Gregory R. BOWMAN, Ph.D.

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Academic Positions

Assistant Professor 2014-present
Washington University in St. Louis
Department of Biochemistry & Molecular Biophysics, Department of Biomedical Engineering, and Center for Biological Systems Engineering

Miller Research Fellow 2011-2014
University of California, Berkeley
Department of Molecular & Cell Biology and Department of Chemistry

Berry Postdoctoral Fellow 2010-2011
Stanford University
Department of Chemistry

Education

Ph.D. Biophysics 2006-2010
Stanford University
Vijay Pande "Markov state models for protein and RNA folding"

BS Computer Science **2002-**2006
Minor in Biomedical Engineering
Cornell University
Summa cum laude

Funding

Packard Fellowship for Science and Engineering 2016-2021
Energy-landscape engineering: Exploiting uncharted protein conformations
$175K/year direct

NSF CAREER Award 2016-2021
FAST methods for protein folding and design
$80K/year direct

U19 NIH/NIAID Project Grant 2016-2018
Therapeutics targeting filoviral interferon-antagonist and replication functions
$130I/year direct

Burroughs Wellcome Fund Career Award at the Scientific Interface 2013-2018
Decrypting cryptic allosteric sites resulting from protein flexibility
$100K/year direct

Honors & Awards

Packard Fellowship for Science and Engineering 2016-2021

NSF CAREER Award 2016-2021

Burroughs Wellcome Fund Career Award at the Scientific Interface 2013-2018

Miller Research Fellow 2011-2014

Genome Technology Young Investigator Award 2011

Berry Postdoctoral Fellow 2010-2011

Thomas Kuhn Paradigm Shift Award 2010
American Chemical Society

NSF Graduate Research Fellowship 2007-2010

Tau Beta Pi 2006

Merrill Presidential Scholar 2006

Computer Science Award for Academic Excellence 2006

Rhodes Scholarship Finalist 2005

Jean Dreyfus Boissevain Undergraduate Scholarship for Excellence in Chemistry 2005

Invited Talks

Union Chimique Belge (UCB) Pharmaceuticals Seminar 2016
Slough, United Kingdom

Markov State Models in Drug Discovery Workshop 2016
Novartis, Boston, MA

Pfizer 2016
Pfizer, Boston, MA

Physical Chemistry Seminar 2016
Kings College, London, United Kingdom

Protein Folding Consortium 2016
St. Louis, MO

SLU Biochemistry Retreat 2016
St. Louis University, St. Louis, MO

Biochemistry & Molecular Biophysics Retreat 2016
Washington University, St. Louis, MO

Theoretical Chemistry Institute (TCI) Seminar 2015
University of Wisconsin-Madison

Free Energy Calculation Workshop 2015
Snowmass, CO

Science for Life Lab Seminar 2015
Karolinska Institute, Stockholm, Sweden

Structure, Dynamics, and Allostery in Drug Target Interaction Platform Session 2014
Biophysical Society

Endowed Scholars Program 2014
University of Texas, Southwestern

Chemistry & Biochemistry Seminar 2014
University of California, Los Angeles

Chemistry Seminar 2014
University of Illinois Urbana-Champaign

Biophysics Seminar 2014
University of Texas, Southwestern

Biochemistry & Molecular Biophysics Seminar 2014
Washington University School of Medicine

Chemistry & Biochemistry Seminar 2014
University of Colorado, Boulder

Chemistry & Biochemistry Seminar 2014
University of Arizona, Tucson

Biochemistry Seminar 2014
Brandeis University

Dr. George W. Raiziss Seminar 2014
University of Pennsylvania

Integrative Biology & Physiology Seminar 2014
University of California, Los Angeles

Advanced Light Source User Meeting 2013
Lawrence Berkeley National Labs

Computational Medicine Seminar 2013
University of Michigan

Theoretical Chemistry Seminar 2013
Cornell University

Molecular Kinetics Workshop 2013
Freie Universitat Berlin

Enzyme Dynamics Workshop 2013
Telluride Science Research Center

Biophysics Seminar 2013
University of Michigan

Physical Chemistry Seminar 2013
University of California, Berkeley

Physical Chemistry Seminar 2013
University of Pennsylvania

Physical Chemistry Seminar 2012
ETH Zurich

Biophysics Seminar 2012
University of California, San Francisco

Biophysics Seminar 2012
Johns Hopkins University

Protein Folding Consortium 2012
Stony Brook

Folding@home Consortium 2012
Stanford University

Protein Folding Consortium 2011
University of California, Berkeley

Rosetta Conference 2011
University of Washington, Seattle

Protein Folding Symposium 2011
Hong Kong University of Science & Technology

Thomas Kuhn Paradigm Shift Award Symposium 2010
American Chemical Society

Protein Folding & Stability Platform Session 2010
Biophysical Society

France-Stanford Exchange Program 2010
Institute Pasteur

Protein Folding Symposium 2010
Notre Dame

GPU Workshop 2010
Lawrence Berkeley National Laboratory

Biomedical Computation at Stanford 2010
Stanford University

Stanford High Performance Computing 2010
Stanford University

Conferences Organized

Markov State Models in Drug Discovery Workshop 2016
Novartis, Boston, MA

Teaching

Chemistry & Physics of Biomolecules 2004-**present**
Washington University in St. Louis

Computational Biophyics Journal Club 2004-**present**
Washington University in St. Louis

MSMBuilder Workshop 2009-2011
Stanford University

Teaching Assistant, Methods in Molecular Biophysics 2009
Stanford University

Constructing an Alternate Universe: Computer Simulation of Protein Folding 2008-2010
Stanford University

Software

MSMBuilder
http://msmbuilder.org/
Open source software for building Markov state models, which are maps of the conformational space a biomolecule can explore that consist of structural states and the rates of transitioning between them.

Research Articles (* denotes corresponding author)

1. Hart KM, Ho CMW, Duta S, Gross ML, **Bowman GR***. Modeling proteins' hidden conformations to predict antibiotic resistance. ***Nat Commun*** 2016;7:12965.

2. **Bowman GR***. Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. ***J Comput Chem*** 2016;37:558-566.
3. Hart KM, Reck M, **Bowman GR***, Wencewicz TA. Tabtoxinine-β-lactam is a "stealth" β-lactam antibiotic that evades β-lactamase-mediated antibiotic resistance. ***Med Chem Comm*** 2016;7:118-127.
4. Pascolutti R, Sun X, Kao J, Maute R, Ring AM **Bowman GR**, Kruse AC. Structure and dynamics of PD-L1 and an ultra-high-affinity PD-1 receptor mutant. ***Structure*** 2016;24:1719+1728.
5. Warfarin traps human vitamin K epoxide reductase in an intermediate state during electron transfer. ***Nat Struct Mol Bio*** 2016 accepted.Zimmerman MI, **Bowman GR***. FAST conformational searches by balancing exploration/exploitation tradeoffs. ***J Chem Theory Comput*** 2015;11:5747-5757.
7. **Bowman GR*,** Bolin ER, Hart KM, Maguire BC, Marqusee S. Discovery of multiple hidden allosteric sites by combining Markov state models and experiments. ***Proc Natl Acad Sci U S A***, 2015:112;2734-2739.
8. **Bowman GR***, Geissler PL. Extensive structural heterogeneity within protein cores. ***J Phys Chem B*** 2014;118:6417-6423.
9. Kohlhoff KJ, Shukla D, Lawrenz M, **Bowman GR**, Konerding DE, Belov D, Altman RB, Pande VS. Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. ***Nature Chemistry,*** 2014;6:15-21.
10. **Bowman GR*,** Meng L, Huang X. Quantitative comparison of alternative methods for coarse-graining biological networks. ***J Chem Phys*** 2013;139:121905.
11. Yao Y, Cui RZ, **Bowman GR**, Silva DA, Sun J, Huang X. Hierarchical Nystrom methods for constructing Markov state models for conformational dynamics. ***J Chem Phys*** 2013;138:174106.
12. Qiao Q, **Bowman GR**, Huang X. Dynamics of an intrinsically disordered protein reveal metastable conformations that potentially seed aggregation. ***J Am Chem Soc*** 2013;135:16092-16101.
13. **Bowman GR*,** Geissler PL. Equilibrium fluctuations of a single folded protein reveal a multitude of potential cryptic allosteric sites. ***Proc Natl Acad Sci U S A*** 2012;29:11681-11686.
14. **Bowman GR***. Improved coarse-graining of Markov state models via explicit consideration of statistical uncertainty. ***J Chem Phys*** 2012;137;134111.
15. Levin AM, Bates DL, Ring AM, Krieg C, Lin JT, Su L, Moraga I, Raeber ME, **Bowman GR**, Novick P, Pande VS, Fathman CG, Boyman O, Garcia KC. Exploiting a natural conformational switch to engineer an interleukin-2 'superkine'. ***Nature*** 2012;484:529-533.
16. Ring AM, Lin J, Feng D, Mitra S, Rickert M, **Bowman GR**, Pande VS, Li P, Moraga I, Spolski R, Özkan E, Leonard WJ, Garcia KC. Mechanistic and structural insight into the functional dichotomy between IL-2 and IL-15. ***Nature Immunology*** 2012;13:1187-1195.
17. Voelz VA, Jager M, Yao S, Chen Y, Zhu L, Waldauer SA, **Bowman GR**, Friedrichs M, Bakajin O, Lapidus LJ, Weiss S, Pande VS. Slow unfolded-state structuring in ACBP folding revealed by theory and experiment. ***J Am Chem Soc*** 2012;134:12565-12577.
18. **Bowman GR**, Voelz VA, Pande VS. Atomistic folding simulations of the five-helix bundle protein λ_{6-85}. ***J Am Chem Soc*** 2011;133:664-667.
19. Silva D, **Bowman GR**, Sosa-Peinado A, Huang X. A role for both conformational selection and induced fit in ligand binding by the LAO protein. ***PLoS Comput Biol*** 2011;7:e1002054.
20. Beauchamp KA, **Bowman GR**, Lane TJ, Maibaum L, Haque IS, Pande VS. MSMBuilder2: Modeling conformational dynamics at the picosecond to millisecond scale. ***J Chem Theory Comput*** 2011;7:3412-3419.
21. Lane TJ, **Bowman GR**, Beauchamp KA, Voelz VA, Pande VS. Markov state model reveals folding and functional dynamics in ultra-long MD trajectories. ***J Am Chem Soc*** 2011;113:18413-18419.

22. Lin Y, **Bowman GR**, Beauchamp KA, Pande VS. Investigating how peptide length and a pathogenic mutation modify the structural ensemble of amyloid beta monomer. ***Biophys J*** 2011;102:315-324.
23. Pronk S, Larsson P, Pouya I, **Bowman GR**, Haque IS, Beauchamp KA, Hess B, Pande VS, Kasson PM, Lindahl E. Copernicus: A new paradigm for parallel adaptive molecular dynamics. ***In SC '11: Proc Conf High Perf Computing, Networking, Storage and Analysis***, New York, NY, USA, 2011. ACM.
24. **Bowman GR**, Pande VS. Protein folded states are kinetic hubs. ***Proc Natl Acad Sci U S A*** 2010;107:10890-10895.
25. **Bowman GR**, Ensign DL, Pande VS. Enhanced modeling via network theory: adaptive sampling of Markov state models. ***J Chem Theory Comput*** 2010;6:787-794.
26. Voelz VA, **Bowman GR**, Beauchamp KA, Pande VS. Molecular simulation of *ab initio* protein folding for a millisecond folder NTL9(1-39). ***J Am Chem Soc*** 2010;132:1526-1528.
27. Huang X, Yao Y, Sun J, **Bowman GR**, Guibas L, Carlsson G, Pande VS. Constructing multi-resolution Markov state models (MSMs) to elucidate RNA hairpin folding mechanisms. ***Pac Symp Biocomput*** 2010;15:228-239.
28. **Bowman GR**, Beauchamp KA, Boxer G, Pande VS. Progress and challenges in the automated construction of Markov state models for full protein systems. ***J Chem Phys*** 2009;131:124101.
29. **Bowman GR**, Huang X, Pande VS. Using generalized ensemble simulations and Markov state models to identify conformational states. ***Methods*** 2009;49:197-201.
30. **Bowman GR**, Pande VS. Simulated tempering yields insight into the low-resolution Rosetta scoring functions. ***Proteins*** 2009;74:777-788.
31. **Bowman GR**, Pande VS. The roles of entropy and kinetics in structure prediction. ***PLoS One*** 2009;4:e5840.
32. Huang X, **Bowman GR**, Bacallado S, Pande VS. Rapid equilibrium sampling initiated from nonequilibrium data. ***Proc Natl Acad Sci U S A*** 2009; 106:19765-19769.
33. Voelz VA, Luttmann E, **Bowman GR**, Pande VS. Probing the nanosecond dynamics of a designed three-stranded beta-sheet with a massively parallel molecular dynamics simulation. ***Int J Mol Sci*** 2009;10:1013-1030.
34. Yao Y, Sun J, Huang X, **Bowman GR**, Singh G, Lesnick M, Guibas LJ, Pande VS, Carlsson G. Topological methods for exploring low-density states in biomolecular folding pathways. ***J Chem Phys*** 2009;130:144115.
35. **Bowman GR**, Huang X, Yao Y, Sun J, Carlsson G, Guibas LJ, Pande VS. Structural insight into RNA hairpin folding intermediates. ***J Am Chem Soc*** 2008;130:9676-9678.
36. Huang X, **Bowman GR**, Pande VS. Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. ***J Chem Phys*** 2008;128:205106.
37. Zwick ME, Mcafee F, Cutler DJ, Read TD, Ravel J, **Bowman GR**, Galloway DR, Mateczun A. Microarray-based resequencing of multiple Bacillus anthracis isolates. ***Genome biology*** 2005;6:R10.

Review Articles

38. DuBay KH, **Bowman GR,** Geissler PL. Fluctuations within folded proteins: Implications for thermodynamics and allosteric regulation. ***Acc Chem Res*** 2015;48:1098-1105.
39. Cui RZ, Silva DA, Song J, **Bowman GR**, Zhuang W, Huang X. Bridging the gap between optical spectroscopic experiments and computer simulations for fast protein folding dynamics. ***Curr Phys Chem*** 2012;2:45-58.
40. **Bowman GR**, Voelz VA, Pande VS. Taming the complexity of protein folding. ***Curr Opin Struct Biol*** 2011;21:4-11.
41. **Bowman GR**, Huang X, Pande VS. Network models for molecular kinetics and their initial applications to human health. ***Cell Research*** 2010;20:622–630.

42. Pande VS, Beauchamp KA, **Bowman GR**. Everything you wanted to know about Markov state models but were afraid to ask. ***Methods*** 2010;52:99-105.

Books

43. Zimmerman MI, **Bowman GR**[*]. "How to run FAST simulations." In Methods in enzymology. Edited by Voth GA. Elsevier, submitted.
44. **Bowman GR**. "An overview and practical guide to building Markov state models" in An introduction to Markov state models and their application to long-timescale molecular simulation. Edited by **Bowman GR,** Pande VS, and Noe F. Springer Press, 2014.
45. **Bowman GR**. "Tutorial on building Markov state models with MSMBuilder and coarse-graining them with BACE" in Protein dynamics. Edited by Livesay DR. Humana Press, 2014.