Brenda M. Rubenstein, Ph.D.

Associate Professor of Chemistry and Physics

Brown University

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(Last Updated January 2024)

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 predicted how beta-lactamase, an enzyme involved in drug resistance, evolves. Other past and recurring research interests include problems in computational biology and neuroscience, data science, information theory, computational linear algebra, stochastics, and condensed matter physics. We frequently collaborate with experimentalists to realize our theories regarding quantum materials, quantum sensing, and alternative computing strategies.

APPOINTMENTS

Brown University, Providence, RI — *Associate Professor of Chemistry and Physics*

January 2022 - Present, 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

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. 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. *Accepted for Phys. Chem. Chem. Phys.* (2024). arXiv:2308.05310. [Electronic Structure]
2. [$]Monteiro da Silva, G., Cui, J., Dalgarno, D., Lisi, G., and *[#]**B.M. Rubenstein.** Predicting Relative State Populations of Protein Conformations without a Physics Engine Using AlphaFold 2. *Accepted for Nature Communications* (2023). BioRxiv:10.1101/2023.07.25.550545v2. [Biophysics]
3. [$]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. *Accepted for Chemical Physics Letters* (2023). arXiv:2310.00916. [Electronic Structure]
4. [$]Staros, D., Ganesh, P., and *[#]**B.M. Rubenstein.** A First-Principles Study of Bilayer 1T'-WTe2/CrI3: A Candidate Topological Spin Filter. *Accepted for npj Spintronics* (2023). arXiv:2308.06415. [Electronic Structure]
5. DiScala, M.F., [$]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]

6. Shen, M., [$]Afshar, A., Sinai, N., Guan, H., Harris, C., **Rubenstein, B.M.,** and S. Sun. Tuning Pd Catalytic Selectivity on Intermetallic B2-CuPd@Pd Core/Shell Structures for High-Performance Polymer Synthesis. *ACS Nano,* **18(1):** 178-185 (2024). [Electronic Structure]
7. Baiz, C.R., Berger, R.F., Donald, K.J., de Paula, J.C., Fried, S.D., [#]**Rubenstein, B.M.,** Stokes, G.Y., Takematsu, K., and C. Londergan. Lowering Activation Barriers to Success in Physical Chemistry (LABSIP): A Community Project. *J. Phys. Chem. A,* **128(1)**: 3-9 (2024). [Education]
8. [$]Shen, T., Barghati, H., [$]Yu, J., Del Maestro, A., and *[#]**B.M. Rubenstein.** A Stable, Recursive Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble: Applications to Thermometry and the Hubbard Model. *Phys. Rev. E*: **107**, 055302 (2023). arXiv:2212.08654. [Electronic Structure]
9. Agiza, A., Oakley, K., Rosenstein, J., **Rubenstein**, **B.M.,** Kim, E., Riedel, M., and S. Reda.Digital Circuits and Neural Networks Based on Acid-Base Chemistry Implemented Using Robotic Fluid Handling. *Nature Communications,* **14:** 496 (2023). [Molecular Computing]
10. [$]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]
11. Li, S., Patel, J. S., Crabtree, A., [$]Yang, H., **Rubenstein**, **B.M.,** Lund-Andersen, P., Ytreberg, F. M., and P.A. Rowley. Defining the HIV Capsid Binding Site of Nucleoporin 153. *mSphere,* **7(5)**: e00310-22 (2022). bioRXiv:2022.05.06.490988v1. [Biophysics]
12. [$]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]
13. [$]Monteiro da Silva, G., [$]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]
14. Tang, W.-S., [$]Monteiro da Silva, G., Kirveshlahti, H., [$]Skeens, E., [$]Feng, B., Sudijono, T., Yang, K., Mukherjee, S., *[#]**Rubenstein, B.M**., and L. Crawford (Dual Corresponding Authors). A Topological Data Analytic Approach for Discovering Biophysical Signatures in Protein Dynamics. *PLoS Comput Biol.* **18(5)**: e1010045 (2022). bioRXiv:10.1101/2021.07.28.454240. [Biophysics]
15. [$]Foulon, B., Ray, K., Kim, C., [$]Liu, Y., *[#]**Rubenstein**, **B.M.**, and V. Lordi (Dual Corresponding Authors). 1/w Electric-Field Noise in Surface Ion Traps from Correlated Adsorbate Dynamics. *Phys. Rev. A,* **105**, 013107 (2022). arXiv:2107.01177. [Alternative Computing]
16. Lai, J., [$]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]
17. [$]Staros, D., Hu, G., [$]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]
18. 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]
19. [$]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]
20. 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]

21. 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]
22. $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]
23. $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]
24. 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]
25. 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]
26. $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]
27. $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]
28. 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]
29. 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]
30. $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]
31. 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]
32. $Foulon, B. L., $Liu, Y., Rosenstein, J. K., and *#**B.M. Rubenstein.** A Language for Molecular Computation. *Chem*, **5**, 306-319 (2019). [Alternative Computing]
33. 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]
34. 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]
35. $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]

36. 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]
37. $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]
38. 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]
39. 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]
40. $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]
41. $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]
42. 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]
43. 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]
44. 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]
45. 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)*
46. ***#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]
47. $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

48. ***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]
49. ***#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]
50. ***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]
51. ***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

52. 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. *Submitted to Nature Computational Science (Review)* (2024). [Electronic Structure]
53. [$]Iyer, G., [+]Whelpley, N., Tiihonen, J., Krogel, J.T., Kent, P.R.C., and *[#]**B.M. Rubenstein.** Force-free Identification of Minimum-Energy Pathways and Transition States forSstochastic Electronic Structure Theories. *Submitted to the Journal of Chemical Theory and Computation* (2024). [Electronic Structure]
54. [$]Kabengele, T., [$]Lokare, Y., Marston, J.B., and *[#]**B.M. Rubenstein.** Modeling Stochastic Chemical Kinetics on Quantum Computers. *Submitted to Quantum Science and Technology* (2024). [Electronic Structure and Alternative Computing]
55. [$]Lokare, Y.,[+$]Wei, Dingding, [+]Chan, L., ***[#]Rubenstein, B.M,** and J.B. Marston. Steady-State Statistics of Classical Nonlinear Dynamical Systems from Noisy Intermediate-Scale Quantum Devices. *Submitted to Quantum Science and Technology* (2024). [Electronic Structure and Alternative Computing]
56. [$]Monteiro da Silva, G., [+]Lam, K., Dalgarno, D., and *[#]**B.M. Rubenstein.** Mutations in a Human Kinase Cause Drug Resistance by Shifting Conformational State Distributions. *Submitted to PLOS Computational Biology* (2024). [Biophysics]
57. Khan, A.,[$] Vaish, P., [$]Pang, Y., [+]Kowshik, N., Chen, M.S., Clark, B., ***[#]Rubenstein, B.M.**, and N.M. Tubman. Molecular Dynamics on Quantum Hardware through Machine Learning. *Submitted to PRX Quantum* (2024). [Electronic Structure and Alternative Computing]
58. [$]Wang, L. and *[#]**B.M. Rubenstein.** Sparse Full Configuration Interaction. *Submitted to the Journal of Chemical Theory and Computation* (2023). [Electronic Structure]
59. [$]Staros, D., Gasperich, K., Annaberdiyev, A., Benali, A., Ganesh, P., and *[#]**B.M. Rubenstein.** Exciton Binding Energies in Monolayer CrI_3 from Diffusion Monte Carlo. *Submitted to J. Chem. Phys.* (2023). [Electronic Structure]
60. [$]Foulon, B., [$]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]
61. [$]Shen, T., Barghati, H., Del Maestro, A., and *[#]**B.M. Rubenstein.** Disentangling the Physics of the Attractive Hubbard Model via the Accessible and Symmetry-Resolved Entanglement Entropies. *Submitted to Physical Review B* (2023). arXiv:2312.11746. [Electronic Structure]
62. Wolpert, D., Korbel, J., Lynn, C., Tasnim, F., Grochow, J., Kardes, G., Aimone, J., Balasubramanian, V., de Giuli, E., Doty, D., Freitas, N., Marsili, M., Ouldridge, T.E., Richa, A., Riechers, P., Roldan, E., **Rubenstein, B.M**., Toroczkai, Z., and J. Paradiso. Is Stochastic Thermodynamics the Key to Understanding the Energy Costs of Computation? *Under Review at PNAS* (2023). arXiv:2311.17166. [Alternative Computing]
63. [$]Gumus, S., Biechele-Speziale, D., Manz, K., Pennell, K., *[#]**Rubenstein, B.M.**, and Rosenstein, J. Repurposing Waste Chemicals for Sustainable and Durable Molecular Data Storage. *Under Review at ACS Omega* (2023). [Alternative Computing]

64. [$]Somani, D., Pham, J., [$]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]
65. [$]Liu, N., Ho, J., [$]Monteiro da Silva, G., [$]Daru, S., Incandela, J., Reda, S., Rosenstein, J., Larkin, J., and ***B.M. Rubenstein.** Computing Using Biofilm Oscillations. *Submitted to Natural Computing* (2022). [Alternative Computing]
66. [$]Landinez-Borda, E. and *[#]**B.M. Rubenstein.** Gaussian Processes for Finite-Size Extrapolation of Many-Body Simulations. *Submitted to J. Chem. Phys.* (2021). arXiv:2112.10334. [Electronic Structure]
67. [$]Fichera, J., Stratt, R., and ***B.M. Rubenstein.** Accelerating Equilibration via Sampling the Potential Energy Landscape Ensemble. *Submitted to J. Phys. Chem.* (2022). [Statistical Mechanics]
68. [$]Vaish, P.,[$]Shen, T.,[$]Landinez-Borda, E.,[$]Kabengele, T., and **B.M. Rubenstein.** Modern Finite Temperature Electronic Structure Theory. *Invited Review for Journal of Computational and Theoretical Chemistry* (2022). [Electronic Structure]
69. [$]Song, J.-P., [$]Sprague, L., Clay, R. T., and *[#]**B.M. Rubenstein**. High Accuracy Variational Slater-Jastrow Wave Functions for the Stochastic Gradient Algorithm. *Submitted to Phys. Rev. B* (2020). [Electronic Structure]
70. Mamikon, G., [$]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]

Books

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, 2023 Release. *https://molecularprogrammers.org/#aomp*

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

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 Fellowship — *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 TALKS (SINCE STARTING AT BROWN, JULY 2016)

1. TREX COE in Exascale Computing symposium: Bridging Quantum Monte Carlo and High-Performance Simulations, Luxembourg, February 2024.
2. **Winter School Lecturer (and Organizer):** Brown-University of Puerto Rico Winter School, January 2024.
3. QuEra Applications Group Seminar, December 2023.
4. CUNY Graduate Center Theoretical and Computational Chemistry Workshop, December 2023.

5. **Student-Invited Endowed Lecture:** Caltech University, December 2023.
6. Center for the Predictive Simulation of Functional Materials All-Hands Meeting, November 2023.
7. **Student-Invited Chemistry Alumni Fund Lecturer:** Johns Hopkins University, October 2023.
8. Brown University Quantum Computing Club, September 2023.
9. New York University Chemistry Department/Simons Flatiron Institute Colloquium, September 2023.
10. ***Keynote Speaker:*** Tapia-MolSSI Workshop in Computational Chemistry, Summer 2023.
11. ACS Fall 2023 Meeting in San Francisco Invited Speaker, August 2023.
12. NIST Artificial Intelligence in Materials Science Invited Speaker, July 2023.
13. Telluride Science Workshop on Stochastic Electronic Structure Methods, June 2023.
14. Berkeley Lab Molecular Foundry Colloquium, June 2023.
15. Pittsburgh Quantum Initiative Invited Seminar, May 2023.
16. Stony Brook University Chemistry Department Colloquium, April 2023.
17. University of Rochester Department Colloquium, February 2023.
18. ***Keynote Speaker:*** University of Western Kentucky Annual Math Sumposium, November 2022.
19. University of Tennessee Condensed Matter Physics Seminar, October 2022.
20. QMC Methods in the Next Decade, Simons Flatiron Institute, September 2022.
21. PsiK 2022 Conference, Lausanne, Switzerland, August 2022.
22. 7th International Conference on Chemical Bonding (ICCB), Hawaii, August 2022.
23. Biennial Conference on Chemical Education, Purdue, August 2022.
24. ***Keynote Speaker:*** 20th Mercury Symposium on Computational Chemistry, July 2022.
25. Chemical Physics Colloquium, Lahore University of Management Science, June 2022.
26. McGill University Theoretical Chemistry Conference, June 2022.
27. Monte Carlo and Machine Learning Approaches in Quantum Mechanics, IPAM, Los Angeles, CA, May 2022.
28. Rhode Island College Physical Science Department Colloquium, April 2022.
29. University of Colorado - Boulder Department of Chemistry Colloquium, March 2022.
30. The 1st International Workshop on Data Storage in Molecular Media (DSMM), University of Marburg, March 2022.
31. Sanibel Electronic Structure Sympmosium, February 2022.
32. Simons Collaboration on the Many Electron Problem Annual Meeting, February 2022.
33. Pacifichem, Hawaii, December 2021.
34. CUNY Graduate Center, Quantum Information in Chemistry Symposium, December 2021.
35. Queens College Department of Chemistry Colloquium, October 2021.
36. IBM Unconventional Paradigms in Computing Virtual Conference, September 2021.
37. Simons CCQ Virtual Electronic Structure Workshop, New York, NY, July 2021.
38. Complex Active and Adaptive Material Systems GRC/GRS, Ventura, CA, June 2021.
39. Quantum Effects in Condensed Phase Systems, Telluride, CO, June 2021.
40. New Frontiers in Electron Correlation Workshop, Telluride, CO, June 2021.
41. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2021.
42. University of Maryland, Chemistry Department Seminar, April 2021.
43. Predictive Synthesis and Decisive Characterization of Emerging Quantum Materials Symposium, Materials Research Society Meeting, April 2021.
44. Cornell University, Chemistry Department Seminar, April 2021.
45. Stanford University Chemistry Department Seminar, April 2021.
46. ***Student-Invited Speaker:*** Spring 2021 ACS Meeting, Pitt-CMU ACS Graduate Student Symposium, April 2021.

47. University of California, Santa Cruz, Chemistry Department Seminar, March 2021.
48. Brown/Dartmouth Quantum Computing Winter School, December 2020.
49. University of California, Los Angeles, Chemistry Department Seminar, November 2020.
50. Molecular Programming Interest Group (MolPIGS) Seminar, November 2020.
51. Brown University Data Science Initiative Faculty 2 Faculty Talk, November 2020.
52. Brandeis University Chemistry Department Seminar, November 2020.
53. University of California, Berkeley Theoretical Chemistry Seminar, October 2020.
54. Psi-K 2020 Meeting, Lausanne, Switzerland, September 2020. [*Postponed Due to COVID*].
55. 7th International Conference on Chemical Bonding, Kaui, Hawaii, August 2020. [*Postponed Due to COVID*].
56. Quantum Effects in Condensed-Phase Systems Workshop, Telluride Science Research Center, Telluride, CO, July 2020.
57. *Ab Initio* Simulations of Correlated Fermions Workshop, Kiel, Germany, July 2020.
58. Molecular and Cell Biology Graduate Program Seminar, Brown University, June 2020.
59. University of Houston Chemistry Department Seminar, June 2020.
60. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2020.
61. Electrochemical Society Meeting, Montreal, CA, May 2020 [*Canceled Due to COVID*].
62. Iona College Chemistry Colloquium, New Rochelle, NY, March 2020 [*Postponed Due to COVID*].
63. Spring 2020 American Chemical Society Meeting, Philadelphia, PA, March 2020 [*Canceled Due to COVID*].
64. American Physical Society March Meeting, Denver, CO, March 2020 [*Canceled Due to COVID*].
65. DARPA Defense Sciences Office, San Diego, CA, November 2019.
66. Caltech Department of Chemistry Colloquium, Pasadena, CA, October 2019.
67. Southwest Theoretical and Computational Chemistry Conference, Norman, OK, October 2019.
68. Texas A&M University Department of Chemistry Colloquium, College Station, TX, October 2019.
69. 2019 Utah Workshop [on Electronic Structure Theory], Park Slope, UT, September 2019.
70. University of New Haven Chemistry Colloquium, New Haven, CT, September 2019.
71. C&EN Talented 12 Recipient Symposium, ACS Fall 2019 National Meeting in San Diego, CA, August 2019.
72. Penn Conference on Theoretical Chemistry, UPenn, Philadelphia, PA, August 2019.
73. Oak Ridge National Laboratory, Oak Ridge, TN, August 2019.
74. MOLSSI School on Stochastic Approaches to Electronic Structure, Pittsburgh, PA, July 2019.
75. 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP-X) in the "Emergent Electronic Structure Methods" Track, Tromso, Norway, July 2019.
76. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2019.
77. New Frontiers in Electron Correlation Workshop, Telluride, CO, June 2019.
78. Spring 2019 ACS Meeting Symposium in Honor of Ken Jordan, Orlando, FL, April 2019.
79. Spring 2019 ACS Meeting Symposium on Modeling Dynamics in Dense Manifolds of Electronic States, Orlando, FL, April 2019.
80. APS March Meeting Symposium on Periodic Quantum Chemistry Beyond DFT, Boston, MA, March 2019.
81. University of Maryland - Baltimore County Physics Colloquium, Catonsville, MY, October 2018.
82. ***Keynote Speaker***: Quantum Monte Carlo Workshop in Honor of James Gubernatis, Los Alamos, NM, October 2018.
83. Lawrence Livermore Computational Chemistry and Materials Science Summer Institute Lecture Series, Livermore, CA, July 2018.

84. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2018.
85. ***Keynote Speaker:*** *Computing with Molecules*, Rhode Island American Chemical Society Annual Meeting, University of Rhode Island, May 2018.
86. Strongly Correlated Materials: Experiments and Computation CECAM Workshop, Tel Aviv University, Tel Aviv, April 2018.
87. Center for Computational and Molecular Biology Seminar, Brown University, Providence, RI, April 2018.
88. American Physical Society March Meeting, Los Angeles, CA, March 2018.
89. Quantum Cafe, Simons Center for Computational Quantum Physics, Flatiron Institute, New York, NY, February 2018.
90. New Vistas in Molecular Thermodynamics: Experimentation, Molecular Modeling, and Inverse Design, UC Berkeley, January 2018.
91. Boston University Physical Chemistry Seminar Series, Boston University, Boston, MA, November 2017.
92. Kean University Chemistry Colloquium. Kean University, Union, NJ, November 2017.
93. Fall Materials Research Society Meeting. Boston, MA, November 2017.
94. Brooklyn College Chemistry Colloquium. Brooklyn College, Brooklyn, NY, November 2017.
95. University of Massachusetts, Dartmouth Chemistry Colloquium. University of Massachusetts, Dartmouth, North Dartmouth, MA, September 2017.
96. Electronic Structure of Complex Chemical Systems Symposium. ACS National Meeting, Washington, DC, August 2017.
97. Stochastic Methods in Electronic Structure Theory Workshop. Telluride Science Research Center, Telluride, CO, July 2017.
98. Quantum Effects in Condensed-Phase Systems Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
99. New Frontiers of Electron Correlation Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
100. Stony Brook University Applied Mathematics Colloquium. Stony Brook University, Stony Brook, NY, April 2017.
101. Materials Issues for Quantum Computing. Materials Research Society Meeting. Boston, MA, November 2016.
102. Greater Boston Area Statistical Mechanics Meeting Table Talk. Brandeis University, Waltham, MA, October 2016.
103. Brown Applied Mathematics Department Colloquium. Providence, RI, August 2016.
104. 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 (1 Current, 8 Past)

Daniel Julian Nader, Postdoc/Fulbright Scholar, Brown — *2022-2023*

Amir Afshar, Postdoc, Brown — *2020-2022*

Ehsan Barati, Postdoc, Brown — *2017-2022*

Matthew Church, Postdoc, Brown [now Assistant Professor at the Hobart and William P. Smith Colleges] — *2019-2022*

Ravindra Nanguneri, Postdoc, Brown — *2017-2020*

Jeong-Pil Song, Postdoc, Brown [now Research Assistant Professor at University of Arizona] — *2016-2020*

Can Ataca, Postdoc, Brown [now Assistant Professor at UMBC] — *2016-2017*

Edgar Landinez-Borda, Postdoc, LLNL — *2015-2016, 2020-2021 (Returned to Group)*

Chia-Chen Chang, Postdoc, UC Davis and LLNL — *2014- 2016*

GRADUATE STUDENTS MENTORED (12 Current Full-Time Graduate Students)

Andrew Reynoso, PhD Candidate (Physics), Brown — *2024-PRESENT*

Kenneth Berard, PhD Candidate (Chemistry), Brown — *2024-PRESENT*

Alan Bidart, PhD Candidate (Chemistry), Brown — *2024-PRESENT*

Octavia Florent, PhD Candidate (Chemistry), Brown — *2023-PRESENT*

Gustavo Ramirez, PhD Candidate (Chemistry), Brown — *2023-PRESENT*

Esther Webber, PhD Candidate (Chemistry), Brown — *2022-PRESENT*

Yaoqi Pang, PhD Candidate (Chemistry), Brown — *2022-PRESENT*

Xiaohang Jia, PhD Candidate (Chemistry), Brown — *2022-PRESENT*

Tilas Kabengele, PhD Candidate (Chemistry), Brown — *2021-PRESENT*

Prateek Vaish, PhD Candidate (Chemistry), Brown — *2020-PRESENT*

Annette Lopez, PhD Candidate (Physics), Brown — *2021-PRESENT*

Gabriel Monteiro da Silva, PhD Candidate (Molecular and Cell Biology), Brown — *2020-PRESENT*

Daniel Staros, PhD Candidate (Chemistry), Brown — *2019-PRESENT*

Gopal Iyer, PhD Candidate (Chemistry), Brown — *2019-PRESENT*

Tong Shen, PhD Candidate (Chemistry and Applied Mathematics), Brown [Now a Postdoc at USC] — *2018-2023*

Cancan Huang, PhD Candidate (Chemistry), Brown [Now a Research Scientist at Applied Materials] — *2017-2022*

Benjamin Foulon, PhD Candidate (Chemical Engineering), Brown — *2017-2023*

Haobo ("Jordan") Yang, PhD Candidate (Chemistry and Computer Science), Brown [Now a Biomedical Consultant at Nuvera] — *2017-2022*

Leonard Sprague, PhD Candidate (Chemistry), Brown [Now a JET Language Fellow in Japan] — *2016-2021*

Yuan Liu, PhD Candidate (Chemistry and Electrical Engineering w/Lai-Sheng Wang), Brown [Now a Professor at NC State] — *2016-2020*

Mamikon Gulian, PhD (Applied Math w/George Karniadakis), Brown [Now The Von Neumann Fellow at Sandia National Laboratory] — *2016-2019*

Hongxia Hao, PhD Candidate (Chemistry), Brown [Now a Research Scientist at Microsoft Research Shanghai] — *2016-2019*

Marie Kirkegaard, Department of Homeland Security Graduate Fellow, LLNL — Summer *2016*

MASTERS/POST-BAC STUDENTS MENTORED

Xiaohang Jia, Masters Candidate (Physics), Brown [Now a Graduate Student in the Rubenstein Group] — *2019-2021*

Joseph Fichera, Post-Bac Student (Geophysics), Brown [Now a Graduate Student in the University of Florida Department of Physics] — *2018-2021*

Lijun Wang, Masters Candidate (Physics), Brown — *2018-2020*

Benjamin L. Davis, Masters Candidate (Electrical Engineering), Brown [Now a Graduate Student in the University of Washington Division of Engineering] — *2018-2019*

Carl Romines, Masters Candidate (Physics), Brown — *2017-2018*

Nnenna Elechi, Masters Student, Prairie View University and LLNL — Summer *2015*

UNDERGRADUATE STUDENTS MENTORED (12 Current Brown Students)

Winston Li, Brown Class of 2025 — *2022-PRESENT*

Orion Bloomfield, Brown Class of 2024 — *2022-PRESENT*

Yungeun Kim, Brown Class of 2025 — *2022-PRESENT*

Anjali Srinivasan, Brown Class of 2024 — *2022-PRESENT*

Alberto Lopez Resendiz, Brown Class of 2024 — *2022-PRESENT*

Kevin Rapp, Brown Class of 2025 — *2022-PRESENT*

Jeffrey Tejada Peralta, Brown Class of 2024 — *2022-PRESENT*

Suraj Daru, Brown Class of 2024 — *2022-PRESENT*

Conenicus Weeden, Brown Class of 2024— *2021-PRESENT*

Nicholas Liu, Biophysics Concentrator, Brown Class of 2023— *2021-PRESENT*

Noah Feng, Chemical Physics Concentrator, Brown Class of 2023— *2020-PRESENT*

Logan Dooley, Chemical Physics Concentrator, Class of 2023— *2020-PRESENT*

Minsik Cho, Chemical Physics Concentrator, Brown Class of 2020 [Now MIT Presidential Graduate Fellow] — *2016-2022 (On South Korean Military Leave, 2017-2019)*

Jungho "Daniel" Choi, Chemical Physics and Mathematics Concentrator, Brown Class of 2020 [Now Flatiron Graduate Fellow at NYU] — *2017-2022*

Bunlong Leang, Class of 2022— *2018-2022*

Joseph Cavanagh, Chemical Physics Concentrator, Brown Class of 2022 [Now Chemistry PhD Student at UC Berkeley] — *2020-2021*

Dylan Sam, Computer Science Concentrator, Brown Class of 2021 [Now Computer Science PhD Student at CMU] — *2017-2021*

Kevin Guo, Applied Mathematics Concentrator, Brown Class of 2019— *2018-2020* [Now MD/PhD Student at Stanford University]

Hersh Gupta, Molecular and Cellular Biology and Chemistry Concentrator, Brown Class of 2020 [Now MD/PhD Student at Mount Sinai] — *2017-2020*

Batia Friedman-Shaw, Physics Concentrator, Brown Class of 2022 [Now Physics PhD Student at Perimeter] — *2019*

Liyaan Miskaati, Applied Mathematics Concentrator, Brown Class of 2021 — *2018*

Heesoo Kim, Chemical Physics and Mathematics Concentrator, Brown Class of 2019 — *2017-2018*

David Mayans, Chemistry and Computer Science Concentrator, Brown Class of 2018 — *2017-2018*

Adarsh Sridhar Narayanan, Engineering-CS Concentrator, Brown Class of 2018 [Now at Microsoft] — *2016-2017*

HIGH SCHOOL STUDENTS MENTORED (4 Current)

Hannah Smith, Johnston High School — *2022*

Brian Nguyen, Gatton Academy — *2022*

Casey Lambert, Moses Brown — *2021*

Aneekah Younus, The Wheeler School — *2021-2023*

Cody Comyns, Philips Andover — *2021*

Vaibhav Duggirala (Project SEED), Moses Brown [Brown PLME Class of 2025] — *2019-PRESENT*

Vishwas Duggirala (Project SEED), Moses Brown [Brown PLME Class of 2025] — *2019-PRESENT*

Tahseen Younus, The Wheeler School [Now Undergrad at University of Illinois - Urbana-Champaign] — *2019-PRESENT*

Omar Martinez (Project SEED), Blackstone Valley Academy High School [Now at University of Rhode Island studying Computer Engineering] — *2017-2019*

VISITING UNDERGRADUATES MENTORED

Yuvraj Misra, Engineering, IIT Mandi — *2021*

Jade Kemp, Chemistry, Austin College (Leadership Alliance) — *2021*

Deepak Somani, IIT Kharagpur (IIT International Relations Cell) — *2021*

Abhikhya Tripathy, IIT Kharagpur (IIT International Relations Cell) — *2021*

Shriya Sharma, IIT Dehli — *2021*

Jenel Fraij, Applied Mathematics, Hartnell Community College (Leadership Alliance) — *2020*

Bin Liu, Materials Science, USTC — *2020*

Vinit Singh, Physics, IIT Karaghpur — *2020*

Yang Yu, Materials Science, USTC [Now at University of Michigan Theoretical Physics] — *2019*

Luke MacHale, Chemistry Major, Montana State University [Now at University of Colorado Physical Chemistry] — *2019*

Swati Bodh, Bioinformatics Major, Amity University, India — *2018*

Hang Zhang, Chemistry Major, USTC [Now at Princeton Theoretical Chemistry] — *2018*

Jorge Estrada, Physics Major, University of Cantabria— *2018*

Jessie Huang, Chemistry and Computer Science Major, Wellesley College — *2018 - PRESENT*

Carson Cole, Chemistry Major, Weber State University [Now at Rice Biophysical Chemistry] — *2018*

Xuechen Zheng, Zhejiang University [Now at Johns Hopkins Theoretical Chemistry] — *2017*

SELECTED STUDENT HONORS

Brown Open Masters Program Acceptance, Tilas Kabengele— *2023*

Brown University Blavatnik Fellow, Gabriel Monteiro da Silva — *2023*

Kwanjeong Graduate Fellowship, MinSik Cho — *2022*

Poster Prize, Progress in Many-Body Theories XXI Meeting at UNC, Tong Shen — *2022*

MIT Presidential Graduate Fellowship, MinSik Cho — *2022*

Department of Energy Science Graduate Student Research (SCGSR) Award, Daniel Staros — *2021*

Goldwater Scholarship, Joseph Cavanagh — *2021*

NASA RI Space Grant Graduate Student Fellowship, Daniel Staros — *2021*

Potter Prize for Best PhD Thesis in the Brown Department of Chemistry, Yuan Liu — *2020*

RI State Science and Engineering Fair Finalists (Top Ten), Tahseen Younus, Vaibhav Duggirala, and Vishwas Duggirala — *2020*

ACS Division of Chemical Computing Group Excellence Award for Graduate Students, Yuan Liu — *2019*

Brown Open Masters Program Acceptance, Tong Shen — *2019*

RI ACS Science Fair Award at the Rhode Island Science and Engineering Fair, Omar Martinez — *2019*

Brown University Sigma Xi Award for Research Excellence, Yuan Liu — *2019*

ACS Division of Chemical Computing Group Excellence Award for Graduate Students, Hongxia Hao — *2018*

APS/DCOMP Travel Award to the APS March Meeting, Hongxia Hao — *2018*

IBM Zerner Graduate Student Award, Hongxia Hao — *2018*

Brown University King Prize for Teaching Excellence, Leonard Sprague — *2018*

GRANTS FUNDED [Total Funding as PI, Co-PI, or Co-I: >$32,303,992; Funding as PI: >$6,052,000; Funding as Single Investigator: >$1,902,000]

Current Grants

Wellcome Leap Quantum For Bio Program: Leveraging Near-Term Quantum Computers and Machine Learning for the Simulation of Biomolecular Processes (Co-PI w/Norman Tubman and Grant Rotskoff)— $4.11 M, $300 K/yr to group
October 2023 - October 2026

DEPSCoR Collaboration Grant: Probing Electron Nematicity in Multilayer Graphene Heterostructures— $600 K, $100 K/yr to group
July 2023 - July 2025

LABSIP: Lowering the Activation Barrier to Success in PChem (Co-PI w/Casey Londergan), Cottrell Collaborative Grant— $25 K
September 2022 - September 2024

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

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) — $650 K for Group
May 2021 - April 2026

Hybrid Biofilm Semiconductor Information Systems (Co-PI), NSF SemiSynthBio Program— $150 K for Group, $1.5 M Total
September 2020 - August 2024

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

Stochastic Electronic Structure Methods for Cluster Catalysis (PI), Subcontract from the Oak Ridge Laboratory Center for Predictive Simulation of Functional Materials — $125 K/yr
September 2019 - September 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 - September 2024

Completed Grants

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

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 (AT BROWN)

Brown University, Providence, RI — *CH0970, Introduction to Quantum Computing*
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 — *Equitable Learning Inquiry Program*
January 2022 - May 2022
Designed educational interventions to ensure Chemistry students with less rigorous backgrounds can succeed in our Chemistry sequence as part of the equitable learning inquiry program, organized by the Sheridan Center. Also, learned from colleagues in the Physical and Biological Sciences about the equity issues they face in their classrooms and their interventions.

Brown University, Providence, RI — *CH0156oQ, Accelerating Chemical Discovery*
January 2022 - May 2022
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
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.

Brown University, Providence, RI — *CH0330, Equilibrium, Rate, and Structure*
September 2020 - December 2021
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 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/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 comprised 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

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

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 — *SRPINT 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 off of Szabo's textbook, and quantum dynamics, largely based off of of 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 off of 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 - *National Academies of Science, Engineering, and Medicine Committee on Identifying Opportunities at the Interface of Chemistry and Quantum Information Science* (2021-2023)

Reviewer -

Programs: National Academies of Science, Engineering, and Medicine Committee on Identifying Opportunities at the Interface of Chemistry and Quantum Information Science (2021-Present), Ford Foundation Fellowship (2021-Present), NSF Chemical Models, Theory, and Computation Program (2018-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, Science, Nature, Chemical Communications, Chemical Science, Nature Computational 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

Cottrell Scholars Diversity, Equity, and Inclusion Committee— *Member*

July 2020- PRESENT

Participated and led meetings of Cottrell scholars in Departments across the nation interested in exchanging ideas regarding diversity, equity, and inclusion.

Cottrell Scholars 2021-2023 Northeast Corridor Meetings— *Organizer*

July 2020- PRESENT

Helped organize the 2021-2023 Cottrell Scholars Northeast Corridor Meetings with a cohort of other Northeastern Cottrell Scholars.

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 University Faculty Leadership Program— *Inaugural Member*

August 2022 - PRESENT

Named one of 15 Brown faculty to participate in its inaugural research and administrative leadership training program.

Brown University College Curriculum Committee — *Member*

August 2022 - PRESENT

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 202

Computational Chemistry: Chair, July 2022 - April 2023

Reviewed applications, interviewed candidates, and assisted with recruitment.

Brown University Chemistry Department Diversity and Inclusion Action Committee — *Chair*

August 2016 - PRESENT

Chaired the Brown University Chemistry Department Diversity and Inclusion Action Committee. With the help of many committed graduate students, faculty, and lecturers, organized monthly meetings, invited and hosted an array of diverse speakers, conducted graduate student climate surveys, developed an undergraduate climate survey, and acted on students' concerns about underrepresented populations within the Chemistry Department.

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 Assistanceship (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

September 2018 - PRESENT

Participated in board discussions and drafted documents 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 15 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 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

- Jisoo Kim (Wang Group, PhD 2026)
- Hyun Wook Choi (Wang Group, PhD 2025)
- John Pham (Kim Group, PhD 2025)
- Hanwen Gao (Wang Group, PhD 2024)
- Mia Zhang (Wang Group, PhD 2023)
- Lingyu Ma (Weber Group, PhD 2023)
- Eleftherios Mainas (Stratt Group, PhD 2023)
- Dawei Si (Stratt Group, PhD 2023)
- Weijia Chen (Wang Group, PhD 2022)
- 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)

Previous

- 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.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/