Benjamin Rudshteyn, Ph.D.

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Chemistry Department
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Summary of Qualifications

- Quantum mechanical simulations of molecules and molecules attached to surfaces.
- DFT, CASSCF, QMC, tight-binding methods, comparison to spectroscopy, dielectric continuum solvent models, solar fuels, singlet-oxygen reactions, QM/MM. *ab initio* MD.
- Structure and ligand based drug design, in particular rigid-receptor docking and shape similarity screening.
- Highly collaborative and capable of teamwork – collaborated directly with and published papers with 15 professors, mostly with experimental expertise.
- Highly productive – 37 published manuscripts, 14 first- or co-first-author.
- Highly self-motivated – successfully applied for prestigious fellowships.
- Highly organized – successfully juggled multiple projects, training of students, teaching, service and volunteer activities, and professional development.
- Leadership experience – successfully held leadership positions in a variety of groups.
- Experienced in mentorship – successfully mentored both undergraduates and graduates.

Technical Skills

- Computational chemistry programs: Gaussian, PySCF, ORCA, Schrödinger Suite, Q-Chem, VASP, Quantum Espresso, SIESTA, ADF.
- Programming/scripting languages and software skills: C++, Python, Fortran, Bash, Git, LaTeX, High Performance Computing.

Employment/Research Experience

Columbia University, New York, NY (Advisor: Richard A. Friesner, Chemistry Department)
Postdoctoral Research Fellow, 2020-Present
Postdoctoral Research Scientist, 2018-2020

- Developing protocols for and applying an auxiliary field quantum Monte Carlo on GPU's for the accurate prediction of thermochemical properties of strongly correlated systems with the goal of pushing the method towards applications to metalloproteins and providing accurate transition metal reference data for the development of new functionals and force fields:
  - Bond dissociation energy of metal ligand diatomics in the gas phase.
  - Bond dissociation energy of coordination complexes in the gas phase.
  - Potential energy surfaces for reactions in the troposphere.
  - Ionization potentials of organic and transition metal molecules in the gas phase.
  - Properties of electrolytes in lithium battery related materials.
  - Solution phase properties of coordination complexes in solution.

Yale University, New Haven, CT (Advisor: Victor S. Batista, Chemistry Department)
Graduate Researcher, 2014-2018

- Researched the mechanism of action and of electrode binding of catalysts for water oxidation catalysts and carbon dioxide reaction catalysts using a combination of density functional theory and tight-binding methods in direct comparison to spectroscopic measurements by collaborators:
  - Identified the mechanism of the Cu^{II} pyridine alkoxide water oxidation catalyst.
  - Identified the binding mode of hydroxamic acid catalysts to TiO_2 electrodes in comparison to IR and UV-Vis measurements.

- Identified patterns in the redox properties of tungsten-alkylidyne complexes and iridium pyridine alkoxide model complexes in solution.
- Identified binding modes, vibrational energy relaxation, and Stark shifts of the $Re(bpy)(CO)_3Cl$ catalyst with various anchoring groups to TiO_2, $SrTiO_3$, and Au electrodes by direct comparison to sum frequency generation spectroscopy (SFG).
- Identified the role of electrode-ligand noncovalent interactions in controlling the behavior of Ni(cyclam) catalysts on different electrodes.
- Used inverse design to optimize a catalyst subject to synthetic constraints.

Macaulay Honors College at Brooklyn College of the City University of New York, Brooklyn, NY (Advisor: Alexander Greer, Chemistry Department)
*Undergraduate Researche*r, 2011-2013

- Identified the mechanism of the reaction of hydrazones and singlet oxygens leading to anticancer nitrosamines to complement photodynamic therapy (PDT).
- Identified the potential of nonpeptidic polydisulfide alpha-helices for carrying information.
- Contributed to studies identifying patterns of singlet oxygen reactivity with the natural product hyperforin and the implications of aggregation in photosensitizers for PDT.

Education

Yale University, New Haven, CT, Ph.D. Chemistry, May 2018
Yale University, New Haven, CT, M.S. Chemistry, May 2016
Macaulay Honors College at Brooklyn College of the City University of New York, Brooklyn, NY, B.S. in Chemistry *summa cum laude* May 2013

Professional Development

Schrödinger Inc., New York, NY
Online Course: "High-Throughput Virtual Screening for Hit Finding and Evaluation" May 2021
Online Course: "Introduction to Molecular Modeling Concepts for Polymers" November 2020
Online Course: "Introduction to Molecular Modeling in Drug Discovery" January 2020

Selected Grants and Awards

- NIH/NIGMS Ruth L. Kirschstein NRSA Postdoctoral Fellow (F32), February 2020
- 2nd International Solar Fuels Conference Poster Award, July 2017
- National Science Foundation Graduate Research Fellowship, April 2015
- Barry M. Goldwater Scholarship February 2012

Teaching Experience

Yale Sprout, Columbia Splash, Rainstorm, Wave Learning Festival, Columbia Engineering the Next Generation
Volunteer Instructor 2015-Present
Yale University, New Haven, CT
Teaching Assistant, Department of Chemistry 2013-2015

Selected Leadership and Volunteer Experience

University Senate, Columbia University, New York, NY
Senator for Postdoctoral Research Scientists, Fellows, and Scholars 2019-2021
Columbia University Postdoctoral Society, Columbia University, New York, NY
Co-President 2020-Present
Co-Vice President 2019-2020
Scientific Reviewer for *The Journal of Physical Chemistry C*, *Molecules, Molecular Simulation, Computation, and Nanomaterials*. 2017-Present