Jason A. Wagoner

New York, New York • jawagoner@gmail.com • https://jwagoner.org

EDUCATION

2006–2012 **Ph.D., Chemistry,** Stanford University
Advisor: Vijay Pande
- National Science Foundation Graduate Research Fellowship
- Department of Energy Computational Science Graduate Fellowship (declined)

2002–2006 **B.S in Biomedical Engineering, Chemistry; Minor in Mathematics**
Washington University in St. Louis
- Graduate *magna cum laude*
- Tau Beta Pi Engineering Honor Society, AHMB Biomedical Engineering Honor Society
- Calvin M. Woodward Scholar

POSITIONS

2013– **Junior Laufer Fellow**, Laufer Center for Physical and Quantitative Biology
Stony Brook University
- Research: Designed research projects and computational models for molecular machines, mechano-biological networks, protein folding, protein-ligand interactions. Work published in high-impact journals including Nature Comms, PNAS, and Mol. Biol. Evol. (impact factor=15).
- Mentoring: Mentored 4 Laufer Center graduate students and postdocs in research design, molecular simulation, machine learning, and software engineering.
- Grants: Collaborated on teams of 3-6 to write grants (successfully funded) for Laufer Center supercomputing resources (Blue Waters, XSEDE) and funding through the Keck Foundation.
- Teaching: Instructor for Physical and Quantitative Biology Graduate Course (15-30 students in person at Stony Brook, 10-15 students remote at Rutgers University).

2012–2013 **Postdoctoral Research Fellow**, Department of Chemistry,
Stanford University
Advisor: Vijay Pande
- Derived and wrote code for new methods in molecular simulations that gave 2 publications.

2006–2012 **Graduate Student**, Department of Chemistry,
Stanford University
Advisor: Vijay Pande
- Thesis research in designing new theories, software implementations, and applications of multi-scale molecular simulation methods.

2003–2006 **Undergraduate Researcher**, Department of Biochemistry and Molecular Biophysics
Washington University in St. Louis
Advisor: Nathan Baker
- Three years of independent undergraduate research in biomolecular solvation that gave 4 publications (2 first author).
- Funding received: NIH Summer Undergraduate Research Fellowship; HHMI Summer Undergraduate Research Fellowship

TEACHING

Instructor 2015-2020
Physical and Quantitative Biology
Stony Brook University

Teaching Assistant 2006-2010
Department of Chemistry
Stanford University

Tutor 2007-2008
A+ Home Tutors
Palo Alto, California

Cornerstone Mentor 2005-2006
Washington University in St. Louis

HONORS AND AWARDS

Washington University in St. Louis CBSE Visiting Fellow	2015
National Science Foundation Graduate Research Fellowship	2008-2011
Department of Energy Computational Science Graduate Fellowship	2008 (declined)
AHMB Biomedical Engineering Honor Society	2006-present
Tau Beta Pi Engineering Honor Society	2005-present
NIH Summer Undergraduate Research Fellowship	2004
HHMI Summer Undergraduate Research Fellowship	2003
Calvin M. Woodward Scholar	2002-2006
Robert C. Byrd Scholarship	2002-2006
James R. Hoffa Memorial Scholarship	2002-2006
Missouri Bright Flight Scholar	2002-2006

SELECTED INVITED TALKS

ASCB/EMBO Cell Bio Meeting 2020
Evolutionary principles for the actions of molecular machines

Gordon Research Conference: Stochastic Physics in Biology 2019
The biological catch bond suppresses fluctuations in nonequilibrium systems

Simons Center Workshop on Nonequilibrium Physics in Biology 2018
The biological catch bond suppresses fluctuations in nonequilibrium systems

UTSW Computational and Systems Biology Seminar 2018
Principles of evolution and design for optimizing speed, efficiency, and power in molecular machines

Biophysical Society Thematic Meeting 2016
Engineering Approaches to to Biomolecular Motors
The nonequilibrium statistical mechanics of biomolecular motors

Biophysical Society 60th Annual Meeting 2016
The nonequilibrium statistical mechanics of biomolecular motors

Center for Biological Systems Engineering Special Seminar 2015
Washington University in St. Louis
Advanced simulation methods in multiscale modeling

Center for Biological Systems Engineering Special Seminar 2015
Washington University in St. Louis
A nonequilibrium perspective on the design of biological cycles

Biophysical Society 59th Annual Meeting 2015
Advanced simulation methods in multiscale modeling

Telluride Science Research Center 2014
Advances in Enhanced Sampling Algorithms
Multiscale modeling: adaptive boundaries and transferable potentials

PUBLICATIONS

14. **Wagoner JA** and Dill KA, Evolution of mechanical cooperativity among myosin II motors. *Proc. Natl. Acad. Sci. USA* **118**, e2101871118, 2021
13. Cubik J, Alston JJ, *et. al.*, The SARS-CoV-2 nucleocapsid protein is dynamic, disordered, and phase separates with RNA. *Nat. Commun.* **12** (1936), 1-17, 2021
12. **Wagoner JA** and Dill KA, Opposing pressures of speed and efficiency guide the evolution of molecular machines. *Mol. Biol. Evol.*, **36** (12), 2813-2822, 2019
11. **Wagoner JA** and Dill KA, Mechanisms for achieving high speed and efficiency in biomolecular machines. *Proc. Natl. Acad. Sci. USA* **116** (13), 5902-5907, 2019
10. **Wagoner JA** and Pande VS, Communication: Adaptive boundaries in multiscale simulations. *J. Chem. Phys.* **148** (14), 141104, 2018
9. Dixit P, **Wagoner JA**, Ghosh K, Weistuch C, Presse S, and Dill KA, Perspective: Maximum caliber is a general variational principle for dynamical systems. *J. Chem. Phys.* **148** (1), 010901, 2018
8. **Wagoner JA** and Dill KA, Molecular motors: Power strokes outperform Brownian ratchets. *J. Phys. Chem. B* **120** (26), 6327-6336, 2016
7. **Wagoner JA** and Pande VS, Finite domain simulations with adaptive boundaries: accurate potentials and nonequilibrium movesets. *J. Chem. Phys.* **139** (23), 234114, 2013
6. **Wagoner JA** and Pande VS, Reducing the effect of Metropolization on mixing times in molecular dynamics simulations. *J. Chem. Phys.* **137** (21), 214103, 2012
5. **Wagoner JA** and Pande VS, A smoothly decoupled particle interface: New methods for coupling explicit and implicit solvent. *J. Chem. Phys.* **134** (21), 214103, 2011
4. Dong F, **Wagoner JA**, and Baker NA, Assessing the performance of implicit solvation models at a nucleic acid surface. *Phys. Chem. Chem. Phys.* **10**, 4889-4902, 2008
3. Swanson JMJ, **Wagoner JA**, Baker NA, and McCammon JA, Optimizing the Poisson dielectric boundary with explicit solvent forces and energies: Lessons learned with atom-centered dielectric functions. *J. Chem. Theory Comput.* **3**, 170-184, 2007

2. **Wagoner JA** and Baker, NA, Assessing implicit models for nonpolar mean solvation forces: the importance of dispersion and volume terms. *Proc. Natl. Acad. Sci. USA* **103** (22), 8331-8336, 2006

1. **Wagoner JA** and Baker NA, Solvation forces on biomolecular structures: a comparison of explicit solvent and Poisson-Boltzmann models. *J. Comput. Chem.* **25** (13), 1623-1629, 2004