Michael E Wall

List of Publications by Year
in descending order

55 papers	1,847 citations	279701 23 h-index	276775 41 g-index
72 all docs	72 docs citations	72 times ranked	2100 citing authors

#	Article	IF	Citations
1	Design of gene circuits: lessons from bacteria. Nature Reviews Genetics, 2004, 5, 34-42.	7.7	206
2	Allostery in a Coarse-Grained Model of Protein Dynamics. Physical Review Letters, 2005, 95, 198103.	2.9	146
3	Motions of calmodulin characterized using both Bragg and diffuse X-ray scattering. Structure, 1997, 5, 1599-1612.	1.6	95
4	Quantifying allosteric effects in proteins. Proteins: Structure, Function and Bioinformatics, 2005, 59, 697-707.	1.5	82
5	Scaling molecular dynamics beyond 100,000 processor cores for largeâ€scale biophysical simulations. Journal of Computational Chemistry, 2019, 40, 1919-1930.	1.5	79
6	Multiple Functions of a Feed-Forward-Loop Gene Circuit. Journal of Molecular Biology, 2005, 349, 501-514.	2.0	75
7	LARGE-SCALESHAPECHANGES INPROTEINS ANDMACROMOLECULARCOMPLEXES. Annual Review of Physical Chemistry, 2000, 51, 355-380.	4.8	70
8	Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 2380-2385.	3.3	69
9	Activation of the Escherichia coli marA/soxS/rob Regulon in Response to Transcriptional Activator Concentration. Journal of Molecular Biology, 2008, 380, 278-284.	2.0	62
10	Three-dimensional diffuse x-ray scattering from crystals of Staphylococcal nuclease. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 6180-6184.	3.3	57
11	Mix-and-inject XFEL crystallography reveals gated conformational dynamics during enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25634-25640.	3.3	56
12	Conformational dynamics of a crystalline protein from microsecond-scale molecular dynamics simulations and diffuse X-ray scattering. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17887-17892.	3.3	55
13	Design Principles for Regulator Gene Expression in a Repressible Gene Circuit. Journal of Molecular Biology, 2003, 332, 861-876.	2.0	50
14	Interactions in Native Binding Sites Cause a Large Change in Protein Dynamics. Journal of Molecular Biology, 2006, 358, 213-223.	2.0	49
15	Measuring and modeling diffuse scattering in protein X-ray crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4069-4074.	3.3	48
16	A model of troponinâ€I in complex with troponinâ€C using hybrid experimental data: The inhibitory region is a Î²â€hairpin. Protein Science, 2000, 9, 1312-1326.	3.1	47
17	Literature mining of protein-residue associations with graph rules learned through distant supervision. Journal of Biomedical Semantics, 2012, 3, S2.	0.9	35
18	Biomolecular Solvation Structure Revealed by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2019, 141, 4711-4720.	6.6	33

#	Article	IF	Citations
19	High-resolution macromolecular structure determination using CCD detectors and synchrotron radiation. Structure, 1995, 3, 835-844.	1.6	30
20	Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101.	1.2	29
21	Bringing diffuse X-ray scattering into focus. Current Opinion in Structural Biology, 2018, 50, 109-116.	2.6	29
22	Fast dynamics perturbation analysis for prediction of protein functional sites. BMC Structural Biology, 2008, 8, 5.	2.3	28
23	Text Mining Improves Prediction of Protein Functional Sites. PLoS ONE, 2012, 7, e32171.	1.1	27
24	Methods and Software for Diffuse X-Ray Scattering from Protein Crystals. Methods in Molecular Biology, 2009, 544, 269-279.	0.4	26
25	Domain motions of Argonaute, the catalytic engine of RNA interference. BMC Bioinformatics, 2007, 8, 470.	1.2	25
26	Internal protein motions in molecular-dynamics simulations of Bragg and diffuse X-ray scattering. IUCrJ, 2018, 5, 172-181.	1.0	25
27	Efficient Parallel Linear Scaling Construction of the Density Matrix for Bornâ€“Oppenheimer Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 4644-4654.	2.3	23
28	Reconstruction of Metabolic Networks from High-Throughput Metabolite Profiling Data: In Silico Analysis of Red Blood Cell Metabolism. Annals of the New York Academy of Sciences, 2007, 1115, 102-115.	1.8	22
29	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. Journal of Chemical Theory and Computation, 2022, 18, 1359-1381.	2.3	22
30	Model of Transcriptional Activation by MarA in Escherichia coli. PLoS Computational Biology, 2009, 5, e1000614.	1.5	20
31	Protein structure determination using a database of interatomic distance probabilities. Protein Science, 1999, 8, 2720-2727.	3.1	19
32	Recursive Factorization of the Inverse Overlap Matrix in Linear-Scaling Quantum Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3063-3073.	2.3	19
33	Quantum crystallographic charge density of urea. IUCrJ, 2016, 3, 237-246.	1.0	17
34	Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597.	2.4	15
35	Genome Majority Vote Improves Gene Predictions. PLoS Computational Biology, 2011, 7, e1002284.	1.5	14
36	Predicting X-ray diffuse scattering from translationâ€“librationâ€“screw structural ensembles. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1657-1667.	2.5	14

#	Article	IF	Citations
37	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. Structural Dynamics, 2019, 6, 064704.	0.9	14
38	Consistency of gene starts among Burkholderia genomes. BMC Genomics, 2011, 12, 125.	1.2	11
39	Dynamical Model of Drug Accumulation in Bacteria: Sensitivity Analysis and Experimentally Testable Predictions. PLoS ONE, 2016, 11, e0165899.	1.1	8
40	Ligand Binding, Protein Fluctuations, And Allosteric Free Energy. AIP Conference Proceedings, 2006, , .	0.3	7
41	Structureâ€"function relations are subtle in genetic regulatory networks. Mathematical Biosciences, 2011, 231, 61-68.	0.9	7
42	Hidden structure in protein energy landscapes. Physical Review E, 2008, 77, 021902.	0.8	6
43	Detection of protein catalytic sites in the biomedical literature. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2013, , 433-44.	0.7	6
44	Reproducibility of protein x-ray diffuse scattering and potential utility for modeling atomic displacement parameters. Structural Dynamics, 2021, 8, 044701.	0.9	5
45	Pattern Learning through Distant Supervision for Extraction of Protein-Residue Associations in the Biomedical Literature. , 2011, , .		3
46	Predicting Binding Sites by Analyzing Allosteric Effects. Methods in Molecular Biology, 2012, 796, 423-436.	0.4	3
47	Selected papers from the Fourth Annual q-bio Conference on Cellular Information Processing. Physical Biology, 2011, 8, 050301.	0.8	2
48	Special section dedicated to The Sixth q-bio Conference: meeting report and preface. Physical Biology, 2013, 10, 030301.	0.8	2
49	Interactions that know no boundaries. IUCrJ, 2018, 5, 120-121.	1.0	2
50	DETECTION OF PROTEIN CATALYTIC SITES IN THE BIOMEDICAL LITERATURE. , 2012, , .		2
51	Prediction of Functional Sites in SCOP Domains using Dynamics Perturbation Analysis. Nature Precedings, 2008, , .	0.1	1
52	The Seventh q-bio Conference: meeting report and preface. Physical Biology, 2014, 11, 040301.	0.8	1
53	The Fifth Annual q-bio Conference on Cellular Information Processing. Physical Biology, 2012, 9, 050201.	0.8	0
54	Diffuse X-Ray Scattering for Ensemble Modeling of Crystalline Proteins. Biophysical Journal, 2014, 106, 384a.	0.2	0

#	Article	IF	Citations
55	The eighth q-bio conference: meeting report and special issue preface. Physical Biology, 2015, 12, 060401.	0.8	0