Benjamin Rudshteyn, Ph.D.

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Life Science Software | Force Fields Team
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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.
- Force field development and molecular dynamics calculations.
- Structure- and ligand-based drug design, in particular relative and absolute binding FEP.
- Highly collaborative and capable of teamwork – collaborated directly with and published papers with 15 professors, mostly with experimental expertise.
- Highly productive – 39 published manuscripts, 15 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: Schrödinger Suite, Gaussian, PySCF, ORCA, Q-Chem, VASP, Quantum Espresso, SIESTA, ADF.
- Programming/scripting languages and software skills: Python, Fortran, C++, Bash, Git, LaTeX, High Performance Computing.

Employment/Research Experience

Schrödinger, New York, NY (Force Fields Team, Life Science Software)
Senior Scientist II, 2023-Present
Senior Scientist I, 2021-2022

- Improvement of force fields for difficult cases such as those containing transition metals to improve drug discovery and materials discovery projects, mainly using molecular dynamics (MD) and free energy perturbation (FEP).

Columbia University, New York, NY (Advisor: Richard A. Friesner, Chemistry Department)
Postdoctoral Research Fellow, 2020-2021
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 and ionization energies of metal diatomics and complexes.
  - Potential energy surfaces for reactions in the troposphere.
  - Properties of electrolytes in lithium battery related materials.

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 binding modes of hydroxamic acid, $Re(bpy)(CO)_3Cl$, and Ni(cyclam) catalysts to electrodes in comparison to spectroscopy and electrochemistry.
- Identified patterns in the redox properties of tungsten-alkylidyne complexes and iridium pyridine alkoxide model complexes in solution.
- 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: "Visualizing Science with PyMOL 3" September 2024
Online Course: "Free Energy Calculations for Drug Design with FEP+" November 2022
Online Course: "Introduction to Computational Antibody Engineering" December 2021
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

Coursera Inc., Mountain View, CA
Online Course: "Machine Learning (Andrew Ng)" November 2021

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

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-Vice President, Co-President 2019-2021

Scientific Reviewer for the *National Science Foundation*, *The Journal of Physical Chemistry C, Molecular Simulation, and the Journal of Computer-Aided Molecular Design* 2017-Present