

Benjamin Rudshteyn, PhD

Schrödinger Inc.
Life Science Software | Force Fields Team
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Education:

6/2016 – 5/2018	Yale University, New Haven, CT Ph.D. in Chemistry
8/2013 – 5/2016	Yale University, New Haven, CT M.S. in Chemistry
8/2009 – 5/2013	Macaulay Honors College at Brooklyn College (CUNY), Brooklyn, NY Bachelor of Science (B.S.), Chemistry Summa Cum Laude

Research Interests and Projects:

- Improvement of classical and machine-learned force fields for modeling metalloprotein-small molecule ligand binding
- Usage of approximate quantum chemical methods for drug and materials discovery projects, particularly including transition metals.
- Structure-based and ligand-based drug design.
- Identification and resolution of outliers vs. experiment including FEP binding affinities, AFQMC thermodynamic predictions, and DFT redox potentials.
- Screening and inverse design methods for catalyst and drug molecules.
- Development and application of Auxiliary Field Quantum Monte Carlo for transition metal catalysts in biology and materials science.
- Density functional theory mechanistic studies of water oxidation and CO₂ reduction catalysts and of singlet-oxygen- sensitized reactions.
- Theoretical prediction of vibrational spectroscopy.
- Identification of binding modes of anchoring groups to electrode surfaces.

Research Experience:

1/2023 – Present	Senior Scientist II Force Fields Team, Life Science Software Supervisor: Edward Harder Schrödinger, Inc., Cambridge, Massachusetts (New York, New York before December 2024)
9/2021 – Present	Senior Scientist I Force Fields Team, Life Science Software Schrödinger, Inc., New York, New York

6/2018 – 8/2021	NIH F32 Postdoctoral Research Fellow/Scientist Dr. Richard A. Friesner Theoretical Chemistry Group, Chemistry Department, Columbia University, New York, NY
2/2014 – 5/2018	National Science Foundation Graduate Research Fellow and Ph.D. Student Dr. Victor S. Batista Theoretical Chemistry Group, Chemistry Department, Yale University, New Haven, CT Thesis Title: <i>Computational Molecular Design of Electrocatalysts for Water Oxidation and Carbon Dioxide Reduction</i> Thesis Committee: Dr. Gary W. Brudvig Dr. Charles A. Schmuttenmaer (deceased)
3/2011 - 8/2013	Goldwater Scholar and Undergraduate Researcher Dr. Alexander Greer Photochemistry Group, Brooklyn College, Brooklyn, NY
Teaching Experience:	
7/2019-8/2019	Facilitator for research skills workshops on statistics, careers, and data analysis with the Engineering the Next Generation (ENG) program at Columbia
10/2015 – Present	Volunteer instructor for Yale Sprout, Columbia Splash, Rainstorm, Wave Learning Festival to high school students. Taught the following one hour courses: <ul style="list-style-type: none"> • “Chemophobia: What is a Chemical?” • “Introduction to Solar Fuels” • “Everything You Wanted to Know About Being a Scientist, but Were Too Afraid to Ask” • “Introduction to Computational Chemistry” • “The Unscientific Method: Challenges Facing Science As A Discipline” • “Introduction to Computer-Aided Drug Design” • “Chemical Origins of Life”
9/2013 – 5/2015	Teaching Fellow (TF) Chemistry Department, Yale University, New Haven, CT
References:	<ul style="list-style-type: none"> • Richard A. Friesner: raf8@columbia.edu, 212-854-7606 • Victor S. Batista: victor.batista@yale.edu, 203-432-6672. • David R. Reichman: dr2103@columbia.edu, 212-854-0469. • Shiwei Zhang: szhang@flatironinstitute.org, 646-876-5916 • Gary W. Brudvig: gary.brudvig@yale.edu, 203-432-5202. • John C. Tully: john.tully@yale.edu, 203-432-3934. • Robert H. Crabtree: robert.crabtree@yale.edu, 203-432-3925. • Alexander Greer: agreer@brooklyn.cuny.edu, 718-951-5000 x2830.
Awards and Honors:	
2/2020	NIH F32 Postdoctoral Fellowship
7/2017	Induction into full membership of Sigma Xi

7/2017	2 nd International Solar Fuels Conference Poster Award.
7/2017	2 nd International Solar Fuels-Young Conference Diversity Award.
3/2017	Yale Graduate Student Assembly Conference Travel Fund to attend National ACS Meeting at San Francisco, CA
6/2016	Travel grant to attend Excited State Processes Conference at Santa Fe, NM
3/2015	National Science Foundation Graduate Research Fellowship
5/2013	Jeanette Trum Granoff, '35, Brooklyn College Chemistry Department Graduate Award for Applied Sciences
5/2012	Dr. Franklin H. Epstein Brooklyn College Chemistry Department Scholarship Award
3/2012	Barry M. Goldwater Scholarship
5/2011	Dr. Franklin H. Epstein Brooklyn College Chemistry Department Scholarship Award
5/2011	Arnold and Ruth T. Kaufman Brooklyn College Chemistry Department Summer Research Award
5/2011 2009-2013	Brooklyn College Modern Languages Department Award Brooklyn College Dean's List
2009-2013	Macauley Honors College Scholarship

Publications:

40. Damm, W. *et al.*, OPLS5: Addition of Polarizability and Improved Treatment of Metals. *ChemRxiv.*, **2024**, DOI: 10.26434/chemrxiv-2024-2svr7
<https://doi.org/10.26434/chemrxiv-2024-2svr7>
39. Debnath, S., Neufeld, V.A., Jacobson, L.D., **Rudshteyn, B.**, Weber, J.L., Berkelbach, T.C., Friesner, R.A., Accurate Quantum Chemical Reaction Energies For Lithium-Mediated Electrolyte Decomposition and Evaluation of Density Functional Approximations. *J. Phys. Chem. A.*, **2023**, 127, 9178–9184.
<https://pubs.acs.org/doi/10.1021/acs.jpca.3c04369>
38. **Rudshteyn, B.**, Weber, J.L., Coskun, D., Devlaminck, P., Zhang, S., Reichman, D.R., Shee, J., Friesner, R.A., Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Towards Benchmark Quantum Chemistry for Transition Metals. *J. Chem. Theory Comput.*, **2022**, 18, 2845–2862.
<https://pubs.acs.org/doi/10.1021/acs.jctc.1c01071>
37. Kumar, M., Shee, J., **Rudshteyn, B.**, Reichman, D.R., Friesner, R.A., Miller, C.E., Francisco, J.S., Multiple Stable Isoprene–Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. *J. Am. Chem. Soc.*, **2020**, 142, 10806–10813.
<https://pubs.acs.org/doi/abs/10.1021/jacs.0c02360>

36. **Rudshteyn, B.**,[†] Coskun, D.,[†] Weber, J.L., Arthur, E.J., Zhang, S., Reichman, D.R., Friesner, R.A., and Shee, J., Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. *J. Chem. Theory Comput.*, **2020**, 16, 3041-3054.
<https://pubs.acs.org/doi/abs/10.1021/acs.jctc.0c00070>
35. Li, G., **Rudshteyn, B.**, Shee, J., Weber, J.L., Coskun, D., Bochevarov, A.D. and Friesner, R.A., Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. *J. Chem. Theory Comput.*, **2020**, 16, 2109-2123.
<https://pubs.acs.org/doi/abs/10.1021/acs.jctc.9b00875>
34. Ge, A.,[†] **Rudshteyn, B.**,[†] Videla, P.E., Miller, C.J., Kubiak, C.P., Batista, V.S., and Lian, T., Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. *Acc. Chem. Res.*, **2019**, 52, 1289-1300.
<https://pubs.acs.org/doi/abs/10.1021/acs.accounts.9b00001>
33. Shee, J., **Rudshteyn, B.**, Arthur, E.J., Zhang, S., Reichman, D.R. and Friesner, R.A., On Achieving High Accuracy in Quantum Chemical Calculations of 3d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. *J. Chem. Theory Comput.*, **2019**, 15, 2346-2358.
<https://pubs.acs.org/doi/10.1021/acs.jctc.9b00083>
32. Spies, J.A.,[†] Perets, E.A.,[†] Fisher, K.J.,[†] **Rudshteyn, B.**,[†] Batista, V.S., Brudvig, G.W. and Schmittenmaer, C.A. Collaboration Between Experiment and Theory in Solar Fuels Research. *Chem. Soc. Rev.*, **2019**, 48, 1865-1873.
<https://pubs.rsc.org/en/content/articlelanding/2019/cs/c8cs00819a>
31. Chang, A.M., **Rudshteyn, B.**, Warnke, I. and Batista, V.S. Inverse Design of a Catalyst for Aqueous CO/CO₂ Conversion Informed by the Ni^{II}-Iminothiolate Complex. *Inorg. Chem.*, **2018**, 57, 15474-15480.
<https://pubs.acs.org/doi/10.1021/acs.inorgchem.8b02799>
30. Clark, M.L.,[†] Ge, A.,[†] Videla, P.E.,[†] **Rudshteyn, B.**, Miller, C.J., Song, J., Batista, V.S., Lian, T. and Kubiak, C.P., CO₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. *J. Am. Chem. Soc.*, **2018**, 140, 17643-17655.
<https://pubs.acs.org/doi/abs/10.1021/jacs.8b09852>
29. **Rudshteyn, B.**, Fisher, K.J., Lant, H.M.C., Yang, K.R., Mercado, B.Q., Brudvig, G.W., Crabtree, R.H. Batista, V.S., Water-Nucleophilic Attack Mechanism for the Cu^{II}(pyalk)₂ Water-Oxidation Catalyst. *ACS Catal.* **2018**, 8, 7952-7960.
<https://pubs.acs.org/doi/10.1021/acscatal.8b02466>
28. Ge, A.,[†] Videla, P.E.,[†] **Rudshteyn, B.**, Liu Q., Batista, V.S., Lian, T. Dopant-Dependent SFG Response of Rhenium CO₂ Reduction Catalysts Chemisorbed on SrTiO₃ (100) Single Crystals. *J. Phys. Chem. C* **2018**, 122, 13944-13952.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.8b01123>

27. Ge, A.,[†] **Rudshteyn, B.**,[†] Zhu, J., Maurer, R.J., Batista, V.S., and Lian, T. Electron-Hole-Pair-Induced Vibrational Energy Relaxation of Rhenium Catalysts on Gold Surfaces. *J. Phys. Chem. Lett.* **2018**, 9, 406-412.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcclett.7b02885>
26. **Rudshteyn, B.**, Acharya, A., and Batista, V.S. Is the Supporting Information the Venue for Reproducibility and Transparency? *J. Phys. Chem. A., (B., and C.)* **2017**, 121, 9680-9681.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpca.7b11663>
25. Wu, Y.,[†] **Rudshteyn, B.**,[†] Warnke, I., Xiao, D., and Batista, V.S. Mechanistic Study of CO/CO₂ Conversion Catalyzed by a Biomimetic Ni(II)-Iminothiolate Complex. *Int. J. Quant. Chem.* **2018**, 118, e25555.
<http://onlinelibrary.wiley.com/doi/10.1002/qua.25555>
24. Hedström, S.,[†] Chaudhuri, S.,[†] La Porte, N.T., **Rudshteyn, B.**, Martinez, J.F., Wasielewski, M.R., and Batista, V.S. Thousandfold Enhancement of Photoreduction Lifetime in Re(bpy)(CO)₃ via Spin-dependent Electron Transfer from a Perylene-diimide Radical Anion Donor. *J. Am. Chem. Soc.* **2017**, 139, 16466-16469.
<http://pubs.acs.org/doi/abs/10.1021/jacs.7b09438>
23. Ge, A.,[†] Videla, P.E.,[†] Lee, G.L., **Rudshteyn, B.**, Song, J., Kubiak, C.P. Batista, V.S., and Lian, T. Interfacial Structure and Electric Field Probed by *in situ* Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling. *J. Phys. Chem. C* **2017**, 121, 18674-18682.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.7b05563>
22. **Rudshteyn, B.**, Vibbert, H.B., May, R., Wasserman, E., Warnke, I., Hopkins, M.D. and Batista, V.S. Thermodynamic and Structural Factors that Influence the Redox Potentials of Tungsten-Alkylidyne Complexes. *ACS Catal.* **2017**, 7, 6134-6143.
<http://pubs.acs.org/doi/abs/10.1021/acscatal.7b01636>
21. Wu, Y.,[†] **Rudshteyn, B.**,[†] Zhanaidarova, A., Froehlich, J.D., Ding, W., Kubiak, C.P. and Batista, V.S. Electrode-Ligand Interactions Dramatically Enhance CO₂ Conversion to CO by the [Ni(cyclam)](PF₆)₂ Catalyst. *ACS Catal.* **2017**, 7, 5282-5288.
<http://pubs.acs.org/doi/abs/10.1021/acscatal.7b01109>
20. **Rudshteyn, B.**, Negre, C.F., Oliboni, R.S., Monti, A., Chen, J., Crabtree, R.H., Rego, L.G.C. and Batista, V.S., Inferring Protonation States of Hydroxamate Adsorbates on TiO₂ Surfaces. *J. Phys. Chem. C* **2017**, 121, 11985-11990.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.7b01272>
19. Chaudhuri, S., **Rudshteyn, B.**, Prémont-Schwarz, M., Pines, D., Pines, E., Huppert, D., Nibbering, E.T. and Batista, V.S. Ultrafast Photo-induced Charge Transfer of 1-Naphthol and 2-Naphthol to Halocarbon Solvents. *Chem. Phys. Lett.* **2017**, 683, 49-56.
<http://www.sciencedirect.com/science/article/pii/S0009261417303044>
18. Chase, H.M., Chen, S., Fu, L., Upshur, M.A., **Rudshteyn, B.**, Thomson, R.J., Wang, H.F., Batista, V.S. and Geiger, F.M., Chase, Orientations of Nonlocal Vibrational Modes from Combined Experimental and Theoretical Sum Frequency Spectroscopy. *Chem. Phys. Lett.* **2017**, 683, 199-204.
<http://www.sciencedirect.com/science/article/pii/S000926141730026X>

17. La Porte, N.T.,[†] Martinez, J.F.,[†] Hedström, S., **Rudshteyn, B.**, Phelan, B.T., Mauck, C.M., Young, R.M., Batista, V.S. and Wasielewski, M.R., Photoinduced Electron Transfer from Rylenediimide Radical Anions and Dianions to Re(bpy)(CO)₃ using Red and Near-Infrared light. *Chem. Sci.* **2017**, 8, 3821-3831.
<http://pubs.rsc.org/en/content/articlelanding/2017/sc/c6sc05103k>
16. Abramova, I., **Rudshteyn, B.**, Liebman, J.F., Greer, A., Computed Regioselectivity and Conjectured Biological Activity of Ene Reactions of Singlet Oxygen with the Natural Product Hyperforin. *Photochem. Photobiol.* **2017**, 93, 626-631.
<http://onlinelibrary.wiley.com/doi/10.1111/php.12706/>
15. Shopov, D.Y., **Rudshteyn, B.**, Campos, J., Vinyard, D.J., Batista, V.S., Brudvig, G.W. Crabtree, R.H. A Full Set of iridium(IV) Pyridine-Alkoxide Stereoisomers: Highly Geometry-Dependent Redox Properties. *Chem. Sci.* **2017**, 8, 1642-1652.
<https://pubs.rsc.org/en/content/articlelanding/2017/sc/c6sc03758e>
14. Schloss, A.C.,[†] Liu, W.,[†] Williams, D.M.,[†] Kaufman, G., Hendrickson, H.P., **Rudshteyn, B.**, Fu, L., Wang, H., Batista, V.S., Osuji, C. and Yan, E.C.Y., Fabrication of Modularly Functionalizable Microcapsules Using Protein-Based Technologies. *ACS Biomater. Sci. Eng.* **2016**, 2, 1856-1861.
<http://pubs.acs.org/doi/abs/10.1021/acsbiomaterials.6b00447>
13. Fishman, Z.S., **Rudshteyn, B.**, He, Y., Liu, B., Chaudhuri, S., Askerka, M., Haller, G.L., Batista, V.S. and Pfefferle, L.D. Fundamental Role of Oxygen Stoichiometry in Controlling the Band Gap and Reactivity of Cupric Oxide Nanosheets. *J. Am. Chem. Soc.* **2016**, 138, 10978-10985.
<http://pubs.acs.org/doi/abs/10.1021/jacs.6b05332>
12. Materna, K.L., **Rudshteyn, B.**, Brennan, B.J., Kane, M.H., Bloomfield, A.J., Huang, D.L., Shopov, D.Y., Batista, V.S., Crabtree, R.H., Brudvig, G.W. Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. *ACS Catal.* **2016**, 6, 5371-5377.
<http://pubs.acs.org/doi/abs/10.1021/acscatal.6b01101>
11. Ge, A.,[†] **Rudshteyn, B.**,[†] Psciuk, B.T., Xiao, D., Song, J., Anfusio, C.L., Ricks, A.M., Batista, V.S. and Lian, T., Surface-Induced Anisotropic Binding of a Rhenium CO₂-Reduction Catalyst on Rutile TiO₂ (110) Surfaces. *J. Phys. Chem. C.* **2016**, 120, 20970-20977.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03165>
10. Ho, J.,[†] Psciuk, B.T.,[†] Chase, H.M., **Rudshteyn, B.**, Upshur, M.A., Fu, L., Thomson, R.J., Wang, H.-F., Geiger, F.M., Batista, V.S. Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal A Rotationally Fluid Adsorption State of α -Pinene on Silica. *J. Phys. Chem. C.* **2016**, 120, 12578-12589.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03158>
9. Brennan, B.J., Chen, J., **Rudshteyn, B.**, Chaudhuri, S., Mercado, B.Q., Batista, V.S., Crabtree, R.H. and Brudvig, G.W., Molecular Titanium–Hydroxamate Complexes as Models for TiO₂ Surface Binding. *Chem. Commun.* **2016**, 52, 2972-2975.
<http://pubs.rsc.org/en/content/articlelanding/2016/cc/c5cc09857b>

8. Clark, M.L., **Rudshteyn, B.**, Ge, A., Chabolla, S.A., Machan, C.W., Psciuk, B.T., Song, J., Canzi, G., Lian, T., Batista, V.S., Kubiak, C.P. Orientation of Cyano-Substituted Bipyridine Re (I) *fac*-Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. *J. Phys. Chem. C*. **2016**, 120, 1657-1665.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b10912>
7. Chen, J., Wu, K., **Rudshteyn, B.**, Jia, Y., Ding, W., Xie Z., Batista, V.S., Lian, T. Ultrafast Photoinduced Interfacial Proton Coupled Electron Transfer from CdSe Quantum Dots to 4, 4'-Bipyridine. *J. Am. Chem. Soc.* **2016**, 138, 884-892.
<http://pubs.acs.org/doi/abs/10.1021/jacs.5b10354>
6. Chase, H.M., **Rudshteyn, B.**, Psciuk, B.T., Upshur, M.A., Strick, B.F., Thomson, R.J., Batista, V.S., Geiger, F.M. Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. *J. Phys. Chem. B*. **2016**, 120, 1919-1927.
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b09769>
5. Shopov, D.Y., **Rudshteyn, B.**, Campos, J., Batista, V.S., Crabtree, R.H., Brudvig, G.W. Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. *J. Am. Chem. Soc.* **2015**, 137, 7243-7250.
<http://pubs.acs.org/doi/abs/10.1021/jacs.5b04185>
4. Li, C.,[†] Koenigsmann, C.,[†] Ding, W., **Rudshteyn, B.**, Yang, K.R., Regan, K.P., Konezny, S.J., Batista, V.S., Brudvig, G.W., Schmuttenmaer, C.A., Kim, J-H. Facet-Dependent Enhancement of Photoelectrochemical Performance in TiO₂ Nanostructures: An Experimental and Computational Study. *J. Am. Chem. Soc.* **2015**, 137, 1520-1529.
<http://pubs.acs.org/doi/abs/10.1021/ja5111078>
3. **Rudshteyn, B.**, Castillo, Á., Ghogare, A. A., Liebman, J. F., Greer, A. Theoretical Study of the Reaction Formaldehyde with Singlet Oxygen. Fragmentation of the C=N Bond, Ene Reaction and Other Processes. *Photochem. Photobiol.* **2014**, 90, 431-438.
<http://onlinelibrary.wiley.com/doi/10.1111/php.12199>
2. **Rudshteyn, B.**, Castillo, Á., Greer, A., Theoretical Study of a Nonpeptidic Polydisulfide α -Helix. *J. Sulfur Chem.* **2013**, 34, 3-6.
<http://www.tandfonline.com/doi/full/10.1080/17415993.2012.700457>
1. Kimani, S., Ghosh, G., Ghogare, A.A., **Rudshteyn, B.**, Bartusik, D., Hasan, T., Greer, A. Synthesis and Characterization of Mono-, Di-, and Tri-Polyethylene Glycol Chlorin e₆ Conjugates for the Photokilling of Human Ovarian Cancer Cells. *J. Org. Chem.* **2012**, 77, 10638-10647.
<http://pubs.acs.org/doi/abs/10.1021/jo301889s>

[†]Equal Contributions

External Oral Presentations:

3/3/2021

Yale University Energy Sciences Institute
Rudshteyn, B., Weber, J.L., Coskun, D., Zhang, S., Reichman, D.R., Shee, J., Friesner, R.A., Benchmark Quantum Chemical Calculations for Transition Metal Complexes via Auxiliary Field Quantum Monte Carlo.

11/26/2019 Flatiron Institute, Center for Computational Physics, Quantum Monte Carlo Group Meeting

10/10/2019 Yale University Physical Chemistry Club Seminar

9/13/2019 20th Anniversary Alexander Greer Research Symposium
Rudshiteyn, B., Shee, J., Coskun, D., Weber, J.L., Arthur, E.J., Zhang, S., Reichman, D.R. and Friesner, R.A.
 “Accurate Quantum Chemistry of Transition Metal Compounds using Auxiliary-Field Quantum Monte Carlo”

7/10/2017 2017 EFRC-Hub CMS Principal Investigators Meeting
Rudshiteyn, B., Materna, K.L., La Porte, N.T., Fisher, K. J., Yang, Ke.R., Hedström, S., Martinez, J.F., Kwon, G., Hong, J., Tiede, D.M., Chen, L.X., Wasielewski, M.R., Crabtree, Robert H., Brudvig, G.W., Batista, V.S.
 “The Pyridine Alkoxide Ligand Works for Water Oxidation Catalysts Both in Theory and in Practice.”

4/6/2017 2nd International Solar Fuels Conference
Rudshiteyn, B. Ge, A., Helm, M.L., Maurer, R. J., Psciuk, B.T., Song, J., Kubiak, C.P., Lian, T., Batista, V.S. “Determination of Orientation of Bipyridine Re(I) *fac*-Tricarbonyl Electrocatalysts on Au, on SrTiO₃, and on TiO₂ Surfaces Through Computational and Experimental SFG Spectroscopy”

4/4/2017 253rd American Chemical Society National Meeting San Francisco: PHYS Division
 Batista, V.S., **Rudshiteyn, B.**, Videla, P.E., Hendrickson, H.P. “Sum Frequency Generation Spectra from Density Functional Theory” (given on Victor S. Batista’s behalf)

4/3/2017 253rd American Chemical Society National Meeting San Francisco: PHYS Division
Rudshiteyn, B., Azoz, S., Ding, W., Ran, F., Askerka, M., Matula, A.J., Marinkovic, N.S., Haller, G.L., Pfefferle, L.D., Batista, V.S. “Strong Binding of CdSe Quantum Dots to Single-Walled Carbon Nanotubes”

4/3/2017 253rd American Chemical Society National Meeting San Francisco: ENFL Division
Rudshiteyn, B., Vibbert, H.B., May, R., Wasserman, E., Warnke, I., Hopkins, M.D., Batista, V.S. “Regulation of the Redox Properties of Tungsten-Alkylidyne Complexes by Ligand Design”

7/16/2016 Vibrational Spectroscopy Gordon Research Seminar

4/22/2016 Connecticut Valley Quantum Chemistry Meeting
Rudshiteyn, B. Ge, A., Clark, M.L., Psciuk, B.T., Kubiak, C.P., Lian, T., Batista, V.S. “Determination of Orientation of Bipyridine Re(I) *fac*-Tricarbonyl Electrocatalysts on Au and on TiO₂ Surfaces Through Computational SFG Spectroscopy”

3/15/2015 251st American Chemical Society National Meeting San Diego: COMP Division
Rudshiteyn, B., Chen, J., Brennan, B.J., Negre, Christian F.A., Chaudhuri, S., Mercado, B.Q., Silva, R., Monti, A., Rego, L. Brudvig, G.W., Crabtree, R.H. Batista, V.S. “Computational Exploration of How Hydroxamate Groups Bind to TiO₂ Surfaces”

5/10/2013 61st Annual Undergraduate Research Symposium of the New York Chemistry Students Association of the American Chemical Society's New York Section
Rudshiteyn, B.; Choudhury, R.; Ghosh, G.; Ghogare, A.; Bartusik, D.; Greer, A.
 “Computed Design of a PEGylated Photosensitizer Drug for the Killing of Ovarian Cancer Cells”

5/5/2012 60th Annual Undergraduate Research Symposium of the New York Chemistry Students Association of the American Chemical Society's New York Section
Rudshteyn, B.; Castillo, A.; Ghogare, A.; Greer, A.: "The Reaction of Hydrazone with Singlet Oxygen with an Aim Toward Drug-Delivery via the Photorelease of Nitroso Compounds"

5/7/2011 59th Annual Undergraduate Research Symposium of the New York Chemistry Students Association of the American Chemical Society's New York Section
Rudshteyn, B.; Castillo, A.; Ghogare, A.; Greer, A.: "The Reaction of Hydrazone with Singlet Oxygen with an Aim Toward Drug-Delivery via the Photorelease of Nitroso Compounds"

Media Coverage

- Featured in a Oak Ridge Leadership Computing Facility Highlight
<https://www.olcf.ornl.gov/2020/06/24/summit-helps-predict-molecular-breakups/>
- Featured in the ACS New Haven Local Newsletter for Activities with the Younger Chemists Committee
http://ursula.chem.yale.edu/~batista/personal/ben_in_ACS_December2015_newsletter.pdf
- Featured in advert for CUNY called "His work is a gas" in NYPost:
<http://www.pressreader.com/usa/new-york-post/20150927/282157880054919/TextView>
- Featured in the article "Chemistry Student Scores Big Prize" on the Brooklyn College website:
http://www.brooklyn.cuny.edu/web/news/bcnews/bcnews_120412.php
- Featured in the article "Searching for the Origins of Life" on the CUNY website:
<http://www2.cuny.edu/about/alumni-students-faculty/outstanding-students/os-profile/?sid=benjaminrudshteyn>

Certifications:

- 09/2024 Schrödinger Inc., New York, NY
Online Course:
 - "Visualizing Science with PyMOL 3"
- 11/2022 Schrödinger Inc., New York, NY
Online Course:
 - "Free Energy Calculations for Drug Design with FEP+"
- 12/2021 Schrödinger Inc., New York, NY
Online Course:
 - "Introduction to Computational Antibody Engineering"
- 11/2021 Coursera Inc., Mountain View, CA
 - "Machine Learning (Andrew Ng)"
- 5/2021 Schrödinger Inc., New York, NY
Online Course:
 - "High-Throughput Virtual Screening for Hit Finding and Evaluation"

11/2020 Schrödinger Inc., New York, NY
Online Course:

- “Introduction to Molecular Modeling Concepts for Polymers”

1/2020 Schrödinger Inc., New York, NY
Online Course:

- “Introduction to Molecular Modeling in Drug Discovery”

Professional Affiliations:

2011 - Present
2015-2016 American Chemical Society

- Younger Chemist’s Committee

Volunteer Activities:

03/2025 Boston Public Schools STEM Fair Judge

9/2022 – Present Mentor for Undergraduate Students, Macaulay Honors College, Graduate Students, Yale University, and junior employees at Schrödinger Inc.,

9/2020 – 8/2021 President of the Columbia University Postdoctoral Society for the Morningside/Lamont campuses, Chair of the Advocacy Subcommittee

5/2019 – 5 / 2021 Representative for Postdoctoral Research Scientists, Fellows, and Scholars in the Columbia Senate.

3/2019 – 3/2021 Judge for the New York Science & Engineering Fair (NYCSEF) and Virtual Regeneron International Science and Engineering Fair in Chemistry, Earth and Environmental Sciences, and Energy: Sustainable Materials and Design

1/2019 – 9/2020 Vice President of the Columbia University Postdoctoral Society for the Morningside/Lamont campuses

8/2017 – 5/2018 Non-Resident Graduate Fellow at Benjamin Franklin College at Yale

3/2017 – Present Reviewer for *National Science Foundation*, *The Journal of Physical Chemistry C*, *Molecular Simulation*, *Journal of Computer-Aided Molecular Design*

9/2016 – 5/2018 Co-President of YANIS: Young Associates of Newly Independent States (Russian-speaking club)

3/2016 Technical Session Presider and Undergraduate Poster Judge at the ACS Meeting

8/2015 – 12/2017 Webmaster for Joint Safety Team of the Yale Chemistry Department

6/2014 – 5/2017 Graduate Student Assembly Representative for Chemistry Department

- Participated in Summer Steering Committee to help get ready for the upcoming semester and collect general concerns from survey reports.
- Participated in Transit and Security Subcommittee with focus on lab safety.

5/2014 Yale University Science Pathways Event Guide

- Guided students and their parents between labs in the department.

5/2014-5/2018

New Haven Science Fair Judge/Team Leader

- Judged local high school team physical science projects.

Languages:

- English: Native proficiency
- Russian: Bilingual oral proficiency