Michael E Wall

List of Publications by Year
in descending order

55 papers	1,847 citations	279487 23 h-index	276539 41 g-index
72 all docs	72 docs citations	72 times ranked	2100 citing authors

#	Article	IF	Citations
1	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
2	Reproducibility of protein x-ray diffuse scattering and potential utility for modeling atomic displacement parameters. Structural Dynamics, 2021, 8, 044701.	0.9	5
3	Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597.	2.4	15
4	Scaling molecular dynamics beyond 100,000 processor cores for largeâ€scale biophysical simulations. Journal of Computational Chemistry, 2019, 40, 1919-1930.	1.5	79
5	Biomolecular Solvation Structure Revealed by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2019, 141, 4711-4720.	6.6	33
6	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. Structural Dynamics, 2019, 6, 064704.	0.9	14
7	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
8	Bringing diffuse X-ray scattering into focus. Current Opinion in Structural Biology, 2018, 50, 109-116.	2.6	29
9	Internal protein motions in molecular-dynamics simulations of Bragg and diffuse X-ray scattering. IUCrJ, 2018, 5, 172-181.	1.0	25
10	Interactions that know no boundaries. IUCrJ, 2018, 5, 120-121.	1.0	2
11	Dynamical Model of Drug Accumulation in Bacteria: Sensitivity Analysis and Experimentally Testable Predictions. PLoS ONE, 2016, 11, e0165899.	1.1	8
12	Quantum crystallographic charge density of urea. IUCrJ, 2016, 3, 237-246.	1.0	17
13	Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101.	1.2	29
14	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
15	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
16	Predicting X-ray diffuse scattering from translationâ€“librationâ€“screw structural ensembles. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1657-1667.	2.5	14
17	The eighth q-bio conference: meeting report and special issue preface. Physical Biology, 2015, 12, 060401.	0.8	0
18	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

#	Article	IF	Citations
19	The Seventh q-bio Conference: meeting report and preface. Physical Biology, 2014, 11, 040301.	0.8	1
20	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
21	Diffuse X-Ray Scattering for Ensemble Modeling of Crystalline Proteins. Biophysical Journal, 2014, 106, 384a.	0.2	0
22	Special section dedicated to The Sixth q-bio Conference: meeting report and preface. Physical Biology, 2013, 10, 030301.	0.8	2
23	Detection of protein catalytic sites in the biomedical literature. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2013, , 433-44.	0.7	6
24	The Fifth Annual q-bio Conference on Cellular Information Processing. Physical Biology, 2012, 9, 050201.	0.8	0
25	Predicting Binding Sites by Analyzing Allosteric Effects. Methods in Molecular Biology, 2012, 796, 423-436.	0.4	3
26	Literature mining of protein-residue associations with graph rules learned through distant supervision. Journal of Biomedical Semantics, 2012, 3, S2.	0.9	35
27	Text Mining Improves Prediction of Protein Functional Sites. PLoS ONE, 2012, 7, e32171.	1.1	27
28	DETECTION OF PROTEIN CATALYTIC SITES IN THE BIOMEDICAL LITERATURE. , 2012, , .		2
29	Pattern Learning through Distant Supervision for Extraction of Protein-Residue Associations in the Biomedical Literature. , 2011, , .		3
30	Structureâ€“function relations are subtle in genetic regulatory networks. Mathematical Biosciences, 2011, 231, 61-68.	0.9	7
31	Consistency of gene starts among Burkholderia genomes. BMC Genomics, 2011, 12, 125.	1.2	11
32	Selected papers from the Fourth Annual q-bio Conference on Cellular Information Processing. Physical Biology, 2011, 8, 050301.	0.8	2
33	Genome Majority Vote Improves Gene Predictions. PLoS Computational Biology, 2011, 7, e1002284.	1.5	14
34	Model of Transcriptional Activation by MarA in Escherichia coli. PLoS Computational Biology, 2009, 5, e1000614.	1.5	20
35	Methods and Software for Diffuse X-Ray Scattering from Protein Crystals. Methods in Molecular Biology, 2009, 544, 269-279.	0.4	26
36	Fast dynamics perturbation analysis for prediction of protein functional sites. BMC Structural Biology, 2008, 8, 5.	2.3	28

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37	Hidden structure in protein energy landscapes. Physical Review E, 2008, 77, 021902.	0.8	6
38	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
39	Prediction of Functional Sites in SCOP Domains using Dynamics Perturbation Analysis. Nature Precedings, 2008, , .	0.1	1
40	Domain motions of Argonaute, the catalytic engine of RNA interference. BMC Bioinformatics, 2007, 8, 470.	1.2	25
41	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
42	Interactions in Native Binding Sites Cause a Large Change in Protein Dynamics. Journal of Molecular Biology, 2006, 358, 213-223.	2.0	49
43	Ligand Binding, Protein Fluctuations, And Allosteric Free Energy. AIP Conference Proceedings, 2006, , .	0.3	7
44	Quantifying allosteric effects in proteins. Proteins: Structure, Function and Bioinformatics, 2005, 59, 697-707.	1.5	82
45	Allostery in a Coarse-Grained Model of Protein Dynamics. Physical Review Letters, 2005, 95, 198103.	2.9	146
46	Multiple Functions of a Feed-Forward-Loop Gene Circuit. Journal of Molecular Biology, 2005, 349, 501-514.	2.0	75
47	Design of gene circuits: lessons from bacteria. Nature Reviews Genetics, 2004, 5, 34-42.	7.7	206
48	Design Principles for Regulator Gene Expression in a Repressible Gene Circuit. Journal of Molecular Biology, 2003, 332, 861-876.	2.0	50
49	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
50	LARGE-SCALESHAPECHANGES INPROTEINS ANDMACROMOLECULARCOMPLEXES. Annual Review of Physical Chemistry, 2000, 51, 355-380.	4.8	70
51	A model of troponinâ€‰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
52	Protein structure determination using a database of interatomic distance probabilities. Protein Science, 1999, 8, 2720-2727.	3.1	19
53	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
54	Motions of calmodulin characterized using both Bragg and diffuse X-ray scattering. Structure, 1997, 5, 1599-1612.	1.6	95

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55	High-resolution macromolecular structure determination using CCD detectors and synchrotron radiation. Structure, 1995, 3, 835-844.	1.6	30