

# Benjamin Rudshteyn, PhD

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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 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:

9/2021 – Present	Senior Scientist I Force Fields Team 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:**

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. *ChemRxiv*, **2021**.  
<https://doi.org/10.26434/chemrxiv.14751684.v1>
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.**,<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., **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.,<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 Schmittenmaier, 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.* **2017**, 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, 11985-11190.  
<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.,<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. Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. *Chem. Sci.* **2017**, 8, 1642-1652.  
<http://pubs.acs.org/doi/abs/10.1021/jacs.5b04185>
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., Anfusio, 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.* **2015**, *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., **Rudshiteyn, 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. **Rudshiteyn, 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. **Rudshiteyn, 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., **Rudshiteyn, 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:

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| 3/3/2021   | Yale University Energy Sciences Institute<br><b>Rudshiteyn, B.</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<br><b>Rudshiteyn, B.</b> , Shee, J., Coskun, D., Weber, J.L., Arthur, E.J., Zhang, S., Reichman, D.R. and Friesner, R.A.<br>“Accurate Quantum Chemistry of Transition Metal Compounds using Auxiliary-Field Quantum Monte Carlo “  |
| 7/10/2017  | 2017 EFRC-Hub CMS Principal Investigators Meeting<br><b>Rudshiteyn, B.</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.<br>“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<br><b>Rudshiteyn, B.</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) <i>fac</i> -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:**

4/2021-5/2021	Schrödinger Inc., New York, NY Online Course: <ul style="list-style-type: none"> <li>• “High-Throughput Virtual Screening for Hit Finding and Evaluation”</li> </ul>
10/2020-11/2020	Schrödinger Inc., New York, NY Online Course: <ul style="list-style-type: none"> <li>• “Introduction to Molecular Modeling Concepts for Polymers”</li> </ul>
12/2019-1/2020	Schrödinger Inc., New York, NY Online Course: <ul style="list-style-type: none"> <li>• “Introduction to Molecular Modeling in Drug Discovery”</li> </ul>

#### **Professional Affiliations:**

2011 - Present 2015-2016	American Chemical Society <ul style="list-style-type: none"> <li>• Younger Chemist’s Committee</li> </ul>
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#### **Volunteer Activities:**

9/2020 – President	President of the Columbia University Postdoctoral Society for the Morningside/Lamont campuses, Former Vice President, Former Chair of the Advocacy Subcommittee
5/2019 – 5 / 2021	Representative for Postdoctoral Research Scientists, Fellows, and Scholars in the Columbia Senate.
3/2019 – Present	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
5/2018 – Present	Judge for the Midwood High School Science Fair
8/2017 – 5/2018	Non-Resident Graduate Fellow at Benjamin Franklin College at Yale
3/2017 – Present	Reviewer for <i>The Journal of Physical Chemistry C</i> , <i>Molecules</i> , <i>Molecular Simulation</i> , <i>Computation</i> , <i>Nanomaterials</i> , <i>Pharmaceuticals</i>
9/2016 – 5/2018	Co-President of YANIS: Russian Club of Yale Students

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 <ul style="list-style-type: none"> <li>• Participated in Summer Steering Committee to help get ready for the upcoming semester and collect general concerns from survey reports.</li> <li>• Participated in Transit and Security Subcommittee with focus on lab safety.</li> </ul>
5/2014	Yale University Science Pathways Event Guide <ul style="list-style-type: none"> <li>• Guided students and their parents between labs in the department.</li> </ul>
5/2014-5/2018	New Haven Science Fair Judge/Team Leader <ul style="list-style-type: none"> <li>• Judged local high school team physical science projects.</li> </ul>
2011 – Present	Committee of Concerned Scientists <ul style="list-style-type: none"> <li>• Vice Chair of the Young Scholars Council, which advises the co-chairs on current events, particularly the cases of academics in Turkey and in former USSR republics.</li> </ul>
<b>Languages:</b>	<ul style="list-style-type: none"> <li>• English: Native proficiency</li> <li>• Russian: Bilingual oral proficiency</li> </ul>