

# Benjamin Rudshteyn, PhD

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Schrödinger Inc.  
Life Science Software | Force Fields Team  
1540 Broadway, 24<sup>th</sup> Floor, New York, NY 10036  
[benjamin.rudshteyn@schrodinger.com](mailto:benjamin.rudshteyn@schrodinger.com)  
[benjamin.rudshteyn@gmail.com](mailto:benjamin.rudshteyn@gmail.com)  
ORCID: 0000-0002-9511-6780  
<https://br2575.github.io/>

## 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 force fields and approximate quantum chemical methods for drug and materials discovery projects, particularly including transition metals.
- Structure-based and ligand-based drug design.
- 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<sub>2</sub> 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 Schrödinger, Inc., New York, New York
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:  
*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](mailto:raf8@columbia.edu), 212-854-7606
- Victor S. Batista: [victor.batista@yale.edu](mailto:victor.batista@yale.edu), 203-432-6672.
- David R. Reichman: [dr2103@columbia.edu](mailto:dr2103@columbia.edu), 212-854-0469.
- Shiwei Zhang: [szhang@flatironinstitute.org](mailto:szhang@flatironinstitute.org), 646-876-5916
- Gary W. Brudvig: [gary.brudvig@yale.edu](mailto:gary.brudvig@yale.edu), 203-432-5202.
- John C. Tully: [john.tully@yale.edu](mailto:john.tully@yale.edu), 203-432-3934.
- Robert H. Crabtree: [robert.crabtree@yale.edu](mailto:robert.crabtree@yale.edu), 203-432-3925.
- Alexander Greer: [agreer@brooklyn.cuny.edu](mailto: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<sup>nd</sup> International Solar Fuels Conference Poster Award.

7/2017 2<sup>nd</sup> 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	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., **Rudshiteyn, 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. **Rudshiteyn, 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., **Rudshiteyn, 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. **Rudshiteyn, B.**,<sup>†</sup> Coskun, D.,<sup>†</sup> 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., **Rudshiteyn, 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.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> 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.,<sup>†</sup> Perets, E.A.,<sup>†</sup> Fisher, K.J.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> 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/CO<sub>2</sub> Conversion Informed by the Ni<sup>II</sup>-Iminothiolate Complex. *Inorg. Chem.*, **2018**, 57, 15474-15480.  
<https://pubs.acs.org/doi/10.1021/acs.inorgchem.8b02799>
30. Clark, M.L.,<sup>†</sup> Ge, A.,<sup>†</sup> Videla, P.E.,<sup>†</sup> **Rudshteyn, B.**, Miller, C.J., Song, J., Batista, V.S., Lian, T. and Kubiak, C.P., CO<sub>2</sub> 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<sup>II</sup>(pyalk)<sub>2</sub> Water-Oxidation Catalyst. *ACS Catal.* **2018**, 8, 7952-7960.  
<https://pubs.acs.org/doi/10.1021/acscatal.8b02466>
28. Ge, A.,<sup>†</sup> Videla, P.E.,<sup>†</sup> **Rudshteyn, B.**, Liu Q., Batista, V.S., Lian, T. Dopant-Dependent SFG Response of Rhenium CO<sub>2</sub> Reduction Catalysts Chemisorbed on SrTiO<sub>3</sub> (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.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> 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.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> Warnke, I., Xiao, D., and Batista, V.S. Mechanistic Study of CO/CO<sub>2</sub> 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.,<sup>†</sup> Chaudhuri, S.,<sup>†</sup> 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)<sub>3</sub> 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.,<sup>†</sup> Videla, P.E.,<sup>†</sup> 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.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> Zhanaidarova, A., Froehlich, J.D., Ding, W., Kubiak, C.P. and Batista, V.S. Electrode-Ligand Interactions Dramatically Enhance CO<sub>2</sub> Conversion to CO by the [Ni(cyclam)](PF<sub>6</sub>)<sub>2</sub> 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<sub>2</sub> Surfaces. *J. Phys. Chem. C* **2017**, *121*, 11985–11990.  
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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.,<sup>†</sup> Martinez, J.F.,<sup>†</sup> 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)<sub>3</sub> 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.,<sup>†</sup> Liu, W.,<sup>†</sup> Williams, D.M.,<sup>†</sup> 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.,<sup>†</sup> **Rudshteyn, B.**,<sup>†</sup> 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<sub>2</sub>-Reduction Catalyst on Rutile TiO<sub>2</sub> (110) Surfaces. *J. Phys. Chem. C.* **2016**, *120*, 20970-20977.  
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03165>
10. Ho, J.,<sup>†</sup> Psciuk, B.T.,<sup>†</sup> 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  $\alpha$ -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<sub>2</sub> 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.,<sup>†</sup> Koenigsmann, C.,<sup>†</sup> 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<sub>2</sub> 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  $\alpha$ -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<sub>6</sub> 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>

<sup>†</sup>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

20<sup>th</sup> 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  
**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 2<sup>nd</sup> 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 SrTiO<sub>3</sub>, and on TiO<sub>2</sub> Surfaces Through Computational and Experimental SFG Spectroscopy”
- 4/4/2017 253<sup>rd</sup> 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 253<sup>rd</sup> 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 253<sup>rd</sup> 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 TiO<sub>2</sub> Surfaces Through Computational SFG Spectroscopy”
- 3/15/2015 251<sup>st</sup> 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 TiO<sub>2</sub> Surfaces”
- 5/10/2013 61<sup>st</sup> 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 60<sup>th</sup> Annual Undergraduate Research Symposium of the New York Chemistry Students Association of the American Chemical Society’s New York Section  
**Rudshiteyn, 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

59<sup>th</sup> Annual Undergraduate Research Symposium of the New York Chemistry Students Association of the American Chemical Society's New York Section  
**Rudshiteyn, 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](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](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=benjaminrudshiteyn>

### 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 American Chemical Society  
2015-2016  
• Younger Chemist’s Committee

**Volunteer Activities:**

9/2022 – President Mentor for Undergraduate Students, Macaulay Honors College

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

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