Benjamin Rudshteyn, PhD

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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-learning 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 CO_2 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 9/2021 – 12/2022	Senior Scientist II Senior Scientist I Force Fields Team, Life Science Software Schrödinger, Inc., Cambridge, Massachusetts (New York, New York before December 2024)

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: *Computational Molecular Design of Electrocatalysts for Water Oxidation and Carbon Dioxide Reduction* 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: ● "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:

- Richard A. Friesner: raf8@columbia.edu, 212-854-7606
- Victor S. Batista: victor.batista@yale.edu, 203-432-6672.
- David R. Reichman: drr2103@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	2nd International Solar Fuels Conference Poster Award.

7/2017	2nd 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	Brooklyn College Modern Languages Department Award
2009-2013	Brooklyn College Dean's List
2009-2013	Macaulay 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 Schmuttenmaer, 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/CO_2 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., CO_2 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 CO_2 Reduction Catalysts Chemisorbed on $SrTiO_3$ (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.jpclett.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/CO_2 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 CO_2 Conversion to CO by the $[Ni(cyclam)](PF_6)_2$ 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 TiO_2 Surfaces. *J. Phys. Chem. C* **2017**, *121*, 11985-11190.
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., Anfuso, C.L., Ricks, A.M., Batista, V.S. and Lian, T., Surface-Induced Anisotropic Binding of a Rhenium CO_2-Reduction Catalyst on Rutile TiO_2 (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 TiO_2 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.jpcb.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 TiO_2 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 Formalhydrazone 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 e_6 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 **Rudshteyn, 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 **Rudshteyn, 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 **Rudshteyn, 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 $SrTiO_3$, and on TiO_2 Surfaces Through Computational and Experimental SFG Spectroscopy"
4/4/2017	253rd American Chemical Society National Meeting San Francisco: PHYS Division Batista, V.S., **Rudshteyn, 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 **Rudshteyn, 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 **Rudshteyn, 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 **Rudshteyn, 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 TiO_2 Surfaces Through Computational SFG Spectroscopy"
3/15/2015	251st American Chemical Society National Meeting San Diego: COMP Division **Rudshteyn, 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 TiO_2 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 **Rudshteyn, 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"

Schrödinger Inc., New York, NY
1/2020 Online Course:
- "Introduction to Molecular Modeling in Drug Discovery"

Professional Affiliations:

2011 - Present American Chemical Society
2015-2016
- 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