uzun, E., *[#]**Rubenstein**, **B.M.**, and I. N. Sarkar. LYRUS: A Machine Learning Model for Predicting the Pathogenicity of Missense Variants. *Bioinformatics Advances,* **2(1)**: vbab045 (2022). *bioRXiv:10.1101/2021.05.10.443497v1*. [Biophysics]

28. [$]Staros, D., Hu, G., [$]Nanguneri, R., Krogel, J., Bennett, M.C., Heinonen, O., Ganesh, P., and *[#]**B.M. Rubenstein.** A Combined First Principles Study of the Structural, Magnetic, and Phonon Properties of Monolayer CrI_3. *J. Chem. Phys.* **156**, 014707 (2022). [Electronic Structure]

29. Kennedy, E., Geiser, J., Arcadia, C., Weber, P., Rose, C., **[#]Rubenstein, B.M.**, and J.K. Rosenstein. Secret Messaging with Endogenous Chemistry. *Scientific Reports,* **11**, 13960 (2021). [Alternative Computing]

30. [$]Church, M.S. and *[#]**B.M. Rubenstein.** Real Time Dynamics of Correlated Fermions via Auxiliary Field Quantum Monte Carlo. *J. Chem. Phys.,* **154**, 184103 (2021). [Electronic Structure]

31. Dombroski, A., Oakley, K., Arcadia, C., Nouraei, F., Chen, S.-L., **[#]Rubenstein, B.M.**, Rose, C., Rosenstein, J., Reda, S., and E. Kim. Implementing Parallel Arithmetic via Acetylation and Its Application to Chemical Image Processing. *Proceedings of the Royal Society A,* **477**, 20200899 (2021). [Alternative Computing]

32. Arcadia, C., Dombroski, A., Oakley, K., Chen, S.-L., Tann, H., Rose, C., Kim, E., Reda, S., *#**Rubenstein, B.M.,** and J. Rosenstein. Leveraging Autocatalytic Reactions for Chemical Domain Image Classification. *Chem. Sci.,* **12,** 5464 (2021). **2021 Chemical Science HOT Article.** [Alternative Computing]

33. $Liu, Y., Zhu, G.-Z., Yuan, D.-F., Qian, C.-H., Zhang, Y.-R., **Rubenstein, B.M.**, and L.-S. Wang. Observation of a Symmetry-Forbidden Excited Quadrupole-Bound State. *J. Am. Chem. Soc.,* **142** (47), 20240 (2020). [Electronic Structure]

34. $Shen, T., $Liu, Y., $Yang, Y., and *#**B.M. Rubenstein**. Finite Temperature Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble. *Invited for the J. Chem. Phys. Special Issue on Frontiers of Stochastic Electronic Structure Calculations, J. Chem. Phys.,* **153**, 204108 (2020). [Electronic Structure]

35. Yuan, D. F., $Liu, Y., Qian, C.-H., Kocheril, G. S., Zhang, Y.-R., **Rubenstein, B.M.**, and L. S. Wang. Polarization of Valence Orbitals by the Intramolecular Electric Field from a Diffuse Dipole-Bound Electron. *J. Phys. Chem. Lett.*, 11, 18, 7914-7919 (2020). [Electronic Structure]

36. Yuan, D. F., $Liu, Y., Qian, C.-H., Zhang, Y.-R., **Rubenstein, B.M.**, and L. S. Wang. Observation of p-type Dipole-Bound States in Molecular Anions. *Phys. Rev. Lett.*, **125**, 073003 (2020). [Electronic Structure]

37. $Liu, Y., $Shen, T., +Zhang, H., and ***#B.M. Rubenstein**. Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo. *J. Chem. Theor. Comput.,* **16**(7), 4298-4314 (2020)*; arXiv:2004.01194.* [Electronic Structure]

38. $Yang, J., Naik, N., Patel, J. S., Wylie, C. S., $Gu, W., +Huang, J., Naik, M., Weinreich, D., and *#**B.M. Rubenstein**. Predicting the Viability of Beta-Lactamase: How Thermodynamic Measures Correlate with Beta-Lactamase Fitness. *PLOS One,* **15** (5): e0233509 (2020)*; BioRXiv/2020/043661.* [Biophysics]

39. Cong, R., $Nanguneri, R., *#**Rubenstein, B.M.**, and V. Mitrovic. First Principles Calculations of the EFG Tensors of Ba_2NaOsO_6, a Mott Insulator with Strong Spin Orbit Coupling. *J. Phys.: Cond. Mat.*, **32** (40) (2020). *arXiv:1908.09014.* [Electronic Structure]

40. Kent, P. R. C. *et al*. QMCPack: Recent Advances in Auxiliary Field and Real-Space Quantum Monte Carlo. **Named Editor's Pick** for the Journal of Chemical Physics*, J. Chem. Phys.,* **152**, 174105 (2020); *arXiv:2003.01831.*[Electronic Structure] *(Rubenstein graduate student Hongxia Hao is author 17; Rubenstein is author 15 out of 19; This is a community software paper, standard in my field.)* [Electronic Structure]

41. $Hao, H., Georges, A., Millis, A. J., ***Rubenstein, B.M.**, Han, Q., and Shi, H. Metal-Insulator and Magnetic Phase Transitions of Ca_2RuO_4 from Auxiliary Field Quantum Monte Carlo and Dynamical Mean Field Theory. *Phys. Rev. B.,* **101**, 235110 (2020)*; arXiv:1911.02702.* [Electronic Structure]

42. Rosenstein, J.K., Rose, C., Reda, S., Weber, P., Kim, E., Sello, J., Geiser, J., Kennedy, E., Arcadia, C., Dombroski, A., Ferguson, K., Chen, S.-L., Tann, H., and *#**B.M. Rubenstein**. Principles of Information Storage in Small-Molecule Mixtures. *IEEE Transactions on NanoBioScience,* **19** (3), 378-384 (2020). *arXiv:1905.02187.* [Alternative Computing]

43. [$]Foulon, B. L., [$]Liu, Y., Rosenstein, J. K., and *[#]**B.M. Rubenstein.** A Language for Molecular Computation. *Chem*, **5**, 306-319 (2019). [Alternative Computing]

44. Arcadia, C., Kennedy, E., Geiser, J., Dombroski, A., Oakley, K., Chen, S.L., [$]Sprague, L., Sello, J., Weber, P., Reda, S., Rose, C., Kim, E., *[#]**Rubenstein, B. M.**, and Rosenstein, J. K. Multicomponent Molecular Memory. *Nature Communications,* **11**, 691 (2020). [Alternative Computing]

45. Cong, R., [$]Nanguneri, R., *[#]**Rubenstein, B.M.,** and V. Mitrovic. Evidence from First-Principles Calculations for Orbital Ordering in Ba_2NaOsO_6, a Mott Insulator with Strong Spin Orbit Coupling, from First Principles. *Phys. Rev. B*, **100** (24), 245141 (2019). [Electronic Structure]

46. [$]Sprague, L., [$]Huang, C., [$]Song, J.-P., and *[#]**B.M. Rubenstein.** Maximizing Thermoelectric Figures of Merit by Uniaxially Straining Indium Selenide. *J. Phys. Chem. C,* **123** (41), 25437-25447 (2019). [Electronic Structure]

47. Kennedy, E., Arcadia, C., Geiser, J., Weber, P., Rose, C., *[#]**Rubenstein, B.M.**, and J.K. Rosenstein. Encoding Information in Synthetic Metabolomes. *PLOS ONE*, **14** (7), e0217364. *bioRxiv: 10.1101/627745v1*. *Among PLOS ONE's most cited papers of 2020.* [Alternative Computing]

48. [$]Hao, H., ***[#]Rubenstein, B.M.**, and H. Shi. Auxiliary Field Quantum Monte Carlo for Multiorbital Hubbard Models: Controlling the Sign and Phase Problems to Capture Hund's Physics. *Phys. Rev. B,* **99**, 235142 (2019). *arXiv:1902.01463*. [Electronic Structure]

49. Ray, K., ***Rubenstein, B.M.**, [$]Gu, W., and V. Lordi. *VdW-Corrected Density Functional Theory Study of Electric Field Noise Heating in Ion Traps Caused by Electrode Surface Adsorbates*. *New J. Phys.*, **21** (5) (2019). *arXiv:1810.10199.* [Alternative Computing]

50. Cai, T., Yang, H., Hills-Kimball, K., [$]Song, J.-P., Zhu, H., Hofman, E., Zheng, W., **Rubenstein, B.M.**, and O. Chen. Synthesis of All-Inorganic Cd^{2+}-Doped $CsPbCl_3$ Perovskite Nanocrystals with a Dual-Wavelength Emission. *J. Phys. Chem. Lett.,* **9** (24), 7079 (2018). [Electronic Structure]

51. [$]Hao, H., Shee, J., [$]Ataca, C., Upadhyay, S., Jordan, K., and *[#]**B.M. Rubenstein**. Accurate Predictions of Dipole-Bound Anion Binding Energies via Quantum Monte Carlo. *J. Phys. Chem. Lett.,* **9** (21), 6185 (2018); *arXiv:1809.09771*. [Electronic Structure]

52. [$]Liu, Y., [+]Cho, M., and ***[#]B.M. Rubenstein**. Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo. *J. Chem. Theor. Comput.,* **14** (9), 4722 (2018); *arXiv:1806.02848*. [Electronic Structure]

53. Zhu, H., Cai, T., Que, M., [$]Song, J.-P., **Rubenstein, B.M.**, Wang, Z., and O. Chen. Pressure-Induced Phase Transformation and Bandgap Engineering of Formamidinium Lead Iodide Perovskite Nanocrystals. *J. Phys. Chem. Lett.,* **9** (15), 4199 (2018). [Electronic Structure]

54. Arcadia, C., Tann, H., Dombroski, A. Ferguson, K., Chen, S.-L., Kim, E., Rose, C., *[#]**Rubenstein, B.M.**, Reda, S., and J. K. Rosenstein. Parallelized Linear Classification with Volumetric Chemical Perceptrons. *IEEE Rebooting Computing* (2018). [Alternative Computing]

55. Rose, C., Reda, S., [#]**Rubenstein, B.M.**, and J. Rosenstein. Computing with Chemicals: Perceptrons Using Small Molecules. *Proceedings of the International Symposium on Information Theory (ISIT) 2018*.

[Alternative Computing]

56. Kim, J. *et al*. QMCPACK: An Open Source Ab Initio Quantum Monte Carlo Package for the Electronic Structure of Atoms, Molecules, and Solids. *J. Phys.: Condens. Mat.*, **30**, 195901 (2018). [Electronic Structure] *(Rubenstein graduate student Hongxia Hao is author 12; Rubenstein is author 36 out of 48; This is a community software paper, standard in my field)*

57. ***#Rubenstein, B.M**. Introduction to the Variational Monte Carlo Method in Quantum Chemistry and Physics. In *Variational Methods in Molecular Modeling*, ed. Jianzhong Wu, Springer (2017). [Electronic Structure]

58. $Chang, C.-C., *#**Rubenstein, B.M.**, and M. Morales-Silva. Auxiliary-Field Based Trial Wave Functions in Quantum Monte Carlo Calculations. *Phys. Rev. B*, **94**, 235144 (2016). [Electronic Structure]

From Before Independent Career Began

59. ***Rubenstein, B.M**., Zhang, S., and D.R. Reichman. Auxiliary-Field Quantum Monte Carlo for Bose-Fermi Mixtures. *Phys. Rev. A*, **86**, 053606 (2012). [Electronic Structure]

60. ***#Rubenstein, B.M.**, Coluzza, I., and M.A. Miller. Controlling the Folding and Binding of Proteins Using Polymer Brushes. *Phys. Rev. Lett.*, **108**, 208104 (2012). [Biophysics]

61. ***Rubenstein, B.M.**, Gubernatis, J.E., and J.D. Doll. Comparative Monte Carlo Efficiency by Monte Carlo Analysis. *Phys. Rev. E*, **82**, 036701 (2010). [Electronic Structure]

62. ***Rubenstein, B.M.** and L.J. Kaufman**.** The Role of Extracellular Matrix in Glioma Invasion: A Cellular Potts Model Approach. *Biophys. J.*, **95**, 5661-5680 (2008). [Biophysics]

Currently Under Review/Revision

63. $Kabengele, T., $Lokare, Y., Marston, J.B., and *#**B.M. Rubenstein.** Modeling Stochastic Chemical Kinetics on Quantum Computers. *Under Revision at Quantum Science and Technology* (2024). *arXiv:2404.08770.* [Electronic Structure and Alternative Computing]

64. +Galeazzi, F.M., Arantes, P., $Monteiro da Silva, G., $Varghese, I., +Shukla, A., and *#**B.M. Rubenstein.** FastEnsemble: A Standalone Toolkit for Modeling and Analyzing Protein Conformational Ensembles at Scale. *Submitted to the Journal of Chemical Information and Modeling* (2024). [Biophysics]

65. **Rubenstein, B.M.,** Annaberdiyev, A., Panchapakesan, G., $Iyer, G., Krogel, J.T., $Lopez, A., Melton, C.A., Mitas, L., +Nirenberg, S., Kayahan, S., Shin, H., $Staros, D., and P.R.C. Kent. A Practical Guide to Quantum Monte Carlo Calculations Using QMCPACK and Nexus. *Submitted to Electronic Structure* (2025). [Electronic Structure]

66. Sands, I., Xu, H., Zihan, J., Li, P., [$]Florent, O., [$]Ramirez, G., Zhang, W., Zhou, L., Han, M., **Rubenstein. B.M.**, Tian, B., Meng, E., Song, D., and Y. Chen. Novel Electrically Conductive DNA-Inspired Nanotubes for Bioelectronic interface Coating. *Submitted to Nature Nanotechnology* (2025). [Electronic Structure]
67. Batist, G., Farahnak, F., El Deiry, W., Lussier, Y., Kurzrock, R., Magidi, S., Bresson, C., Enger, S., Liu, J., Bar, J., Warner, J., Meissner, T., Rubenin, E., Rueter, J., Gaddipati, H., Kulkarni, M., Chen, Z., Limaye, S., Elsey, R., **Rubenstein, B.M.**, Joshua, A., Al-Shamsi, H., Musallam, K., Wunder, F., Raynaud, J., Berchem, G., Gantenbein, M., Al Omari, A., Dermime, S., Abdel-Razeq, H., Saintigny, P., Cervantes, A., Reddel, R., Aref, A., Martin-Liberal, J., Lazaro, C., Romera, D., Sekacheva, M., Berger, R., Pramesh, C.S., Berindan-Neagoe, I., Girda, E., Farhangfar, C., Salem, M., Dienstmann, R., Salazar, R., and N. Frankel. Worldwide Innovative Network (WIN) Consortium: Building a Common Global Cancer Database. *Submitted to Nature Reviews Clinical Oncology* (2025). [Biophysics]

68. Khan, A.,[$]Vaish, P., [$]Pang, Y., [+]Kowshik, N., Chen, M.S., Batton, C., Rotskoff, G., Mullinax, W., Clark, B., ***[#]Rubenstein, B.M.**, and N.M. Tubman. Quantum Hardware-Enabled Molecular Dynamics via Transfer Learning. *Under Review at Quantum* (2024). *arXiv:2406.08554*. [Electronic Structure and Alternative Computing]

69. [$]Lokare, Y.,[+$]Wei, Dingding, [+]Chan, L., ***[#]Rubenstein, B.M,** and J.B. Marston. Steady-State Statistics of Classical Nonlinear Dynamical Systems from Noisy Intermediate-Scale Quantum Devices. *Submitted to Physical Review E* (2024). [Electronic Structure and Alternative Computing]

70. [$]Vaish, P., [$]Pang, Y., Singh, H., Chen, M., Batton, C., Mullinax, W., Rotskoff, G., Tubman, N., and *[#]**B.M. Rubenstein.** Biophysics on a Quantum Computer: Clarifying the Mechanism of ATP Hydrolysis via Quantum Computation. *Submitted to PNAS* (2024). [Electronic Structure and Alternative Computing]

71. Wu, R., [$]Jia, X., Cai, T., [$]Iyer, G.P., Luo, Q., Jin, N., Liu, Z., Chen, X.-F., Saul, A., Hwang, S., Liu, Y., McDonald, B., Mani, T., Zhao, J., He, J., **Rubenstein, B.M.,** and O. Chen. Synthesis of Palladium Nanocluster-Decorated Cs3Sb2Cl9 Perovskite Heterostructural Nanorods for Enhanced CO2 Photoreduction. *Submitted to Advanced Materials* (2025). [Electronic Structure]

72. Mullinax, W., [$]Vaish, P., Singh, H., Tubman, N., and *[#]**B.M. Rubenstein.** Reducing Qubit Volumes Needed to Model Reactive Dynamics on Quantum Computers Using Double Unitary Coupled Cluster Theory. *Submitted to the Journal of Chemical Physics* (2024). [Electronic Structure and Alternative Computing]

73. [$]Vaish, P. and *[#]**B.M. Rubenstein.** An Active Space Approach to Unitary Coupled Cluster Theory. *Submitted to the Journal of Chemical Theory and Computation* (2024). [Electronic Structure]

74. [$]Wang, L. and *[#]**B.M. Rubenstein.** Sparse Full Configuration Interaction. *Submitted to the Journal of Chemical Theory and Computation* (2023). [Electronic Structure]

75. [$]Staros, D., Gasperich, K., Annaberdiyev, A., Benali, A., Ganesh, P., and *[#]**B.M. Rubenstein.** A Many-Body Characterization of the Fundamental Gap in Monolayer CrI3. *Submitted to J. Chem. Phys.* (2024). arXiv:2506.17038v. [Electronic Structure]

76. [+]Feng, B., Marks, A., Jay, Gregory, and *[#]**B.M. Rubenstein.** Lubricin's Mucin Domain Has Strong Polyproline Type II Character. *Submitted to Biophysical Journal* (2025). bioRxiv:10.1101/2025.06.15.659778. [Biophysics]

77. [$]Foulon, B., [$]Iyer, G., and *[#]**B.M. Rubenstein.** The TCat Database: A Database of Transition State Energies and Geometries of Reactions on Heterogeneous Catalysts. *Submitted to Nature Scientific Data* (2023). [Electronic Structure]

78. [$]Somani, D., Pham, J., [$]Pang, Y., Riedel, M., Rosenstein, J., Reda, S., Kim, E., and *[#]**B.M. Rubenstein.** Multilayer Chemical Circuits Using Autocatalytic Reactions. *Submitted to ACS Central Science* (2022). [Alternative Computing]

79. [$]Liu, N., Ho, J., [$]Monteiro da Silva, G., [$]Daru, S., Incandela, J., Reda, S., Rosenstein, J., Larkin, J., and ***B.M. Rubenstein.** Computing Using Biofilm Oscillations. *Submitted to Natural Computing* (2022). [Alternative Computing]

80. [$]Vaish, P.,[$]Shen, T.,[$]Landinez-Borda, E.,[$]Kabengele, T., and **B.M. Rubenstein.** Modern Finite Temperature Electronic Structure Theory. *Invited Review for Journal of Computational and Theoretical Chemistry* (2024). [Electronic Structure]

81. Mamikon, G., [$]Yang, H., and *[#]**B.M. Rubenstein.** Fractional Path Integral Monte Carlo. *Submitted to JCP, One Reviewer Correctly Pointed Out a Mathematical Flaw We Since Solved* (2017)*; Resubmitted After Rewriting Delays* (2020); *arXiv:1709.09089*. [Electronic Structure]

Refereed Conference Submissions (for Certain Computer Science/Engineering Research)

1. [+]Sam, D., [+]Guo, K., Li, X., Fourches, D., and *[#]**B.M. Rubenstein**. Hierarchical Clustering Analysis of Spectral Fingerprints for Cheminformatics. *Machine Learning for Molecules Workshop @ NeurIPS* (2020).
2. [+]Singh, V. and *[#]**B.M. Rubenstein**. Quantum Neural Networks for Analyzing X-Ray Scattering Data. *IEEE Quantum Week* (2020).
3. [$]Bodner, B. and *[#]**B.M. Rubenstein**. Benchmarking the Adaptive Two Mode Algorithm (ATM). *GECCO 2019 Workshop Black-Box-Optimization Benchmarking* (2018).

Patents

1. Methods of Chemical Computation. *#**Rubenstein, B. M.,** Rosenstein, J. K., Kennedy, E., Chen, S.-L., Dombroski, A., Ferguson, K., Arcadia, A., Reda, S., Rose, C., Sello, J., Kim, E., Geiser, J., Tann, H., and P.M. Weber. U.S. Patent PCT/US2019/038301 (2022).
2. Molecular Data Storage Using Cost-Free Molecular Libraries. Gumus, S., Biechele-Speziale, D., **Rubenstein, B.M.**, and J.K. Rosenstein. U.S. Provisional Application No. 63/531208 (2023).

Refereed Reports

1. Goodson III, T.G., Awschalom, D.D., Babbush, R., Cheuk, L.W., Cushing, S.K., Frank, N.L., Freedman, D.E., Griffin, S.M., Hill, S.O., Liu, H., Garcia, M.P., **Rubenstein, B.M.**, Schelter, E.J., Wasielewski, M.R., Watkins, D., Nhon, N., Bremer, A., Lynch, A., and Wymbs, K. Advancing Chemistry and Quantum Information Science: An Assessment of Research Opportunities at the Interface of Chemistry and Quantum Information Science in the United States. *The National Academies Press* (2023). doi: 10.17226/26850. [Alternative Computing]
2. **Rubenstein, B.M.** and S. Perry. Protecting and Improving Human Health White Paper. *Proceedings of the 2024 Materials Genome Initiative.* (2024)

Books and Book Chapters

1. *Advances in the Computational Sciences: Symposium in Honor of Dr. Berni Alder's 90th Birthday*, eds. Schwegler, E., ***Rubenstein, B.M.**, and S. Libby, World Scientific, 2017.
2. *Art of Molecular Programming,* eds. ***Rubenstein, B.M.** *et al.*, World Scientific, 2024 Release. *https://molecularprogrammers.org/#aomp*
3. Collins, M., Louthain, E., Mohamed, G., Morin, J., Nemerovski, A., Rubenstein, B.M., and R. Tobias. Reimaging Chemistry: Cultivating Conscious Scientists Through Contextual Learning and Diverse Perspectives in STEM Education. *Accepted as a Book Chapter in Book STEM Education and Culturally Sustaining Pedagogies* (2024).

Theses

1. **Rubenstein, B.M**. Novel Quantum Monte Carlo Techniques for Bosons and Fermions (2013).
2. **Rubenstein, B.M**. Protein Folding and Binding Amidst Entropy Sources (2008).
3. **Rubenstein, B.M**. Complex Structure, Complex Dynamics: The Dynamics of Liquid Crystals in the Nematic Phase (2007).

SELECTED HONORS AND AWARDS

NIH Quantum Computing Grand Challenge — *2025*

NSF CHE Committee of Visitors Selection — *2024*

US Defense Science Study Group Selection — *2023*

Brown Meenakshi Narain Award for Undergraduate Research Mentoring (2 per year across the College) — *2023*

Heartland Challenge Venture Prize Recipient (AtomICs Startup) — *2023*

US Fulbright Senior Scholar to the Netherlands — *2023*

DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Allocation Recipient (with QMCPACK Team) — *2022, 2023*

Get Started Rhode Island First-Place Venture Prize Recipient (AtomICs Startup) — *2022*

Brown University First-Place Venture Prize Recipient (AtomICs Startup) — *2022*

Brown University Early Career Research Achievement Award — *2022*

American Chemical Society Petroleum Research Fund Outstanding Reviewer Award — *2021*

Named to *Popular Science's* Brilliant 10 List — *2021*

Research Corporation of America Scialog Fellow (Mitigating Zoonotic Threats) — *2021*

Camille Dreyfus Teacher-Scholar Award — *2021*

ACS Computers in Chemistry Division OpenEye Outstanding Junior Faculty Award in Computational Chemistry — *2020*

Cottrell Teacher-Scholar Award — *2020*

Air Force Young Investigator Award — *2019*

DARPA Defense Sciences Office Futures Innovation Lab Selection — *2019*

Named to *Chemical & Engineering News* Talented 12 — *2019*

Brown University Diversity and Inclusion Action Plan Faculty Award — *2019*

Alfred P. Sloan Fellow — *2019*

NSF Innovation Lab Selection — *2018*

Dell-Intel Young Investigator Award in Quantum Chemistry — *2018*

Society for Science and the Public Fellow — *2017, 2019;* **National Lead Advocate** — *2018*

Lawrence Distinguished Postdoctoral Fellowship — *2013*

Best Poster Award, Berkeley Mini Stat Mech Meeting — *2010*

Best Poster Award, Los Alamos National Laboratory Student Symposium — *2009*

Best Poster Award, ACS Division of Physical Chemistry — *2008*

Department of Energy Computational Science Graduate Fellowship — *2008*

National Science Foundation Graduate Research Fellowship — *2008*

Winston Churchill Foundation of America Scholarship to Cambridge — *2007*

Rhodes Scholarship Finalist (NJ/MA Region) — *2007*

Paul Cross Prize for Best Senior in Physical Chemistry (Brown) — *2007*

Leallyn B. Clapp Thesis Prize for Best Thesis in Physical Chemistry (Brown) — *2007*

Barry Goldwater Scholarship — *2006*

NJ Bloustein Distinguished Scholar — *2003*

National Merit Scholarship Recipient — *2003*

Academy for the Advancement of Science and Technology (AAST) Salutatorian — *2003*

NJ Governor's School Selection — *2002*

NSF/Christopher Columbus Foundation Award for Community Innovation Finalist — *1999*

INVITED EXTERNAL TALKS (SINCE STARTING AT BROWN, JULY 2016)

1. Pacifichem, Quantum Monte Carlo and Quantum Dynamics Sessions, December 2025.
2. **Northeast Quantum Forum: AI in Quantum, Public and Scientific Talks, October 2025.**
3. Novo Nordisk, Copenhagen, September 2025.
4. NC State University Electrical and Computer Engineering Seminar, September 2025.
5. Telluride Science Workshop on Quantum Dynamics, July 2025.
6. DOE CSGF Annual Meeting, July 2025.
7. Telluride Science Workshop on Stochastic Electronic Theory, June 2025.
8. Workshop on Stochastic Thermodynamics, Virtual, May 2025.
9. CECAM Meeting on Finite Temperature Physics, Lausanne, May 2025.
10. SIAM DS25 Conference, May 2025.
11. APS Meeting, Anaheim, CA, March 2025.
12. ACS Meeting, San Diego, CA, March 2025.
13. Iona College Chemistry Seminar, February 2025.
14. **Winter School Lecturer (and Organizer):** Brown-University of Puerto Rico Winter School, January 2025.
15. Legorreta Cancer Center Seminar, December 2024.
16. Barnard College Chemistry Seminar, November 2024.
17. University of Waterloo, November 2024.
18. Foresight Molecular Machines Group, October 2024.
19. DOE Materials Genome Initiative Conference, July 2024.
20. Telluride Science Workshop on Condensed Phase Dynamics, July 2024.

21. Faraday Discussion on Correlated Electronic Structure, the Royal Society, July 2024.
22. Foresight Institute Molecular Machines Group, June 2024 (Online).
23. One Chemistry Symposium, Johns Hopkins, April 2024.
24. University of Twente, Molecules and Materials Colloquium, April 2024.
25. University of Twente, Computational Chemical Physics Colloquium, March 2024.
26. TREX COE in Exascale Computing symposium: Bridging Quantum Monte Carlo and High-Performance Simulations, Luxembourg, February 2024.
27. **Winter School Lecturer (and Organizer):** Brown-University of Puerto Rico Winter School, January 2024.
28. QuEra Applications Group Seminar, December 2023.
29. CUNY Graduate Center Theoretical and Computational Chemistry Workshop, December 2023.
30. **Student-Invited Endowed Lecture:** Caltech University, December 2023.
31. Center for the Predictive Simulation of Functional Materials All-Hands Meeting, November 2023.
32. **Student-Invited Chemistry Alumni Fund Lecturer:** Johns Hopkins University, October 2023.
33. Brown University Quantum Computing Club, September 2023.
34. New York University Chemistry Department/Simons Flatiron Institute Colloquium, September 2023.
35. ***Keynote Speaker:*** Tapia-MolSSI Workshop in Computational Chemistry, Summer 2023.
36. ACS Fall 2023 Meeting in San Francisco Invited Speaker, August 2023.
37. NIST Artificial Intelligence in Materials Science Invited Speaker, July 2023.
38. Telluride Science Workshop on Stochastic Electronic Structure Methods, June 2023.
39. Berkeley Lab Molecular Foundry Colloquium, June 2023.
40. Pittsburgh Quantum Initiative Invited Seminar, May 2023.
41. Stony Brook University Chemistry Department Colloquium, April 2023.
42. University of Rochester Department Colloquium, February 2023.
43. ***Keynote Speaker:*** University of Western Kentucky Annual Math Symposium, November 2022.
44. University of Tennessee Condensed Matter Physics Seminar, October 2022.
45. QMC Methods in the Next Decade, Simons Flatiron Institute, September 2022.
46. PsiK 2022 Conference, Lausanne, Switzerland, August 2022.
47. 7th International Conference on Chemical Bonding (ICCB), Hawaii, August 2022.
48. Biennial Conference on Chemical Education, Purdue, August 2022.
49. ***Keynote Speaker:*** 20th Mercury Symposium on Computational Chemistry, July 2022.
50. Chemical Physics Colloquium, Lahore University of Management Science, June 2022.
51. McGill University Theoretical Chemistry Conference, June 2022.
52. Monte Carlo and Machine Learning Approaches in Quantum Mechanics, IPAM, Los Angeles, CA, May 2022.
53. Rhode Island College Physical Science Department Colloquium, April 2022.
54. University of Colorado - Boulder Department of Chemistry Colloquium, March 2022.
55. The 1st International Workshop on Data Storage in Molecular Media (DSMM), University of Marburg, March 2022.
56. Sanibel Electronic Structure Symposium, February 2022.

57. Simons Collaboration on the Many Electron Problem Annual Meeting, February 2022.
58. Pacifichem, Hawaii, December 2021.
59. CUNY Graduate Center, Quantum Information in Chemistry Symposium, December 2021.
60. Queens College Department of Chemistry Colloquium, October 2021.
61. IBM Unconventional Paradigms in Computing Virtual Conference, September 2021.
62. Simons CCQ Virtual Electronic Structure Workshop, New York, NY, July 2021.
63. Complex Active and Adaptive Material Systems GRC/GRS, Ventura, CA, June 2021.
64. Quantum Effects in Condensed Phase Systems, Telluride, CO, June 2021.
65. New Frontiers in Electron Correlation Workshop, Telluride, CO, June 2021.
66. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2021.
67. University of Maryland, Chemistry Department Seminar, April 2021.
68. Predictive Synthesis and Decisive Characterization of Emerging Quantum Materials Symposium, Materials Research Society Meeting, April 2021.
69. Cornell University, Chemistry Department Seminar, April 2021.
70. Stanford University Chemistry Department Seminar, April 2021.
71. ***Student-Invited Speaker:*** Spring 2021 ACS Meeting, Pitt-CMU ACS Graduate Student Symposium, April 2021.
72. University of California, Santa Cruz, Chemistry Department Seminar, March 2021.
73. Brown/Dartmouth Quantum Computing Winter School, December 2020.
74. University of California, Los Angeles, Chemistry Department Seminar, November 2020.
75. Molecular Programming Interest Group (MolPIGS) Seminar, November 2020.
76. Brown University Data Science Initiative Faculty 2 Faculty Talk, November 2020.
77. Brandeis University Chemistry Department Seminar, November 2020.
78. University of California, Berkeley Theoretical Chemistry Seminar, October 2020.
79. Psi-K 2020 Meeting, Lausanne, Switzerland, September 2020. [*Postponed Due to COVID*].
80. 7th International Conference on Chemical Bonding, Kaui, Hawaii, August 2020. [*Postponed Due to COVID*].
81. Quantum Effects in Condensed-Phase Systems Workshop, Telluride Science Research Center, Telluride, CO, July 2020.
82. *Ab Initio* Simulations of Correlated Fermions Workshop, Kiel, Germany, July 2020.
83. Molecular and Cell Biology Graduate Program Seminar, Brown University, June 2020.
84. University of Houston Chemistry Department Seminar, June 2020.
85. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2020.
86. Electrochemical Society Meeting, Montreal, CA, May 2020 [*Canceled Due to COVID*].
87. Iona College Chemistry Colloquium, New Rochelle, NY, March 2020 [*Postponed Due to COVID*].
88. Spring 2020 American Chemical Society Meeting, Philadelphia, PA, March 2020 [*Canceled Due to COVID*].
89. American Physical Society March Meeting, Denver, CO, March 2020 [*Canceled Due to COVID*].
90. DARPA Defense Sciences Office, San Diego, CA, November 2019.
91. Caltech Department of Chemistry Colloquium, Pasadena, CA, October 2019.

92. Southwest Theoretical and Computational Chemistry Conference, Norman, OK, October 2019.
93. Texas A&M University Department of Chemistry Colloquium, College Station, TX, October 2019.
94. 2019 Utah Workshop [on Electronic Structure Theory], Park Slope, UT, September 2019.
95. University of New Haven Chemistry Colloquium, New Haven, CT, September 2019.
96. C&EN Talented 12 Recipient Symposium, ACS Fall 2019 National Meeting in San Diego, CA, August 2019.
97. Penn Conference on Theoretical Chemistry, UPenn, Philadelphia, PA, August 2019.
98. Oak Ridge National Laboratory, Oak Ridge, TN, August 2019.
99. MOLSSI School on Stochastic Approaches to Electronic Structure, Pittsburgh, PA, July 2019.
100. 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP-X) in the "Emergent Electronic Structure Methods" Track, Tromso, Norway, July 2019.
101. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2019.
102. New Frontiers in Electron Correlation Workshop, Telluride, CO, June 2019.
103. Spring 2019 ACS Meeting Symposium in Honor of Ken Jordan, Orlando, FL, April 2019.
104. Spring 2019 ACS Meeting Symposium on Modeling Dynamics in Dense Manifolds of Electronic States, Orlando, FL, April 2019.
105. APS March Meeting Symposium on Periodic Quantum Chemistry Beyond DFT, Boston, MA, March 2019.
106. University of Maryland - Baltimore County Physics Colloquium, Catonsville, MY, October 2018.
107. ***Keynote Speaker***: Quantum Monte Carlo Workshop in Honor of James Gubernatis, Los Alamos, NM, October 2018.
108. Lawrence Livermore Computational Chemistry and Materials Science Summer Institute Lecture Series, Livermore, CA, July 2018.
109. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2018.
110. ***Keynote Speaker:*** *Computing with Molecules*, Rhode Island American Chemical Society Annual Meeting, University of Rhode Island, May 2018.
111. Strongly Correlated Materials: Experiments and Computation CECAM Workshop, Tel Aviv University, Tel Aviv, April 2018.
112. Center for Computational and Molecular Biology Seminar, Brown University, Providence, RI, April 2018.
113. American Physical Society March Meeting, Los Angeles, CA, March 2018.
114. Quantum Cafe, Simons Center for Computational Quantum Physics, Flatiron Institute, New York, NY, February 2018.
115. New Vistas in Molecular Thermodynamics: Experimentation, Molecular Modeling, and Inverse Design, UC Berkeley, January 2018.
116. Boston University Physical Chemistry Seminar Series, Boston University, Boston, MA, November 2017.
117. Kean University Chemistry Colloquium. Kean University, Union, NJ, November 2017.
118. Fall Materials Research Society Meeting. Boston, MA, November 2017.
119. Brooklyn College Chemistry Colloquium. Brooklyn College, Brooklyn, NY, November 2017.

120. University of Massachusetts, Dartmouth Chemistry Colloquium. University of Massachusetts, Dartmouth, North Dartmouth, MA, September 2017.
121. Electronic Structure of Complex Chemical Systems Symposium. ACS National Meeting, Washington, DC, August 2017.
122. Stochastic Methods in Electronic Structure Theory Workshop. Telluride Science Research Center, Telluride, CO, July 2017.
123. Quantum Effects in Condensed-Phase Systems Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
124. New Frontiers of Electron Correlation Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
125. Stony Brook University Applied Mathematics Colloquium. Stony Brook University, Stony Brook, NY, April 2017.
126. Materials Issues for Quantum Computing. Materials Research Society Meeting. Boston, MA, November 2016.
127. Greater Boston Area Statistical Mechanics Meeting Table Talk. Brandeis University, Waltham, MA, October 2016.
128. Brown Applied Mathematics Department Colloquium. Providence, RI, August 2016.
129. Recent Progress in Numerical Green's Function Methods in Physics and Chemistry. Telluride Science Research Center, Telluride, CO, August 2016.

RESEARCH EXPERIENCE

Lawrence Livermore National Laboratory, Livermore, CA — *Lawrence Distinguished Postdoctoral Fellow*

September 2013 - May 2016

Collaborated with Miguel Morales-Silva to develop the theory and software needed to study solid-state systems and heavy elements using Auxiliary Field Quantum Monte Carlo. Additionally collaborated with Jonathan Dubois and Berni Alder to benchmark and extend exact fermion path integral techniques to plasmas and molecules, and collaborated with Keith Ray and Vince Lordi to develop a microscopic model of anomalous heating in trapped ion quantum computers.

Columbia University, New York, NY — *Doctoral Research*

September 2008 - July 2013

Worked with David Reichman and Shiwei Zhang to create novel Auxiliary Field Quantum Monte Carlo algorithms for bosons and Bose-Fermi mixtures. These techniques are the first capable of studying Bose-Fermi mixtures exactly in any dimension, for any system size. Also explored the possibility of a superglass phase of hydrogen mixtures.

Lawrence Livermore National Laboratory, Livermore, CA — *DOE CSGF Practicum Research*

June 2011 - November 2012

Worked with Jonathan Dubois and Berni Alder to develop new isostress ensemble techniques to identify ground state structures of hydrogen at high pressures. Our quantum isostress methods allow quantum simulations to settle into their equilibrium structures given no initial information about those structures.

Los Alamos National Laboratory, Los Alamos, NM — *DOE CSGF Practicum Research*

May 2009 - August 2009

Worked with James Gubernatis to show how the convergence of Markov chains may be captured by the eigenvalues of their transition matrices. Our work demonstrates how commonly used acceptance ratios do not tell the whole story about the convergence of Monte Carlo algorithms.

University of Cambridge, Cambridge, UK — *Masters Research*

October 2007 - August 2008

Worked with Mark Miller and Ivan Coluzza to demonstrate how grafted polymers may tune the binding and folding of proteins. Employing the Go model and sophisticated parallel-tempering and umbrella sampling techniques, we illustrated the effects of polymers on the binding and folding of proteins of very different natures.

Brown University, Providence, RI — *Undergraduate Honors Thesis Research*

October 2005 - August 2007

Worked with Richard Stratt to study the heterogeneous dynamics of liquid crystals around the isotropic-nematic phase transition. Developed a molecular dynamics code that represents liquid crystals as Gay-Berne ellipsoids to show that the isotropic-nematic phase transition may be identified by monitoring specific signals in Optical Kerr Effect (OKE) spectroscopy.

Columbia University, New York, NY — *REU Summer Research Experience*

May 2006 - August 2006

Worked with Laura Kaufman to mathematically model the invasion of glioblastoma multiforme, one of the most lethal brain tumors. Using a simple Q-Potts model, we showed which chemical and physical attributes of brain tissue promote invasion.

Kimball Research Institute, New York, NY — *Summer Research Experience*

May 2005 - August 2005

Worked with Shibo Zhang to help discover the CP-1 and CP-1m fusion inhibitors for the SARS virus by running HPLCs and electrophoreses of a number of SARS proteins and their related mutants.

POSTDOCS MENTORED (9 Past)

Dr. Daniel Julian Nader Fulbright Scholar from Mexico *Now:* Postdoc, Palacky University Olomouc (Czechia) *2022-2023*	**Dr. Amir Afshar** *Now:* Research Scientist, Palladus *2020-2022*	**Dr. Ehsan Barati** *Now:* Postdoc, Howard University *2019-2021*
Dr. Matthew Church *Now:* Assistant Professor at the	**Dr. Ravindra Nanguneri** *Now:* Assistant Professor at	**Dr. Jeong-Pil Song** *Now:* Research Assistant

Hobart and William P. Smith Colleges *2019-2022*	Amrita Vishwa Vidyapeetham (Chennai) *2017-2020*	Professor at University of Arizona *2016-2020*
Dr. Can Ataca *Now:* Associate Professor at UMBC *2016-2017*	**Dr. Edgar Landinez-Borda,** *Now:* Computational Scientist at Julich Computing Center *2015-2016 (LLNL), 2020-2021 (Brown)*	**Dr. Chia-Chen Chang** *2014- 2016 (LLNL)*

CURRENT PHD STUDENTS MENTORED (14)

Andrew Reynoso (Physics) BS, UC Berkeley *Research Focus:* Correlated Quantum Dynamics and Phase Transitions *2024-PRESENT*	**Iz Varghese** (Therapeutic Sciences, Coadvised with George Lisi) BS, Colby College *Research Focus:* Machine Learning for Protein Dynamics and Drug Binding *2024-PRESENT*	**Yitian Liu** (Chemistry) BS, U. Rochester *Research Focus:* QMC and Surrogate Methods for Correlated Catalysis *2024-PRESENT*
Alan Bidart (Chemistry) BS, Harvard *Research Focus:* Grand Unification of Quantum Algorithms and Compilation *Honors:* MIT iQuHACK Winner, Brown Open Graduate Program *2023-PRESENT*	**Kenneth Berard** (Chemistry) BS, URI; MS, Stony Brook *Research Focus:* Reduced Cost Tensor and ML Approaches for QMC *Honors:* Brown Open Graduate Program, RI NASA Space Grant, NDSEG Fellow, DOE SCGSR Fellow *2023-PRESENT*	**Octavia Florent** (Chemistry) BS, Geneva College *Research Focus:* Ab Initio Modeling of Correlated Quantum Heterostructures *Honors:* Brown IMSD Fellowship *2022-PRESENT*
Gustavo Ramirez (Chemistry) BS, MS National Autonomous University of Mexico (UNAM) *Research Focus:* Predictive Modeling of Biomimetic Polymers *2023-PRESENT*	**Esther Webber** (Chemistry) BS, MS University of Bristol *Research Focus:* Modeling of Host-Guest Complexes 2022-*PRESENT*	**Yaoqi Pang** (Chemistry) BS, MS ShanghaiTech University *Research Focus:* Quantum Computing Biochemical Reaction Dynamics 2022-*PRESENT*

Xiaohang Jia (Chemistry) BS, Jilin University; MS, Brown *Research Focus:* Correlated Magnetism in Low-Dimensional Materials 2021 -*PRESENT*	**Tilas Kabengele** (Chemistry) BS, Voronezh University; MS, Dalhousie *Research Focus:* Quantum Computing Partial Differential Equations *2021-PRESENT*	**Prateek Vaish** (Chemistry) BS, MS, IISER Kolkata *Research Focus:* Quantum Computing Biochemical Reaction Dynamics and UCC for Reactive Events *2020-PRESENT*
Annette Lopez (Physics) BS, MS, Cal State Fresno *Research Focus:* Characterizing Topology within Stochastic Methods *2021-PRESENT*	**Ryan Weiss** (Physics) BS, Stevens Institute of Technology *Research Focus:* Excitons in Low-Dimensional Materials *2024-PRESENT* (Transfer)	

PAST PHD STUDENTS MENTORED (11)

Dr. Gabriel Monteiro da Silva (Molecular and Cell Biology) *Honors:* Blavatnik Fellow *Now*: Research Scientist at OpenEye *2020-2024*	**Dr. Daniel Staros** (Chemistry) *Honors*: RI Space Grant, DOE SCGSR Fellowship *Now*: Research Scientist at LANL *2019-2024*	**Dr. Gopal Iyer** (Chemistry) *Honors:* Vince Wernig Dissertation Fellowship *Now*: Research Scientist at Lam Research *2019-2024*
Dr. Tong Shen (Chemistry and Applied Mathematics) *Honors:* Open Graduate Education Fellow, Poster Prize Progress in Many-Body Theories XXI Meeting at UNC *Now:* Postdoc in the Lidar Group (USC) *2018-2023*	**Dr. Cancan Huang** (Chemistry) *Honors:* Data Science Seed Grant Recipient *Now:* Research Scientist at Applied Materials *2017-2022*	**Dr. Benjamin Foulon** (Chemical Engineering) *Now:* Research Scientist at Johnson Matthey *2017-2023*
Dr. Haobo ("Jordan") Yang (Chemistry and Computer Science) *Now:* Analyst, Eight Roads Venture Capital *2017-2022*	**Dr. Leonard Sprague** (Chemistry) *Honors*: King Prize for Outstanding Graduate Teaching in Chemistry *Now*: Assistant Professor of English for STEM at the	**Dr. Yuan Liu** (Chemistry and Electrical Engineering w/Lai-Sheng Wang) *Honors*: Open Graduate Education Fellow, Potter Prize for Outstanding Thesis Recipient

	University of Tokyo *2016-2021*	*Now:* Assistant Professor of Computer Engineering at NC State *2016-2020*
Dr. Mamikon Gulian (Applied Math w/George Karniadakis) *Now:* Senior Software Engineer, Booz Allen Hamilton *2016-2019*	**Dr. Hongxia Hao** (Chemistry) *Now:* Research Scientist, Microsoft Research Asia *Honors:* ACS Division of Chemical Computing Group Excellence Award for Graduate Students, APS/DCOMP Travel Award to the APS March Meeting, IBM Zerner Graduate Student Award *2016-2019*	

MASTERS/POST-BAC STUDENTS MENTORED (5 Past)

Xiaohang Jia (Physics) *Now:* PhD Student in the Rubenstein Group *2019-2021*	**Joseph Fichera** (Geophysics) *Now:* PhD Student in the University of Florida Department of Physics *2018-2021*	**Lijun Wang** (Physics) *2018-2020, 2023*
Benjamin L. Davis (Electrical Engineering) *Now:* PhD Student in the University of Washington Division of Engineering *2018-2019*	**Nnenna Elechi** (Prairie View University and LLNL) *Now:* STEM Teacher at the Suzhou International Park Foreign Language School *LLNL Summer Student 2015*	

CURRENT UNDERGRADUATE STUDENTS MENTORED (10)

Kevin Rapp Chemical Physics, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, DOE SULI, MIT iQuHACK Winner	**Jeffrey Tejada Peralta** Chemical Physics, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, DOE SULI, ACS Prize in Chemical	**Yungeun Kim** Chemical Physics, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, Amgen Scholar, Junior Prize

2022-PRESENT	Physics, MIT iQuHACK Winner *2022-PRESENT*	in Chemical Physics, Third-Author Publication *2022-PRESENT*
Jasper Lincoln Chemical Physics, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, DOE SULI *2022-PRESENT*	**Faith Kim** Chemistry, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, Third-Author Publication *2022-PRESENT*	**Kyle Lam** Chemistry, Class of 2025 *Honors:* Brown Undergraduate Teaching and Research Assistantship, NYU SURF, Second-Author Publication *2022-PRESENT*
Simon Nirenberg Chemical Physics, Class of 2028 *Honors:* 2025 Lindau Nobel Laureate, RI ACS Poster Prize Recipient *2022-PRESENT (Since HS)*	**Winston Li** Computer Science, Class of 2025 *Honors:* Second-Author Publication, FlexMed Program Acceptance *2022-2024*	**Orion Bloomfield** Computer Science, Class of 2025 *Honors:* Third-Author Publication *2021-2023*
Tarek Razzazz Physics, Class of 2026 *Honors:* Brown Undergraduate Teaching and Research Assistantship	**Flavia Maria Galeazzi** Neuroscience and CS, Class of 2026 *2023-PRESENT*	

PAST UNDERGRADUATE STUDENTS MENTORED (19)

Suraj Daru Computer Science, Class of 2024 *Now:* In Industry at UKG on Gap Year *2022-PRESENT (Continuing After Graduation)*	**Conenicus Weeden** Biochemistry, Class of 2024 *Now:* On Gap Year Before Medical School *2021-PRESENT*	**Noah Whelpley** Chemistry, Class of 2024 *Now:* ACS COMP Undergraduate Poster Award, Chemistry Graduate Student at MIT *Honors:* ACS Prize in Physical Chemistry, Paul Cross Prize in Physical Chemistry, Brown Undergraduate Teaching and Research Assistantship, Second-Author Publication *2022-2024*
Bibo ('Noah') Feng Chemical Physics, Class of 2023	**Nicholas Liu** Biophysics, Class of 2023	**Anvita Bhagavathula (w/ Jia Li)** Physics and Applied Mathematics, Class of 2023

Now: Tufts University School of Medicine *Honors:* Junior Prize in Chemical Physics, Paul Cross Prize in Physical Chemistry, Clapp Prize in Physical Chemistry, Brown Undergraduate Teaching and Research Assistantship, First-Author Publication *2021-2024*	*Now:* Associate at Boston Consulting Group, First-Author Publication *2021-2023*	*Now:* Electrical Engineering Graduate Student at MIT *2021-2023*
Logan Dooley Chemical Physics, Class of 2023 *Now:* Associate Software Engineer at Demiurge Studios *2021— 2023*	**Anjali Srinivasan** Class of 204 *Honors:* Brown Undergraduate Teaching and Research Assistantship *2022*	**Alberto Lopez Resendiz** Applied Mathematics-Biology, Class of 2024 *Now:* Masters of Public Health and the University of Illinois-Chicago *Honors:* Brown Undergraduate Teaching and Research Assistantship *2022*
Minsik Cho Chemical Physics, Class of 2022 Concentrator *Now:* Chemistry Graduate Student at MIT *Honors:* Kwanjeong Graduate Fellowship, MIT Presidential Scholar, Paul Cross Prize in Physical Chemistry, Clapp Prize in Chemical Physics, Junior Prize in Chemical Physics, ACS Prize in Chemical Physics, Brown Undergraduate Teaching and Research Assistantship, Second-Author Publication *2016-2022 (On South Korean Military Leave, 2017-2019)*	**Jungho "Daniel" Choi** Chemical Physics and Mathematics Concentrator, Class of 2020 *Now:* Physics Graduate Student at Flatiron/NYU *2017-2022*	**Bunlong Leang** Human Biology, Class of 2022 *Honors:* Third-Author Publication *2018-2022*
Dylan Sam Computer Science, Class of 2021	**Kevin Guo** Applied Mathematics, Class of 2019	**Hersh Gupta** Chemistry and Computational Biology, Class

Now: CS Graduate Student at Carnegie Mellon *Honors:* NSF GRFP, First-Author Conference Proceeding *2017-2021*	*Now:* MD/PhD Student at Stanford *2018-2020*	of 2020 *Now:* MD/PhD Student at Mount Sinai *Honors:* Junior Prize in Chemistry *2017-2020*
Batia Friedman-Shaw Physics, Brown Class of 2022 *Now:* Physics Graduate Student at the Perimeter Institute *Honors:* Brown Undergraduate Teaching and Research Assistantship *2019*	**Heesoo Kim** Chemical Physics and Mathematics, Brown Class of 2019 *Now:* Physics Graduate Student at Stanford University *2017-2018*	**David Mayans** Chemistry and Computer Science, Class of 2018 *Now:* At Vested Financial Services *Honors:* Brown Undergraduate Teaching and Research Assistantship *2017-2018*
Adarsh Sridhar Narayanan Engineering-CS Concentrator, Class of 2018 *Now:* Software Engineer at Microsoft *2016-2017*		

CURRENT HIGH SCHOOL STUDENTS MENTORED (4)

Ho-Joon ('Stephen') Han Academy for the Advancement of Science and Technology, now NJIT *2023-PRESENT*	**Mayank Konduri** Katy High School, TX *2024-PRESENT*	**Stephen Yoon** Academy for the Advancement of Science and Technology *2024-PRESENT*
Shaun Srirangum Barrington High School 2024-PRESENT		

PAST HIGH SCHOOL STUDENTS MENTORED (9)

Casey Lambert	**Aneekah Younus**	**Cody Comyns**

Moses Brown High School *2021*	The Wheeler School *2021-2023*	Phillips Andover *2021*
Vaibhav Duggirala Moses Brown High School ACS Project SEED *Now:* Brown PLME Class of 2025 *Honors:* 2020 RI State Science and Engineering Fair Finalist (Top Ten) *2019-2021*	**Vishwas Duggirala** Moses Brown High School ACS Project SEED *Now:* Brown PLME Class of 2025 *Honors*: 2020 RI State Science and Engineering Fair Finalist (Top Ten) 2019-2021	**Tahseen Younus** The Wheeler School *Now:* Undergraduate at University of Illinois - Urbana-Champaign *Honors*: 2020 RI State Science and Engineering Fair Finalist (Top Ten) *2019-2021*
Omar Martinez Blackstone Valley Academy High School ACS Project SEED *Now:* University of Rhode Island Computer Engineering *Honors:* RI ACS Science Fair Award at the Rhode Island Science and Engineering Fair *2017-2019*	**Hannah Smith** Johnston High School ACS Project SEED *2022*	**Brian Nguyen** Gatton Academy *2022*

CURRENT VISITING UNDERGRADUATES MENTORED (6)

Nikhil Kowshik IIT Kharagpur *Honors:* Fourth-Author Paper *2023-2024*	**Ananya Shukla** Plaksha University *2023-2024*	**Shirui Li** Mount Holyoke College *2024*
Grace Delaney Brandeis University *2024*	**Tomas Heger** Churchill College, Cambridge *2024*	**Asmita Niyogi** Churchill College, Cambridge *2024*

PREVIOUS VISITING UNDERGRADUATES MENTORED (17)

Ray Zhai Churchill College, Cambridge	**Yuvraj Misra** IIT Mandi *Now:* Graduate Student at	**Jade Kemp** Austin College (Leadership Alliance)

2023	UIUC *2021*	*Now:* Chemistry Graduate Student at Columbia University *2021*
Shriya Sharma IIT Delhi *2021*	**Deepak Somani** IIT Kharagpur (IIT International Relations Cell) *Now:* Graduate Student in Germany *Honors:* First-Author Paper 2021	**Abhikhya Tripathy** IIT Kharagpur (IIT International Relations Cell) *2021*
Jenel Fraij Hartnell Community College (Leadership Alliance) *Now*: Graduate Student at UCLA 2020	**Bin Liu** USTC *2020*	**Vinit Singh** IIT Kharagpur *Now:* Graduate Student at Purdue University *Honors:* First-Author Conference Proceeding *2020*
Luke MacHale Montana State University (Leadership Alliance) *Now:* Chemistry Graduate Student at Colorado State University *2019*	**Yang Yu** USTC *Now:* Physics Graduate at the University of Michigan *Honors:* Second-Author Paper *2019*	**Jessie Huang** Wellesley College *Now:* Medical Student at the University of Rochester *Honors*: Third-Author Paper *2018*
Jorge Estrada University of Cantabria *2018*	**Swati Bodh** Amity University, India *2018*	**Hang Zhang** USTC *Now:* Chemistry Graduate Student at Princeton *Honors:* Second-Author Paper *2018*
Carson Cole Weber State University (Leadership Alliance) *Now:* Just Graduated Rice with a PhD in Biophysical Chemistry, Starting Postdoc *2018*	**Xuechen Zheng** Zhejiang University *Now:* Chemistry PhD Student at Johns Hopkins University *2017*	

GRANTS FUNDED [Total Funding as PI, Co-PI, or Co-I: >$40 M; Funding as PI: >$7 M; Funding as Single Investigator: >$3 M]

Current Grants

Leveraging Near-Term Quantum Computers and Machine Learning for the Simulation of Biomolecular Processes (Co-PI w/Norman Tubman and Grant Rotskoff), Wellcome Leap Quantum4Bio Program — $4.11 M, $300 K/yr to group

October 2023 - October 2026 (Based on Performance)

DEPSCoR Collaboration Grant: Probing Electron Nematicity in Multilayer Graphene Heterostructures (PI w/Jia Li), DOD DEPSCOR Collaboration Grant — $600 K, $100 K/yr to group

July 2023 - July 2025

Exascale Simulations of Quantum Materials (Co-PI w/Paul Kent), DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award — >1 M node-hours/year distributed across leadership computing machines (this is the most prestigious computing allocation award)

October 2022 - September 2024 (Won two award cycles)

LABSIP: Lowering the Activation Barrier to Success in PChem (Co-PI w/Casey Londergan), Cottrell Collaborative Grant— $25 K

September 2022 - September 2024

Broadening and Deepening the ESCIP Network: Infusing Computational Science Concepts into STEM Courses through Multidisciplinary Instructor Collaborative Networks (Co-PI w/Davit Patoyan), Cottrell Collaborative Grant— $25 K

September 2022 - September 2024

Statistics of Classical Nonlinear Dynamics by Quantum Computation (Co-PI w/Brad Marston), Brown University Seed Grant— $70 K

January 2022 - May 2023 (Extension to August 2024)

Accurate and Efficient Stochastic Electronic Structure Algorithms for Materials Design (PI), Camille Dreyfus Teacher-Scholar Award Program — $100 K for Group

May 2021 - April 2026

NSF CAREER: Finite Temperature Electronic Structure Algorithms for Predicting Material Phase Diagrams (PI), NSF Chemical Theory, Models, and Computational Methods Program — $650 K for Group

May 2021 - April 2026

Center for Predictive Simulations of Functional Materials (Co-PI), Department of Energy Computational Materials Science Centers — $140 K/yr for Group, $10 M Total

September 2020 - August 2024, Renewed September 2024 - August 2026

Pending Proposals and Rapidly Approaching Submissions

Exascale Simulations of Quantum Materials Renewal (Co-PI w/Paul Kent), DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award — >1 M node-hours/year distributed across leadership computing machines (this is the most prestigious computing allocation award)

October 2024 - September 2025

Harnessing Nonreciprocity for the Quantum Sensing of Molecules and Nanostructures (PI w/Yusong Bai and Jia Li), Keck Foundation Science and Engineer Grant — $250 K/yr for Group, $1.5 M Total

Submitted June 2024

Leveraging Homology-Based AI and Accelerated Sampling to Model Protein Conformational Distributions and Dynamics (PI), NIH R01

To Be Submitted September 2024

High-Throughput Prediction and Design of Biomimetic Polymers (PI w/Ben McDonald, Sarah Delaney, Nick Fawzi et al.), NSF Research Trainership (NRT) Program

To Be Submitted September 2024 (Rought Title)

Completed Grants

Hybrid Biofilm Semiconductor Information Systems (Co-PI), NSF SemiSynthBio Program— $150 K for Group, $1.5 M Total

September 2020 - August 2024

Stochastic Methods for Carbon Dioxide Catalysis (PI), Air Force Office of Scientific Research Young Investigator Award — $150 K/yr for 3 years

January 2020 - January 2024

RII Track-2 FEC: Harnessing the Data Revolution for the Quantum Leap: From Quantum Control to Quantum Materials (Co-I w/ Vesna Mitrovic (PI), Brad Marston, Dmitri Feldman, and Chandrasekhar Ramanathan), NSF EPSCoR Grant — $3.6 M ($25 K to Group/Year)

September 2019 - August 2023

Bridging the Time Scale in Exascale Computing of Chemical Systems (Co-I w/ Andrew Peterson, Franklin Goldsmith, Zachary Ulissi, Andrew Medford, and Matthew Willard), DOE Computational Chemical Science Research Center — *$3.4 M ($150 K to Group/Year)*

September 2018 - August 2023

Catalyst Design via Data-Enabled Quantum Chemistry and Integrating Data Science into the Chemistry Curriculum (PI), Cottrell Teacher-Scholar Award — $100 K over 2 years

June 2020 - June 2022

Confronting the Data Deluge using Quantum Machine Learning (Co-PI w/ Meenakshi Narrain and Peter Weber), Brown University Tier-2 SEED Award — *$79 K*
April 2020 - May 2022

Critical Chemistry (Co-PI w/Jesse Morin, Micah Selengut, Thedoe Nyunt, and Danielle Blum), Brown University Curriculum Development Funds for Undergraduate STEM Courses — $3 K for Team Course Development
October 2021 - June 2022

Harnessing the Data Revolution for the Quantum Leap: From Quantum Control to Quantum Materials - Postdoctoral Supplement (Co-PI w/Vesna Mitrovic and Brad Marston), NSF EPSCoR Grant — Additional Underrepresented Postdoc for Collaboration
September 2021 - September 2022

Predicting the Course of Chemical Reactions with Deep Reinforcement Learning (Co-PI w/Cancan Huang, Leonard Sprague, and Benjamin Foulon), Brown University Data Science Grant — *$15 K*
February 2020 - May 2021

Synthetic Chemical-Based Information Processing (Co-PI w/ Sherief Reda, Jacob Rosenstein, and Eunsuk Kim), NSF Eager from the CISE Division — *$600 K*
September 2019 - September 2021

Acquisition of a Maskless Lithography Tool for the Brown Nanofabrication Central Facility (Co-PI w/ Alexander Zaslavsky, Anita Shukla, Domenico Pacifici, and Derek Stein), NSF Major Research Instrumentation Grant — *$287,000 in Instrumentation*
August 2018

Chemical CPUs: Chemical Computational Processing via Ugi Reactions (PI w/ Jacob Rosenstein, Christopher Rose, Peter Weber, Sherief Reda, Eunsuk Kim, Joseph Geiser, and Jason Sello), DARPA Molecular Informatics Program — *$4.15 M*
November 2017 - January 2022

Quantum Chemistry That Scales (PI), Alfred P. Sloan Foundation — *$70 K*
June 2019 - May 2021

Genotype to Phenotype (Co-I w/ Marty Ytreberg, Daniel Weinreich, Brandon Ogbunugafor, Craig Miller, Tanya Miura, Holly Wichman, and Others), NSF EPSCoR Program — *$6 M ($1 M to Group)*
September 2017 - September 2021

Beyond DFT: Accurate Simulations of Low Dimensional Materials for Energy and Device Applications (PI w/ Can Ataca), NSF Division of Materials Research Grant — *$420,000 (All to Group, Opted to Subcontract to UMBC)*
May 2018 - April 2021

Biomolecular Condensates: Multi-Functional Liquid-Like Cellular Compartments (PI w/ Jay Tang and Nicholas Fawzi), Brown MRSEC Seed Award — *$38,000 ($17 K to Group)*

July 2018 - May 2019

Fractional PDEs for Conservation Laws and Beyond; Theory, Numerics, and Applications - Fractional Schrodinger Equation Add-On (PI), Army Research Office — *$356,000 ($50 K to Group)*
May 2018 - June 2018

High Accuracy Quantum Monte Carlo Studies of Strongly Correlated Materials (PI), Xtreme Science and Engineering Discovery Environment (XSEDE) Computing Program — *2.5 Million CPU Hours*
June 2017 - June 2018

Rhode Island American Chemical Society Project Seed Grant (PI) — *$17,500 to fund high school student internships in Chemistry at Brown, the University of Rhode Island, and Providence College*
April 2018 - August 2018, April 2019 - August 2019

Society for Science and the Public Advocate Grant (PI) — *$3 K to mentor RI underrepresented students through science competitions*
April 2017 - April 2018; *Renewed* as Lead Advocate April 2018 - April 2019; *Renewed* as Advocate April 2019 - April 2020 [Chose to Let Someone Else Be a Lead Advocate]

Quantum Monte Carlo Studies of Dipole-Bound Anions (PI), Argonne Leadership Computing Facility (ALCF) Computing Program — *5 Million CPU Hours*
April 2017 - September 2017

Unraveling Actinide Structure in the Environment: An Integrated Theoretical, Computational, and Spectroscopic Approach (PI w/ Brad Marston, Lai-Sheng Wang), Brown University Tier-2 SEED Award — *$96 K ($90 K to Group)*
February 2017 - July 2018

Quantum Simulations for Uncertainty Quantification (Co-PI), LLNL Subcontract — *$40 K for Modeling at Brown*
October 2016 - PRESENT

An Ab-Initio Study of Ion-Trap Electric Field Noise Caused by Electrode Surface Adsorbates (Co-PI), LLNL/LPS Subcontract — *$75 K for Modeling at Brown as of 2017; $60 K in 2018; $60 K in 2019*
October 2016 - PRESENT

Biogeochemical Processes at Femtomolar Concentrations and Nanometer Scales (Co-I w/ Annie Kersting, *et al.*), DOE BER Subsurface Biogeochemical Research Program — *$10 Million ($200 K for Modeling)*
August 2015 - PRESENT

Quantum Simulations for Uncertainty Quantification (Co-I w/ Miguel Morales-Silva), LLNL Laboratory Directed Research and Development Grant-Exploratory Research — *$1.5 Million*
October 2014 - July 2016

High-Pressure BCC Iron?: An AFQMC Study of the Iron Phase Diagram (PI), LLNL Grand Challenge

Tier 2 Computing Grant — *10 Million CPU-Hours*
October 2014 - PRESENT

TEACHING EXPERIENCE

University of Twente, Enschede, The Netherlands— *Graduate Electronic Structure Theory*

April 2024 - June 2024
Taught a graduate electronic structure theory course covering Hartree-Fock, Density Functional Theory, the GW Method, and Quantum Monte Carlo to roughly 10 Dutch students. Prepared lectures, led recitations, and graded exercises.

Simons Brown-UPR Winter School in Computational Physics, *The University of Puerto Rico - San Juan*

January 2024, January 2025
Delivered lectures and organized activities for UPR students interested in computational physics and ultimately pursuing research over summers in the Brown Physics Department. The Winter School was funded by the Simons Foundation.

Brown University, Providence, RI — *CH0970, Introduction to Computational Chemistry (Voluntary)*

September 2023 - December 2023
Offered an independent study for five undergraduates who requested an Computational Chemistry course in order to solidify their understanding. While informal, we covered key many-body theories, molecular dynamics, machine learning, and quantum computing.

Brown University, Providence, RI — *CH0970, Introduction to Quantum Computing (Voluntary)*

September 2022 - December 2022
Developed a new quantum computing course aimed at advanced undergraduates in collaboration with a Computer Science student interested in the topic. The course covered the quantum mechanical theory underlying key quantum algorithms, the use of Qiskit, and quantum machine learning and featured numerous hands-on programming projects. Ultimately, the course was piloted as an 8-person **independent study.**

Brown University, Providence, RI — *CH01560Q, Accelerating Chemical Discovery*

January 2022 - May 2022; January 2023 - May 2023
Developed a new course that aims to teach undergraduates in the chemical sciences how data science and computation can be used to accelerate their chemical research. The course consists of four modules on Python, Machine Learning of Molecules, Chemical Spectra, and Chemical Simulation. In its first offering, 30+ students from chemistry, applied mathematics, and chemical engineering have enrolled.

Brown University, Providence, RI — *CH1980, Critical Chemistry*

January 2022 - May 2022; January 2024 - May 2024
Offered a Department Independent Study Project (DISP) for 8 students to design a new Race, Power, and Privilege course for the Chemistry Department focused on critically analyzing the role of chemistry in modern society and how it can be reimagined. This course we developed was finally offered in 2024 and was taught to over 30 students (indicative of the interest) by my colleague, Jesse Morin.

Brown University, Providence, RI — *CH0330, Equilibrium, Rate, and Structure*

September 2020 - December 2021; September 2024 - December 2024, September 2025 - December 2025
Taught the quantum mechanics (quantum, bonding, and orbitals) portion of our primary General Chemistry course (>700 students/year) through all three semesters. With the help of undergraduates who previously took the course, developed a variety of new remote learning materials, including preparatory exercises, scaffolded exercises, research videos, interest videos, and polls to assess student progress.

Brown University, Providence, RI — *Data Science Course Design Institute Participant*

August 2021

Participated in a three-week data science course design institute aimed at faculty developing courses involving data science who may also want assistance from a Data Science Fellow. Shared experiences and advice with other faculty, and developed new materials for my *Accelerating Chemical Discovery* course to be offered Spring 2022. Collaborating with Chemical Physics concentrator and Data Science Fellow Martin Trouilloud during the Fall 2021 semester.

Brown University, Providence, RI — *Accelerating Chemical Discovery Course Design and Textbook*

May 2020 - Present

Engaged 5 undergraduate students (Zach Schapire [CH330], David Garcia [CH330], David Liu [CH1560], Satya Anisetti [CH1560], and Jacquelin Ho [CH1560]) in the course redesign of CH330 to accommodate remote teaching and the course design of CH1560, "Accelerating Chemical Discovery," which will be offered for the first time during the spring of 2021 to 20+ students. For the CH330 course design, we developed work packets on topics either most important to the class or most confusing to students. We met weekly to discuss how to construct these packets. For CH1560, we developed a series of Python notebooks to support the key modules of the course on Machine Learning, Python, Mapping Chemical Space, Computational Spectroscopy, and Atomistic Simulation.

Brown/Dartmouth Winter School on Quantum Computing and Materials, *Remote*

December 2020

Delivered lectures and developed materials on quantum computing and quantum materials for a 100+ advanced undergraduates and beginning graduate students in Chemistry and Physics at Brown and Dartmouth.

Brown University, Providence, RI — *Sheridan Center Seminar for Transformation Around Anti-Racist Teaching (START) Team Leader*

December 2020 - December 2021

Organized Chemistry team consisted of an undergraduate, a graduate student, a lecturer, and myself to successfully apply to participate in the Sheridan Center's START program. As part of the program, we will develop modules for our Chemistry labs that promote antiracism through green chemistry.

Brown University, Providence, RI — *IMSD Module on Applying for and Winning STEM Graduate Fellowships*

September 2020, 2022, 2023

Introduced students to graduate fellowships and their key components over a four session virtual module. Key topics included the variety of fellowships available, why students should apply for fellowships, what are common fellowship components, tips for CVs, strategies for writing research statements, and advice about writing personal statements. The module also featured a panel of Brown fellowship recipients from multiple Departments, multiple writing exercises, and a collection of previous successful applications from across campus. Over 30 students attended.

Brown University, Providence, RI — *Science Center Workshop on Applying to Graduate School*

September 2019, October 2020, April 2022, April 2023, April 2024

Worked with Science Center and SACNAS leadership to develop and advertise a 2-hour workshop for undergraduates about applying to graduate school. Students were taught about key graduate school application components, when to start preparing their applications, how to improve their applications, and how to ask for recommendations. Designed slides to foster discussion in close collaboration with SACNAS students, who ultimately presented them.

Brown University, Providence, RI — *SPRINT Advisor for CH330 and CH1560 Course Design*

June 2020 - August 2020

Engaged 5 undergraduate students (Zach Schapire [CH330], David Garcia [CH330], David Liu [CH1560], Satya Anisetti [CH1560], and Jacquelin Ho [CH1560]) in the course redesign of CH330 to accommodate remote teaching and the course

design of CH1560, “Accelerating Chemical Discovery,” which will be offered for the first time during the spring of 2021. For the CH330 course design, we developed worked packets on topics either most important to the class or most confusing to students. We met weekly to discuss how to construct these packets. For CH1560, we developed a series of Python notebooks to support the key modules of the course on Machine Learning, Python, Mapping Chemical Space, Computational Spectroscopy, and Atomistic Simulation.

Brown University, Providence, RI — *Anchor Course Design Institute Facilitator*

June 2020 - August 2020

Invited to serve as a facilitator for the Anchor Course Design Institute jointly sponsored by the Provost and the Sheridan Center. Alongside a larger cohort of faculty colleagues, I first troubleshot the Anchor remote course design curriculum and participated in conversations about remote pedagogy. I subsequently led group course design discussions as a facilitator for my own group.

Brown University First-Year Advisor

July 2021 - Present

Advised first-year students on their course choices with the help of a Meiklejohn peer advisor.

Brown University Biochemistry Concentration Advisor

July 2020 - Present

Advised potential and declared Biocheistry concentrators about coursework, research, and graduate school.

Brown University, Providence, RI — *CH2780, Graduate Quantum Mechanics II*

January 2018 - May 2018, January 2019 - May 2019

Developed a new graduate Quantum Mechanics course offered to roughly 20 graduate and advanced undergraduate students per year. The new course emphasizes modern electronic structure theory, largely based on Szabo’s textbook, and quantum dynamics, largely based on Nitzan’s textbook. Special topics included tensor network states and equation of motion coupled cluster theory. Course was complemented by many practical computational exercises.

Brown University, Providence, RI — *CH2770, Graduate Quantum Mechanics I*

October 2017, October 2018, October 2020

Guest lectured on the theory underlying and applications of quantum computing.

Brown University, Providence, RI — *Science Center Science Fridays Participant*

September 2016-Present

Actively participated in semimonthly Science Friday discussions on science education. Led several discussions on Engaged Learning and Computing in STEM Education.

Brown University, Providence, RI — *CH2010, Graduate Thermodynamics*

September 2016 - December 2016, September 2017 - December 2017

Taught the Chemistry and Engineering Department’s joint Thermodynamics course offered to roughly 30 graduate (and a few undergraduate) students per year. The course covered equilibrium thermodynamics, largely based on Callen’s related textbook. Special topics including nonequilibrium thermodynamics, renormalization group theory, and statistical mechanics were discussed during the end of the course.

Brown University, Providence, RI — *Scientific Computing Workshop Series Coordinator*

September 2016 - Present

Coordinated a series of workshops in collaboration with Brown Chemistry’s Computing Coordinator, Dr. David Blair, aimed at orienting Brown Chemistry and Geology graduate students with scientific computing concepts. Seminars involved short discussions followed by practicals and covered such topics as Python, Matplotlib, visualization, profiling, and high performance computing.

Brown University Chemical Physics Concentration Advisor

August 2016 - August 2020

Advised potential and declared Chemical Physics concentrators about coursework, research, and graduate school. I moreover represented the Chemical Physics concentration at the Admissions Office and Dean of the College concentration fairs once or twice per semester and attended related Dean of the College concentration advisor lunches.

SERVICE AND LEADERSHIP

To the Scientific Community

International Advisory Board Member - *WIRES Molecular Computational Science*

Committee Member - *NSF CHE Committee of Visitors*

2024

Selected by the NSF to review its programs with a panel of leading chemical researchers. Committee work entailed reviewing key NSF reports for much of the summer of 2024 and serving on an in-person panel in August of 2024.

Committee Member - *United States Defense Science Study Group*

2023 - 2026

Selected via a competitive process to serve on the United States Defense Science Study Group, which aims to familiarize leading researchers with defense science needs and to provide scientific advice to the defense community. Weeklong meetings are held roughly every few months.

Committee Member - *Lawrence Berkeley National Laboratory Review Panel*

2022

Chosen to review LBNL's portfolio of research programs. Analyzed LBNL reports and interviewed researchers.

Committee Member - *National Academies of Science, Engineering, and Medicine Committee on Identifying Opportunities at the Interface of Chemistry and Quantum Information Science*

2021 - 2023

Drafted a report used to advise NSF and DOE funding priorities detailing opportunities at the interface of chemistry and quantum information science with roughly 10 leading researchers in the United States and NASEM staff. I led the writing of Chapter 4 on modeling QIS systems on both classical and quantum computers. Meetings were held 1-2 times per month for nearly two years to complete this report.

Reviewer -

Programs: Ford Foundation Fellowship (2021-Present); NSF Chemical Models, Theory, and Computation Program (2018-Present), Cyberinfrastructure (2024-Present), Partners for Innovation Program (2023-Present), Division of Materials Science (2018-Present), and Graduate Research Fellowship Program (2017); DOE Basic Energy Sciences Division (2016-Present), INCITE High-Performance Computing Program (Panelist 2016-Present), Lawrence Berkeley National Laboratory (Panelist 2022), and LCLS Program (Panelist 2019-Present); Petroleum Research Fund (2017); Air Force Molecular Dynamics Program (2020-Present); Winston Churchill Foundation of America Scholarship Program (2014, 2018, 2019, 2022); Iota Sigma Pi Gladys Anderson Emerson Scholarship (2017-Present)

Journals: *Journal of Chemical Theory and Computation, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Physical Review B, Physical Review Letters, Chemical Engineering Journal, Physical Review A, Physical Review E, Science, Nature, Chemical Communications, Chemical Science, Nature Computational Science, Nature Communications, Proceedings of the National Academy of Science*

Telluride Summer School on Stochastic Approaches to Electronic Structure — *Instructor*

August 2016 - PRESENT

Designed and lectured at the 2017 and 2019 Telluride Schools on Stochastic Approaches. I developed the curriculum, including hours of practical exercises and solutions, with the help of four other experts on stochastic approaches. I delivered a full day of lectures on Auxiliary Field Quantum Monte Carlo to a class of thirty PhD students and postdocs.

Sabbatical Host — *Maricris Mayes (UMass Dartmouth)*

August 2021 - June 2022

To the Larger Community

Rhode Island ACS SEED Program — *Co-Coordinator*

December 2017- PRESENT

Organized this year's Rhode Island ACS Seed Program (to be combined with the Advocate Program) with the help of the Rhode Island local ACS Chapter and other faculty from the University of Rhode Island and Brown.

Leadership Alliance — *Poster Judge and Mentor*

July 2017 - PRESENT

Judged posters and networked with Leadership Alliance students at its Leadership Alliance National Symposium. Mentored Carson Cole, a Leadership Alliance student from rural Idaho, during the Summer of 2018.

Society for Science and the Public Advocate — *Science Research Competition Mentor*

April 2017 - PRESENT

Named one of thirty or so Society for Science and the Public Advocates nationally based upon my ongoing science outreach efforts in 2017 and appointed one of five Lead Advocates in 2018. As part of the Advocate Program, I am in charge of organizing science mentoring for underrepresented high school students across Rhode Island.

Rhode Island Science and Engineering Fair (RISEF) — *Judge*

February 2017 - PRESENT

Judged ten middle school and high school submissions at the Rhode Island Science and Engineering Fair. I entered my own "school" as part of the Advocate Program at the RISEF in 2018 and recruited more than 20 Chemistry students to judge this past year.

Chemistry STEM Outreach Day — *Speaker and Co-Organizer*

January 2016 - PRESENT

Helped organize the Chemistry Department STEM Outreach Day, which brings several classes of high school students to campus to learn about chemistry, college, and science careers. I have been in conversations with the Dean of the College to expand this day across campus in future years.

Lawrence Livermore National Laboratory Ambassador to the HBCUs — *Speaker*

April 2015 - April 2016

Presented research and recruitment talks at HBCUs including Prairie View University and Morehouse College. I also mentored several HBCU students in my group at Livermore.

Brown Alumni Association — *Chair, East Bay Alumni Interviewing Committee*

June 2015 - April 2016

Interviewed applicants to Brown and organized alumni to meet our regional interview needs.

Lawrence Livermore National Laboratory, Livermore, CA — *President, Lawrence Livermore Postdoc Association*

June 2015 - March 2016

Presided over the Lawrence Livermore Postdoc Association, a body of over 150 postdoctoral associates at the lab. As part of the office, I ran the postdoc council, organized social outings, postdoc coffee hours, and informational Brown Bag lunches, and developed the LabList website designed to link postdocs with time to offer to staff members in need of assistance.

Lawrence Livermore National Laboratory, Livermore, CA — *Organizer, Berni Alder 90th Birthday Symposium*

January 2015 - PRESENT

Planned the Berni Alder 90th Birthday Symposium, which was held at LLNL on August 20th, 2015. As part of the planning, I invited and hosted over 20 world-renowned speakers, solicited for and edited manuscripts to be included in the concomitant World Scientific volume, and worked with management to secure funding for the event.

Lawrence Livermore National Laboratory, Livermore, CA — *Coordinator, Lawrence Fellowship Symposium*

August 2014

Brought Lawrence Fellows past and present together for a day of talks to foster community among Lawrence Fellowship recipients.

Columbia University, New York, NY — *President, Women in Science at Columbia*

June 2011 - May 2013

Led the campus's largest student group of over 250 women in science. During my tenure, I helped plan a monthly lecture series, managed a yearly campus symposium on women's issues, recruited for and assisted with our annual Take a Girl to College and Girls' Science Day events, and ran our Science on Saturdays program.

Columbia University, New York, NY — *President, Physical Chemistry Seminar Series*

June 2010 - May 2011

Coordinated the Chemistry Department's twice monthly physical chemistry seminar series, which entailed inviting and hosting speakers from a variety of areas and organizing related social events.

To the Brown Community

Brown Presidential Scholars Program — *Faculty Advisor*

August 2024 - PRESENT

Advised the 2024 cohort of Brown Presidential Scholars, which consists of students from the incoming class selected based upon their socioeconomic status and promise as future scholars.

Churchill College-Brown University Reverse Scholar Exchange — *Coordinator*

January 2023 - PRESENT

Organized the first reverse exchanges of Churchill College, Cambridge undergraduates to the Brown Physical Science Departments. The process involves screening applicants, matching students with labs, and mentoring students during their stays. 5 scholars have been exchanged so far.

Brown University CHIPS Act Committee — *Member*

January 2023 - September 2023

Served on the Brown CHIPS in Science Act Committee charged with developing Brown's contributions to Rhode Island's CHIPS Act proposals.

Brown University Faculty Leadership Program— *Inaugural Member*

August 2022 - May 2023

Named one of 15 Brown faculty to participate in its inaugural research and administrative leadership trainingprogram, which met for an afternoon each month.

Brown University College Curriculum Committee — *Member*

August 2022 - PRESENT (on sabbatical 2023-2024 school year)

Reviewed and refined course proposals and set goals and tone for the overall college curriculum.

Brown University Chemistry Department Fundraising and Alumni Relations Committee — *Chair*

August 2022 - PRESENT

Chaired the Department committee charged with organizing outreach and fundraising endeavors. Set fundraising priorities and worked with Advancement to establish Department fundraising mechanisms.

Brown University Chemistry Department Faculty Searches

Physical Chemistry: Member, August 2021 - April 2022

Computational Chemistry: Chair, July 2022 - April 2023, July 2024 - April 2025

Reviewed applications, interviewed candidates, and assisted with recruitment.

Brown University Chemistry Department Recruiting Committee — *Co-Chair*

August 2016 - PRESENT

Organized the Chemistry Department's Recruitment efforts alongside Prof. Robinson. These efforts included visiting a number of area schools (such as UMass Dartmouth, URI, RIC, Kean University, and Brooklyn College), scheduling Webex Information sessions for interested students, and representing Brown at several national conferences (such as the Spring and Fall 2017 ACS meetings, SACNAS, and the Leadership Alliance National Symposium). As a result of these efforts, the number of students who matriculated during the Spring of 2017 exceeded department expectations by 50%.

Brown University Undergraduate Teaching and Research Assistantship (UTRA) — *Mentor*

August 2016 - PRESENT

Mentored four undergraduates (MinSik Cho, Daniel Choi, David Mayans, and Batia Friedman-Shaw) at different points in their science studies through the summer UTRA program. Worked closely with these students to craft projects of interest to them and to teach them fundamental research and communications skills. Remain in contact with all of these students, some of whom have worked in my group for years and two of whom have published papers with my group.

Brown University Diversity and Inclusion Oversight Board — *Member*

September 2018 - PRESENT

Participated in monthly board discussions and drafted an annual memo aimed at steering the University's diversity and inclusion initiatives.

Brown University Goldwater and Churchill Committees — *Chair*

December 2018 - PRESENT

Chaired the Brown University Goldwater Selection Committee by organizing rounds of review and mentoring applicants. Increased percentage of Brown nominees receiving fellowship dramatically during tenure. The Goldwater Scholarship is the highest national honor for American STEM undergraduates.

Brown University Dean of the Faculty Search Committee — *Member*

December 2021 - PRESENT

Assisted in the search and identification of a new Brown University Dean of the Faculty as part of a cross-campus committee chaired by the Provost.

Brown University Rhodes, Marshall, Mitchell, and Schwartzmann Committees — *Mentor*

September 2016 - PRESENT

Selected students to be nominated by Brown to compete in these national fellowship competitions. Read applications,

served on mock interview panels, and mentored students on how to improve their applications.

Brown University Data Science Initiative Advisory Board

August 2019 - PRESENT

Advises Brown's Data Science Initiative regarding programming, speakers, and curriculum.

Brown University Research Computing Advisory Committee

August 2018 - PRESENT

Led the High Performance Computing subgroup, which meets twice per semester with the charge of drafting explicit recommendations about HPC for the Brown Center for Computation and Visualization.

Brown University Chemistry Department Physical Chemistry Graduate Student Mentoring

August 2017 - PRESENT

Mentored a cohort of roughly 10 graduate students per year through their first year in graduate school at Brown. I specifically assisted students with course selections and advised them on how best to choose research groups.

Brown University Salomon Award Committee — *Referee*

January 2017 - PRESENT

Reviewed applications for Brown's internal grants.

Brown University Molecular and Cell Biology (MCB) Graduate Trainer

June 2020 - Present

Advised MCB graduate students and participated in MCB events.

Initiative to Maximize Student Development T32 Trainer

July 2020 - Present

Assisted with the IMSD program, mentored IMSD students, and contributed to IMSD grant proposals.

Brown University Chemistry Career Series

June 2020 - Present

Helped organize a speaker series that features industry professionals and alumni willing to share their career advice with Chemistry and other graduate students.

Brown Chemistry Department PhD Thesis Committees — *Member*

May 2017 - PRESENT

Current

- Yash Lokare (Coley-O'Rourke Group, PhD 2029)
- An Li (Bai Group, PhD 2029)
- Haoteng Sun (Bai Group, PhD 2029)
- Alexander Lackey (Peterson Group, PhD 2029)
- Changye Zhang (Bai Group, PhD 2029)
- Ken Hong (Bai/Chen Groups, PhD 2028)
- Natalie Warren (Sprague-Klein Group, PhD 2028)
- Stephen Marriott (Kim Group, PhD 2028)
- Camila Molina Roca (Lisi Group, PhD 2027)
- Jisoo Kim (Wang Group, PhD 2026)
- Siddha Sharma (Goldsmith Group, PhD 2026)
- Vinnie Widjaja (Lisi Group, PhD 2026)
- Hyun Wook Choi (Wang Group, PhD 2025)
- John Pham (Kim Group, PhD 2025)

Previous

- Dawei Si (Stratt Group, PhD 2023)
- Lingyu Ma (Weber Group, PhD 2024)
- Hanwen Gao (Wang Group, PhD 2024)
- Mia Zhang (Wang Group, PhD 2023)
- Eleftherios Mainas (Stratt Group, PhD 2023)
- Stephen Kocheril (Wang Group, PhD 2022)
- Nathan Goff (Weber Group, PhD 2022)
- Asami Odate (Weber Group, PhD 2022)
- Catherine Machniki (Wong Group, PhD 2022)
- Yichen Chai (Stratt Group, PhD 2022)
- Chenhui Qian (Wang Group, PhD 2021)
- Rong Cong (Mitrovic Group, PhD 2021)
- Weijia Chen (Wang Group, PhD 2022)
- Xi Chen (Peterson Group, PhD 2022)
- Cheng Zheng (Peterson Group, PhD 2022)

- Aaron Danilack (Goldsmith Group, PhD 2021)
- Qingyu Ye (Williard Group, PhD 2021)
- Xi Chen (Goldsmith Group, PhD 2019)
- Jennifer Ruddock (Weber Group, PhD 2019)
- Elianna Isaacs (Rose-Petruck Group, MS 2019)
- Kat Stephan (Rose-Petruck Group, PhD 2019)
- Vale Cofer-Shabica (Stratt Group, PhD 2018)
- Yan Zhao (Stratt Group, PhD 2018)
- Alireza Korshidi (Peterson Group, PhD 2017)
- Xuan Xu (Weber Group, PhD 2021)

Brown University Chemistry Department DUG Co-Advisor

August 2016 - August 2019

Supervised the Chemistry Department Undergraduate Group, a group of twenty or so undergraduate concentrators that meets throughout the school year to foster community among chemistry majors. Alongside one other faculty advisor, I oversaw and provided advice to the group about how best to plan their events.

Brown University Chemistry Department Scientific Computing Workshops — *Co-Coordinator*

August 2016 - PRESENT

Coordinated a series of workshops in collaboration with Brown Chemistry's Computing Coordinator, Dr. David Blair, aimed to orient Brown Chemistry and Geology graduate students with scientific computing concepts. Seminars involved short discussions followed by practicals and covered such topics as Python, Matplotlib, visualization, profiling, and high performance computing.

Brown University Chemistry and Physics Department Colloquia — *Speaker Host*

August 2016 - PRESENT

Hosted a number of speakers for Brown Chemistry Department Colloquia, the DIAC Seminar Series, and Physical Chemistry Tea Sessions, as well as the Physics Department Condensed Matter and Biophysics Colloquia. Hosted speakers include Ainissa Ramirez (Independent Author), Chris Hendon (University Oregon), David Wolpert (Santa Fe Institute), Daniel Zuckerman (University of Oregon), Malika Jeffries-El (BU), Rigoberto Hernandez (JHU), Ken Jordan (UPitt), Marcia Lester (UPenn), Robert Best (NIH), Nandini Ananth (Cornell), Matthew Reuter (Stony Brook), Laurie Butler (University of Chicago), Yevgeny Bar Lev (Columbia), Anders Sandvik (Boston University), Benjamin Savitzky (Cornell), Bill Wilson (Harvard), Catherine Drennan (MIT), Joseph Subotnik (UPenn), Heather Kulik (MIT), Carlos Jimenez-Hoyos (Wesleyan), Ksenia Bravaya (Boston University), and Toru Shiozaki (Northwestern).

Brown Quantum/Molecular Computing Research Workshop

August 2018 - March 2019

Organized quantum/molecular computing research workshop scheduled for April 2019 aimed at familiarizing key figures and companies in the field with ongoing research in this area at Brown.

SELECTED RECENT PRESS

https://www.brown.edu/news/2025-06-25/testimony
https://www.quantamagazine.org/new-ai-tools-predict-how-lifes-building-blocks-assemble-20240508/
https://www.chemistryworld.com/news/proteins-with-multiple-structures-open-up-alphafolds-black-box/4020210.article
https://www.brown.edu/news/2024-03-27/protein-mod

https://www.haverford.edu/college-communications/news/casey-londergan-and-colleagues-win-cottrell-scholars-collaborative-award
https://www.brown.edu/news/2022-03-24/venture-prize
https://www.popsci.com/science/brilliant-scientists-2021/
https://www.alfa.com/en/chemistry-podcasts/
https://rescorp.org/cottrell-scholars/2020-cottrell-scholars
https://cen.acs.org/people/profiles/Talented-12/97/i33
https://www.nature.com/articles/d41586-019-02070-0
https://phys.org/news/2019-07-molecular-thumb-digital-images-metabolite.html
https://today.brown.edu/announcements/119152?utm_source=todayAtBrown&utm_medium=email&utm_campaign=All%20Staff
https://news.brown.edu/articles/2018/01/chemcpus
https://www.brown.edu/academics/chemistry/news/2018/04/brown-advocate-program-pilots-2017-18-mentors-5-high-school-students-participate-state
https://spectrum.ieee.org/nanoclast/computing/hardware/test-tube-hard-drives-compute-with-chemicals
https://www.wired.com/story/darpa-wants-to-build-an-image-search-engine-out-of-dna/
http://ripr.org/post/brown-researchers-join-study-understand-changing-viruses
http://news.brown.edu/articles/2017/08/phenotypes
https://www.societyforscience.org/advocate-grant
https://www.scientificamerican.com/article/punch-card-dna-could-mean-cheaper-high-capacity-data-storage/