Benjamin Rudshteyn, Ph.D.

1 Main Street, Suite 1120, 11th Floor
Schrödinger Inc.
Cambridge, Massachusetts, 02142
ORCID: 0000-0002-9511-6780

https://br2575.github.io/
Life Science Software | Force Fields Team
benjamin.rudshteyn@schrodinger.com
benjamin.rudshteyn@gmail.com

Summary of Qualifications

- Classical Methods: Molecular Mechanics (MM), Relative and Absolute Binding Free Energy Perturbation (FEP), and Molecular Dynamics (MD) calculations.
- Quantum Mechanical Methods: DFT (density functional theory), Complete Active Space Self-Consistent Field (CASSCF), Auxiliary Field Quantum Monte Carlo (AFQMC), Tight-Binding (TB) methods, dielectric continuum solvent models, Quantum Mechanics/Molecular Mechanics (QM/MM), Machine-Learned Force Fields (MLFF).
- Fields of expertise: Force field development, structure- and ligand-based drug design, metalloproteins, quantum mechanical simulations of molecules and molecules attached to surfaces, solar fuels, reaction mechanism, water oxidation, carbon dioxide reduction, electrochemistry, singlet-oxygen reactions, comparison to vibrational spectroscopy.
- Highly collaborative and capable of teamwork – collaborated directly with and published papers with more than 15 professors, mostly with experimental expertise, and contributed to OPLS5 paper with almost 30 co-authors.
- 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

- Schrödinger Suite: OPLS4/OPLS5 (Force Fields), Force Field Builder (Torsion Parameterization FEP+, Desmond (MD), QSite (QM/MM), Jaguar (QM), Macromodel (MM), Maestro and PyMOL (GUI), Macro-pKa (protonation states and tautomers)
- Molecular computational chemistry programs: Gaussian, PySCF, ORCA, Q-Chem
- Solid-state computational chemistry programs: VASP, Quantum Espresso, SIESTA, ADF.
- Programming/scripting languages and software skills: Python, Fortran, C++, Octave, Bash, Git, LaTeX, High Performance Computing (HPC).
- Python Packages: Numpy, Scipy, Matplotlib, Pandas

Employment/Research Experience

Schrödinger, Cambridge, MA and New York, NY (Manager: Edward Harder, Force Fields Team, Life Science Software)
Senior Scientist II, 2023-Present
Senior Scientist I, 2021-2022

- Scientific investigation, validation and stress-testing of OPLS5 to enable drug discovery on metalloproteins using a combination of FEP, MD, and QM techniques
- Organizing the FEP Outliers Meeting where we help the Schrödinger Therapeutics Group resolve outliers in their predictions

Columbia University, New York, NY (Advisor: Richard A. Friesner, Chemistry Department)
Postdoctoral Research Scientist/Fellow, 2018-2021

- 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 DFT and TB methods in direct comparison to spectroscopic measurements:
  - 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 heavy metal complexes in solution.

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

- Studied reactivity of hydrazones and the natural product hyperforin with singlet oxygen leading to anticancer nitrosamines to complement photodynamic therapy (PDT) efforts.
- Identified the potential of nonpeptidic polydisulfide alpha-helices for carrying information.

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
- 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