

# Brenda M. Rubenstein, Ph.D.

## *Joukowsky Family Assistant Professor of Chemistry*

### *Brown University*

**brenda\_rubenstein@brown.edu**

**603.661.2160**

*(Last Updated October 2020)*

#### 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 solids in the post-DFT era (Electronic Structure); 2) designing new molecular and quantum computing techniques and algorithms (Molecular 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 showed 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, computational linear algebra, stochastics, and condensed matter physics.

#### APPOINTMENTS

**Brown University**, Providence, RI — *Joukowsky Family Assistant Professor of Chemistry*

Assistant Professor, July 2016 - June 2020; Joukowsky Family Assistant Professor, July 2020 - Present

**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 2013

#### EDUCATION

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

September 2008 - July 2013

Advisor: Prof. David Reichman

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

October 2007 - August 2008

Advisors: Prof. Mark Miller, Prof. Daan Frenkel

**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

Summer Research Advisors: Prof. Laura Kaufman (Columbia), Dr. Shibo Zhang (New York Blood Center Virology)

## PUBLICATIONS

### Refereed Journal Articles

1. **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).
2. **Rubenstein, B.M.**, Gubernatis, J.E., and J.D. Doll. Comparative Monte Carlo Efficiency by Monte Carlo Analysis. *Phys. Rev. E*, 82, 036701 (2010).
3. **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).
4. **Rubenstein, B.M.**, Zhang, S., and D.R. Reichman. Auxiliary-Field Quantum Monte Carlo for Bose-Fermi Mixtures. *Phys. Rev. A*, 86, 053606 (2012).

### Since Independent Career Began

**Note:** \*Denotes Main Contributor (i.e., Wrote Paper and/or Contributed Main Ideas); #Denotes PI;

§Denotes Rubenstein Student or Postdoc

5. §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]
6. \*\***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]
7. 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*)
8. 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*. [Molecular Computing]
9. 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). [Molecular Computing]
10. 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]

11. <sup>§</sup>Liu, Y., <sup>§</sup>Cho, M., and **\*#B.M. Rubenstein**. Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo. *JCTC*, 14 (9), 4722 (2018); *arXiv:1806.02848*. [Electronic Structure]
12. <sup>§</sup>Hao, H., Shee, J., <sup>§</sup>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]
13. Cai, T., Yang, H., Hills-Kimball, K., <sup>§</sup>Song, J.-P., Zhu, H., Hofman, E., Zheng, W., **Rubenstein, B.M.**, and O. Chen. Synthesis of All-Inorganic Cd<sup>2+</sup>-Doped CsPbCl<sub>3</sub> Perovskite Nanocrystals with a Dual-Wavelength Emission. *J. Phys. Chem. Lett.*, 9 (24), 7079 (2018). [Electronic Structure]
14. Ray, K., **\*Rubenstein, B.M.**, <sup>§</sup>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*. [Molecular Computing]
15. <sup>§</sup>Hao, H., Shi, H., and **\*#B.M. Rubenstein**. 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]
16. 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*. [Molecular Computing]
17. <sup>§</sup>Sprague, L., <sup>§</sup>Huang, C., <sup>§</sup>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]
18. Cong, R., <sup>§</sup>Nanguneri, R., **\*#Rubenstein, B.M.**, and V. Mitrovic. Evidence from First-Principles Calculations for Orbital Ordering in Ba<sub>2</sub>NaOsO<sub>6</sub>, a Mott Insulator with Strong Spin Orbit Coupling, from First Principles. *Phys. Rev. B*, 100 (24), 245141 (2019). [Electronic Structure]
19. Arcadia, C., Kennedy, E., Geiser, J., Dombroski, A., Oakley, K., Chen, S.L., <sup>§</sup>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). [Molecular Computing]
20. <sup>§</sup>Foulon, B. L., <sup>§</sup>Liu, Y., Rosenstein, J. K., and **\*#B.M. Rubenstein**. A Language for Molecular Computation. *Chem*, 5, 306-319 (2019). [Molecular Computing]
21. 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**. Theory of Information Storage in Molecular Mixtures. *IEEE Transactions on NanoBioScience*. [Molecular Computing]
22. Kent, P. R. C. *et al.* QMCPack: Recent Advances in Auxiliary Field and Real-Space Quantum Monte Carlo. *Accepted and Named Editor's Pick for the Journal of Chemical Physics* (December 2019). [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]
23. Cong, R., <sup>§</sup>Nanguneri, R., **\*#Rubenstein, B.M.**, and V. Mitrovic. First Principles Calculations of the EFG Tensors of Ba<sub>2</sub>NaOsO<sub>6</sub>, a Mott Insulator with Strong Spin Orbit Coupling. *J. Phys.: Cond. Mat.*, 32(40) (2020). *arXiv:1908.09014*. [Electronic Structure]
24. Hao, H., Georges, A., Millis, A. J., **\*Rubenstein, B.M.**, Han, Q., and Shi, H. Metal-Insulator and Magnetic Phase Transitions of Ca<sub>2</sub>RuO<sub>4</sub> from Auxiliary Field Quantum Monte Carlo and Dynamical Mean Field Theory. *Phys. Rev. B.*, 101, 235110; *arXiv:1911.02702*. [Electronic Structure]
25. <sup>§</sup>Yang, J., Naik, N., Patel, J. S., Wylie, C. S., <sup>§</sup>Gu, W., <sup>§</sup>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; *BIORXIV/2020/043661*. [Biophysics]
26. <sup>§</sup>Liu, Y., <sup>§</sup>Shen, T., <sup>§</sup>Zhang, H., and **\*#B.M. Rubenstein**. Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, 16(7) 4298-4314 (2020); *arXiv:2004.01194*. [Electronic Structure]

27. Yuan, D. F., <sup>§</sup>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]
28. Yuan, D. F., <sup>§</sup>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]
29. <sup>§</sup>Shen, T., <sup>§</sup>Liu, Y., <sup>§</sup>Yang, Y., and **\*#B.M. Rubenstein**. Canonical Ensemble Auxiliary Field Quantum Monte Carlo for Bosons and Fermions. *Invited and Accepted for the J. Chem. Phys. Special Issue on Frontiers of Stochastic Electronic Structure Calculations* (2020). [Electronic Structure]
30. <sup>§</sup>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. *Accepted for the Journal of the American Chemical Society* (2020). [Electronic Structure]

### Currently Under Review

31. <sup>§</sup>Song, J.-P., <sup>§</sup>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]
32. Mamikon, G., <sup>§</sup>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 (2020); arXiv:1709.09089*. [Electronic Structure]
33. Arcadia, C., Dombroski, A., Oakley, K., Chen, S.-L., Tann, H., Rose, C., Kim, E., Reda, S., **\*#Rubenstein, B.M.**, and Rosenstein, J. Chemical Image Classification with Autocatalytic Reactions. *Submitted to Philosophical Transactions A* (2020). [Molecular Computing]
34. <sup>§</sup>Liu, Y., <sup>§</sup>Foulon, B., Lordi, V., Chiaverini, J., Sage, J., and **\*#Rubenstein, B. M.** How Anomalous Heating in Ion Traps May Be Explained by Simple Dielectric Models. *Submitted to Phys. Rev. A* (2020). [Molecular Computing]
35. Kennedy, E., Geiser, J., Arcadia, C., Weber, P., Rose, C., **\*#Rubenstein, B.M.**, and Rosenstein, J.K. Secret Messaging with Endogenous Chemistry. *Submitted to Science Advances* (2020). [Molecular Computing]
36. <sup>§</sup>Foulon, B., Kim, C., <sup>§</sup>Liu, Y., Ray, K., Lordi, V., and **\*#B.M. Rubenstein**. How Molecular Adsorbate Dynamics on Realistic Surfaces Can Give Rise to 1/f Noise in Ion Traps. *Submitted to PRX* (2020). [Quantum/Molecular Computing]
37. <sup>§</sup>Sam, D., <sup>§</sup>Guo, K., Li, X., Fourches, D., and **\*#B.M. Rubenstein**. Spectral Fingerprints. *Submitted to Journal of Chemical Information and Modeling* (2020). [Molecular Computing]
38. Dombroski, A., Oakley, K., Arcadia, C., Nouraei, F., Chen, S.-L., **\*#Rubenstein, B.M.**, Rose, C., Rosenstein, J., Reda, S., and Kim, E. Parallel Arithmetic via Acetylation: A Case Study in Image Processing. *Submitted to Philosophical Transactions A* (2020).

### Currently In Preparation (Planned Submission in Next 3 Months)

39. **\*#Rubenstein, B.M.**, <sup>§</sup>Monteiro da Silva, G., <sup>§</sup>Yang, H., Patel, J.-S., Weinreich, D., and M. Ytreberg. Predicting Pheno from Geno: Leveraging Biophysical Simulations to Predict Phenotypes from Genotypes. *Editor-Invited Perspective for J. Phys. Chem. B, Due November 2020*. [Biophysics]
40. <sup>§</sup>Monteiro da Silva, G., <sup>§</sup>Leang, B., <sup>§</sup>Yang, H., <sup>§</sup>Huang, J., and **\*#B.M. Rubenstein**. The A237 Mutants of TEM  $\beta$ -Lactamase: Previously Unreported Resistance-Granting Mutations Revealed through Covalent Docking. *Invited for the International Journal of Molecular Sciences Special Issue on "New Beta-lactams, Beta-lactamase Inhibitors and Targets for Beta-lactamase Production Blockade: Powerful Allies against Multidrug-Resistant Pathogens, Due October 2020*. [Biophysics]

41. \*#**Rubenstein, B.M.** and S. Y. (Albert) Wong. Chemical Computational Supremacy: When Molecules Outperform Silicon. *To be submitted to Chemical Communications*. [Molecular Computing]
42. \$Church, M.S. and \*#**B.M. Rubenstein**. Real Time Dynamics of Correlated Fermions via Auxiliary Field Quantum Monte Carlo. *To be submitted to J. Chem. Phys.* [Electronic Structure]
43. Van Leuven, J.T., Patent, J.-S., \$Yang, J., Beard, C., Wilke, C. O., Scott, L., Knopp, K., Altman, E., Wichman, H.A., \*#**Rubenstein, B.M.**, Ytreberg, M., and Miller, C. Predicting  $\phi$ X174 Bacteriophage Infectivity Using Biophysical Models. *To be submitted to the Journal of Molecular Biology and Evolution*. [Biophysics]
44. \$Fichera, J., Stratt, R., and \*#**B.M. Rubenstein**. Accelerating Equilibration via Sampling the Potential Energy Landscape Ensemble. *To be submitted to the J. of Chem. Phys.* [Statistical Mechanics]
45. Hu, G., \$Nanguneri, R., \$Staros, D., Krogel, J., Bennett, M.C., Heinonen, O., Ganesh, P., \*#**Rubenstein, B.M.** A High-Accuracy Quantum Monte Carlo Study of the Magnetic, Charge, and Phonon Properties of Monolayer CrI<sub>3</sub>. *To be submitted to Phys. Rev. Mat.* [Electronic Structure]
46. Li, S., Patel, J.-S., Crabtree, A., \$Yang, J., Sapozhnikov, Y., \*#**Rubenstein, B.M.**, Miller, C.R., Rowley, P.A., and Ytreberg, M. Nucleoporin 153 Sequence Specificity Dictates HIV-1 Capsid Binding. *To be submitted to PLoS One* (2020).

### 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. **B.M. Rubenstein and J. Rosenstein**, Rose, C., Reda, S., Kim, S., Weber, P., Geiser, J., and J. Sello. Provisional Application Filed June 2018.
2. Encoding Information in Synthetic Metabolomes and Molecular Mixtures. **B.M. Rubenstein and J. Rosenstein**. Provisional Application Filed December 2018.

### 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.

### Theses

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

## **SELECTED HONORS AND AWARDS**

**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 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**

**Lealyn 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**

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

1. Pacifichem, Hawaii, December 2021.
2. The 1st International Workshop on Data Storage in Molecular Media (DSMM), University of Marburg, September 2021.
3. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2021.
4. Stanford University Chemistry Department Seminar, April 2021.
5. **Student-Invited Speaker:** Spring 2021 ACS Meeting, Pitt-CMU ACS Graduate Student Symposium, April 2021.
6. University of California - Los Angeles, Chemistry Department Seminar, November 2020.
7. Molecular Programming Interest Group (MolPIGS) Seminar, November 2020.
8. Brown University Data Science Initiative Faculty 2 Faculty Talk, November 2020.
9. Brandeis University Chemistry Department Seminar, November 2020.
10. UC Berkeley Theoretical Chemistry Seminar, October 2020.
11. Psi-K 2020 Meeting, Lausanne, Switzerland, September 2020. [*Postponed Due to COVID*].
12. 7th International Conference on Chemical Bonding, Kauai, Hawaii, August 2020. [*Postponed Due to COVID*].
13. Quantum Effects in Condensed-Phase Systems Workshop, Telluride Science Research Center, Telluride, CO, July 2020.
14. *Ab Initio* Simulations of Correlated Fermions Workshop, Kiel, Germany, July 2020.
15. Molecular and Cell Biology Graduate Program Seminar, Brown University, June 2020.
16. University of Houston Chemistry Department Seminar, June 2020.
17. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2020.
18. Electrochemical Society Meeting, Montreal, CA, May 2020 [*Canceled Due to COVID*].
19. Iona College Chemistry Colloquium, New Rochelle, NY, March 2020 [*Postponed Due to COVID*].
20. Spring 2020 American Chemical Society Meeting, Philadelphia, PA, March 2020 [*Canceled Due to COVID*].
21. American Physical Society March Meeting, Denver, CO, March 2020 [*Canceled Due to COVID*].
22. DARPA Defense Sciences Office, San Diego, CA, November 2019.
23. Caltech Department of Chemistry Colloquium, Pasadena, CA, October 2019.
24. Southwest Theoretical and Computational Chemistry Conference, Norman, OK, October 2019.
25. Texas A&M University Department of Chemistry Colloquium, College Station, TX, October 2019.
26. 2019 Utah Workshop [on Electronic Structure Theory], Park Slope, UT, September 2019.
27. University of New Haven Chemistry Colloquium, New Haven, CT, September 2019.
28. C&EN Talented 12 Recipient Symposium, ACS Fall 2019 National Meeting in San Diego, CA, August 2019.
29. Penn Conference on Theoretical Chemistry, UPenn, Philadelphia, PA, August 2019.
30. Oak Ridge National Laboratory, Oak Ridge, TN, August 2019.
31. MOLSSI School on Stochastic Approaches to Electronic Structure, Pittsburgh, PA, July 2019.
32. 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP-X) in the "Emergent Electronic Structure Methods" Track, Tromsø, Norway, July 2019.
33. Stochastic Approaches to Electronic Structure Theory Workshop, Telluride, CO, June 2019.
34. New Frontiers in Electron Correlation Workshop, Telluride, CO, June 2019.
35. Spring 2019 ACS Meeting Symposium in Honor of Ken Jordan, Orlando, FL, April 2019.

36. Spring 2019 ACS Meeting Symposium on Modeling Dynamics in Dense Manifolds of Electronic States, Orlando, FL, April 2019.
37. APS March Meeting Symposium on Periodic Quantum Chemistry Beyond DFT, Boston, MA, March 2019.
38. University of Maryland - Baltimore County Physics Colloquium, Catonsville, MD, October 2018.
39. **Keynote Speaker:** Quantum Monte Carlo Workshop in Honor of James Gubernatis, Los Alamos, NM, October 2018.
40. Lawrence Livermore Computational Chemistry and Materials Science Summer Institute Lecture Series, Livermore, CA, July 2018.
41. Low Scaling and Unconventional Electronic Structure Techniques Workshop, Telluride Science Research Center, Telluride CO, June 2018.
42. **Keynote Speaker:** *Computing with Molecules*, Rhode Island American Chemical Society Annual Meeting, University of Rhode Island, May 2018.
43. Strongly Correlated Materials: Experiments and Computation CECAM Workshop, Tel Aviv University, Tel Aviv, April 2018.
44. Center for Computational and Molecular Biology Seminar, Brown University, Providence, RI, April 2018.
45. American Physical Society March Meeting, Los Angeles, CA, March 2018.
46. Quantum Cafe, Simons Center for Computational Quantum Physics, Flatiron Institute, New York, NY, February 2018.
47. New Vistas in Molecular Thermodynamics: Experimentation, Molecular Modeling, and Inverse Design, UC Berkeley, January 2018.
48. Boston University Physical Chemistry Seminar Series, Boston University, Boston, MA, November 2017.
49. Kean University Chemistry Colloquium. Kean University, Union, NJ, November 2017.
50. Fall Materials Research Society Meeting. Boston, MA, November 2017.
51. Brooklyn College Chemistry Colloquium. Brooklyn College, Brooklyn, NY, November 2017.
52. University of Massachusetts, Dartmouth Chemistry Colloquium. University of Massachusetts, Dartmouth, North Dartmouth, MA, September 2017.
53. Electronic Structure of Complex Chemical Systems Symposium. ACS National Meeting, Washington, DC, August 2017.
54. Stochastic Methods in Electronic Structure Theory Workshop. Telluride Science Research Center, Telluride, CO, July 2017.
55. Quantum Effects in Condensed-Phase Systems Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
56. New Frontiers of Electron Correlation Workshop. Telluride Science Research Center, Telluride, CO, June 2017.
57. Stony Brook University Applied Mathematics Colloquium. Stony Brook University, Stony Brook, NY, April 2017.
58. Materials Issues for Quantum Computing. Materials Research Society Meeting. Boston, MA, November 2016.
59. Greater Boston Area Statistical Mechanics Meeting Table Talk. Brandeis University, Waltham, MA, October 2016.
60. Brown Applied Mathematics Department Colloquium. Providence, RI, August 2016.
61. 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 (4 Current, 4 Past)**

Amir Afshar, Postdoc, Brown — 2020-PRESENT

Ehsan Barati, Postdoc, Brown — 2020-PRESENT

Matthew Church, Postdoc, Brown — 2019-PRESENT

Ravindra Nanguneri, Postdoc, Brown — 2017-2020

Jeong-Pil Song, Postdoc, Brown — 2016-2020

Can Ataca, Postdoc, Brown (now Assistant Professor at UMBC) — 2016-2017

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

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

## **GRADUATE STUDENTS MENTORED (8.5 Full-Time Graduate Students Current)**

Cooro Harris (Chemistry w/Shouheng Sun), Brown — 2020-PRESENT

Gabriel Monteiro da Silva (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), Brown — 2019-PRESENT

Cancan Huang, PhD Candidate (Chemistry), Brown — 2017-PRESENT

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

Haobo Yang, PhD Candidate (Chemistry), Brown — 2017-PRESENT

Yuan Liu, PhD Candidate (Chemistry w/Lai-Sheng Wang), Brown — 2016-2020 [Now a Postdoc at the Harvard/MIT Center for Ultracold Atoms]

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

Hongxia Hao, PhD Candidate (Chemistry), Brown — 2016-2019 [Now a Postdoc in T. Head-Gordon's Group at UC Berkeley]

Leonard Sprague, PhD Candidate (Chemistry), Brown — 2016-PRESENT

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

### **MASTERS/POST-BAC STUDENTS MENTORED (2 Current)**

Xiaohang Jia, Masters Candidate (Physics), Brown — 2019-PRESENT

Joseph Fichera, Post-Bac Student (Geophysics), Brown — 2018-PRESENT

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

Benjamin L. Davis, Masters Candidate (Electrical Engineering), Brown — 2018-2019

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

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

### **UNDERGRADUATE STUDENTS MENTORED (4 Current Brown Students)**

Joseph Cavanagh, Chemical Physics Concentrator, Brown Class of 2022 — 2020-PRESENT

Minsik Cho, Chemical Physics Concentrator, Brown Class of 2020 — 2016-PRESENT (On South Korean Military Leave, 2017-2019)

Junggho "Daniel" Choi, Chemical Physics and Mathematics Concentrator, Brown Class of 2020 — 2017-PRESENT

Logan Dooley, Chemical Physics Concentrator, Class of 2022 — 2020-PRESENT

Rohan Gupta, Class of 2022 — 2020-PRESENT

Bunlong Leang, Class of 2021 — 2018-PRESENT

Dylan Sam, Computer Science Concentrator, Brown Class of 2021 — 2017-PRESENT

Kevin Guo, Applied Mathematics Concentrator, Brown Class of 2019 — 2018-2020

Hersh Gupta, Molecular and Cellular Biology and Chemistry Concentrator, Brown Class of 2020  
Prof. Brenda Rubenstein, Brown University

— 2017-2020

Batia Friedman-Shaw, Physics Concentrator, Brown Class of 2022 — 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 (3 Current)**

Vaibhav Duggirala, Moses Brown — 2019-PRESENT

Vishwas Duggirala, Moses Brown — 2019-PRESENT

Tahseen Younus, The Wheeler School — 2019-PRESENT

Omar Martinez, Blackstone Valley Academy High School — 2018-2019

### **VISITING UNDERGRADUATES MENTORED**

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 Theoretical Chemistry) — 2018

Xuechen Zheng, Zhejiang University (Now at Johns Hopkins Theoretical Chemistry) — 2017

## SELECTED STUDENT HONORS

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]**

**Hybrid Biofilm Semiconductor Information Systems (co-PI), NSF SemiSynthBio Program — \$150 K for Group, \$1.5 M Total**  
September 2020 - August 2023

**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

**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 2021

**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

**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 2023

**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

**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

**Implementing Quantum Simulations for the Study of Condensed Matter Physics and Quantum Chemistry Problems Using Nuclear Spins (Co-I w/ Vesna Mitrovic (PI), Brad Marston, Dmitri Feldman, and Tayhas Palmore),** DOE Materials and Chemical Sciences Research for Quantum Information Science Program — \$3.6 M (\$25 K to Group/Year)

September 2019 - September 2022

**Quantum Chemistry That Scales (PI),** Alfred P. Sloan Foundation — \$70 K

June 2019 - May 2021

**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 2022

**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

**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

**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

**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)

Prof. Brenda Rubenstein, Brown University

Full CV

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May 2018 - June 2018

**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

**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 - July 2019

**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**

## **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**

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

September 2020 - August 2021

Taught the quantum mechanics (quantum, bonding, and orbitals) portion of our primary General Chemistry course (>500 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 — 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. 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 — 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 troubleshooted 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, 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 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.

### **Stochastic Approaches to Electronic Structure Theory Summer School, Telluride, CO**

July 2017, July 2019

Developed lectures, lecture notes, and software to instruct roughly 40 PhD students from across the world about Monte Carlo methods in general and Auxiliary Field Quantum Monte Carlo in particular.

### **Prairie View University, Prairie View, TX — Guest Lecturer**

May 2015

Delivered three guest lectures on the history and applications of the Monte Carlo method in the physical sciences as part of a molecular simulation workshop aimed at preparing students from historically black colleges and universities for completing summer practicums at DOE Laboratories. In addition to delivering lectures, I also prepared a series of computational exercises for students to complete after the workshop.

### **San Ramon Valley High School Girls Who Code Club, San Ramon, CA — Instructor/Mentor**

October 2014 - October 2016

Presented weekly lectures on programming and life in computer science to high school girls interested in coding and helped them with their end-of-year project aimed at developing a personalized calendar app for students at their high school in Swift.

### **Elite Educational Institute, Fremont, CA — Science and Mathematics Instructor**

August 2014 - June 2017

Taught AP Biology, Honors Biology, SAT II Biology, AP Chemistry, Honors Chemistry, AP Physics 1 and 2, and a variety of SAT/ACT prep courses to advanced high school students in the Bay Area. Developed tailored lecture notes, exercises, review packets, and exams to accompany each class.

### **On Track Learning, Alamo, CA — STEM Tutor**

November 2013 - June 2016

Tutored middle school through college students during evenings and weekends in such areas as chemistry, physics, mathematics, economics, statistics, and neuroscience.

### **24/7 Tutors and Olympiad Academia, Livermore, CA, New York, NY — Science Fair Mentor**

August 2011 - June 2016

Mentored advanced high school students wishing to compete in the Intel and/or Siemens Competitions on their science research projects. Mentoring involved developing a meaningful project with the students as well as training and assisting them to ensure that they successfully complete their projects. Project topics ranged from computational biology to nuclear physics to quantum chemistry. Varun Venkatesh won first prize in biophysics for our project during the 2015 Bay Area Science Fair. 12 students mentored to date:

1. Kevin Koh (Academy for the Advancement of Science and Technology, 2009 – now at Seoul National University)
2. Kyung-Duk Yoon (The Salisbury School, 2013 – now at Columbia University)
3. Eugene Lee (Stuyvesant, 2014 – now at MIT)
4. Ted Lim (Blair Academy, 2014 – now at Bucknell)
5. Joshua Anh (now at Washington University)
6. Kush Rustogi (Dublin High School, 2015 - now at UC Berkeley)
7. Alex Hong (The Hotchkiss School, 2015 - now at Carnegie Mellon)
8. Thomas Choi (Philips Andover, 2016)
9. Jongyeob Lee (Stuyvesant, 2015 - now at MIT)
10. Milena Gonzalez (San Ramon Valley High School, 2016 - now at RPI)
11. Kevin Wu (Dougherty Valley High School, 2019)
12. Varun Venkatesh (The Lynbrook School, 2017)

### **24/7 Tutors, Livermore, CA — Founder, CEO, and STEM Tutor**

September 2013 - June 2016

Started my own private tutoring company that currently employs four tutors and one web designer. The company serves the Tri-Valley area, but is preparing to expand to a remote service in 2015. 150+ Bay Area clients to date.

### **Dream Acts Academy, Cresskill, NJ — STEM Tutor**

November 2011 - June 2013

Taught SAT II preparatory classes to advanced high school students from Northern New Jersey during evenings and weekends. Teaching these classes involved designing lessons and examination materials.

### **Columbia University, New York, NY — Science on Saturdays/Girls' Day of Science Organizer (WISC)**

September 2010 - June 2013

Developed lab activities to expose Harlem girls to science for both Women in Science at Columbia's weekly Science on Saturdays program and yearly Girls' Day of Science event.

### **University of Cambridge, Cambridge, UK — Chemistry Supervisor**

November 2007 - August 2008

Conducted one-on-one hour-long supervisions (required recitation sessions) for first- and second-year students from Homerton, Girton, and Churchill colleges in General, Physical, and Inorganic Chemistry.

### **Brown University, Providence, RI — Chemistry Department Tutor**

September 2004 - May 2007

Peer tutored Brown University students in chemistry courses including General and Physical Chemistry.

### **Brown University, Providence, RI — Physics Department Meiklejohn Peer Advisor**

September 2004 - May 2007

Peer advised approximately 40 incoming freshmen enrolled in Brown's Honors Mechanics course alongside Humphrey Maris and Jay Tang. Advice pertained to settling in at Brown as well as to what courses each student should take given their backgrounds.

### **Brown University, Providence, RI — Immunology (BI153) TA**

September 2005 - December 2006

TAed Bio153, Brown's largely undergraduate Immunology course for George Yap. TAing involved preparing weekly lessons, slides, and review packets for my 25-person section of the 13-week course.

## **SERVICE AND LEADERSHIP**

### ***To the Scientific Community***

**International Advisory Board Member** - WIRES Molecular Computational Science

### **Reviewer -**

**Programs:** 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), 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); Iota Sigma Pi Gladys Anderson Emerson Scholarship (2017-Present)

**Journals:** *Journal of Chemical Theory and Computation*, *Journal of Chemical Physics*, *Physical Review B*, *Physical Review Letters*, *Science*, *Nature*, *Chemical Communications*

### **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 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 Diversity and Inclusion Oversight Board**

Prof. Brenda Rubenstein, Brown University

Full CV

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 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 Biochemistry Concentration Advisor**

July 2020 - Present

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

### **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](#)

[Previous](#)

- Cooro Harris (Sun Group, PhD 2024)
- 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)
- Xi Chen (Peterson Group, PhD 2022)
- Cheng Zheng (Peterson Group, PhD 2022)
- 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)
- Qingyu Ye (Williard Group, PhD 2021)
- Rong Cong (Mitrovic Group, PhD 2021)
- Aaron Danilack (Goldsmith Group, PhD 2021)
- Xuan Xu (Weber Group, PhD 2021)
- Xi Chen (Goldsmith Group, PhD 2019)
- Jennifer Ruddock (Weber Group, PhD 2019)
- Elianna Isaacs (Rose-Petruck Group, PhD 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)

### **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 Malike 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 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.

### **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://rescorp.org/cottrell-scholars/2020-cottrell-scholars>

<https://cen.acs.org/people/profiles/Talented-12/07/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://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-dna-storage/>