Michael F Crowley

List of Publications by Year
in descending order

119 papers	6,977 citations	41339 49 h-index	62593 80 g-index
120 all docs	120 docs citations	120 times ranked	7006 citing authors

#	Article	IF	Citations
1	Characterization and engineering of a plastic-degrading aromatic polyesterase. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4350-E4357.	7.1	632
2	The implementation of a fast and accurate QM/MM potential method in Amber. Journal of Computational Chemistry, 2008, 29, 1019-1031.	3.3	360
3	Revealing Natureâ€™s Cellulase Diversity: The Digestion Mechanism of Caldicellulosiruptor bescii CelA. Science, 2013, 342, 1513-1516.	12.6	253
4	Experimental and theoretical studies of a coupled chemical oscillator: phase death, multistability and in-phase and out-of-phase entrainment. The Journal of Physical Chemistry, 1989, 93, 2496-2502.	2.9	219
5	Molecular-Level Origins of Biomass Recalcitrance: Decrystallization Free Energies for Four Common Cellulose Polymorphs. Journal of Physical Chemistry B, 2011, 115, 4118-4127.	2.6	185
6	The Mechanism of Cellulose Hydrolysis by a Two-Step, Retaining Cellobiohydrolase Elucidated by Structural and Transition Path Sampling Studies. Journal of the American Chemical Society, 2014, 136, 321-329.	13.7	164
7	Crystal Structure and Computational Characterization of the Lytic Polysaccharide Monooxygenase GH61D from the Basidiomycota Fungus Phanerochaete chrysosporium. Journal of Biological Chemistry, 2013, 288, 12828-12839.	3.4	158
8	Glycosylated linkers in multimodular lignocellulose-degrading enzymes dynamically bind to cellulose. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14646-14651.	7.1	149
9	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. Nature Communications, 2018, 9, 2487.	12.8	135
10	High-Temperature Behavior of Cellulose I. Journal of Physical Chemistry B, 2011, 115, 2155-2166.	2.6	121
11	Applications of computational science for understanding enzymatic deconstruction of cellulose. Current Opinion in Biotechnology, 2011, 22, 231-238.	6.6	121
12	Identification of Amino Acids Responsible for Processivity in a Family 1 Carbohydrate-Binding Module from a Fungal Cellulase. Journal of Physical Chemistry B, 2010, 114, 1447-1453.	2.6	116
13	Predicting Enzyme Adsorption to Lignin Films by Calculating Enzyme Surface Hydrophobicity. Journal of Biological Chemistry, 2014, 289, 20960-20969.	3.4	116
14	Comparison of Cellulose Iβ Simulations with Three Carbohydrate Force Fields. Journal of Chemical Theory and Computation, 2012, 8, 735-748.	5.3	113
15	Multiple Functions of Aromatic-Carbohydrate Interactions in a Processive Cellulase Examined with Molecular Simulation. Journal of Biological Chemistry, 2011, 286, 41028-41035.	3.4	108
16	New faster CHARMM molecular dynamics engine. Journal of Computational Chemistry, 2014, 35, 406-413.	3.3	107
17	A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 9626-9630.	7.1	104
18	Molecular dynamics simulation study of DNA dodecamer d(CGCGAATTCGCG) in solution: conformation and hydration. Journal of Molecular Biology, 1997, 272, 553-572.	4.2	100

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19	Adventures in Improving the Scaling and Accuracy of a Parallel Molecular Dynamics Program. Journal of Supercomputing, 1997, 11, 255-278.	3.6	99
20	Electrically coupled Belousov-Zhabotinskii oscillators. 1. Experiments and simulations. The Journal of Physical Chemistry, 1986, 90, 1907-1915.	2.9	98
21	The O-Glycosylated Linker from the Trichoderma reesei Family 7 Cellulase Is a Flexible, Disordered Protein. Biophysical Journal, 2010, 99, 3773-3781.	0.5	96
22	Carbohydrateâ€"Protein Interactions That Drive Processive Polysaccharide Translocation in Enzymes Revealed from a Computational Study of Cellobiohydrolase Processivity. Journal of the American Chemical Society, 2014, 136, 8810-8819.	13.7	95
23	Passive membrane transport of lignin-related compounds. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23117-23123.	7.1	94
24	Towards a molecular-level theory of carbohydrate processivity in glycoside hydrolases. Current Opinion in Biotechnology, 2014, 27, 96-106.	6.6	89
25	Cellulase Linkers Are Optimized Based on Domain Type and Function: Insights from Sequence Analysis, Biophysical Measurements, and Molecular Simulation. PLoS ONE, 2012, 7, e48615.	2.5	88
26	Effects of Lytic Polysaccharide Monooxygenase Oxidation on Cellulose Structure and Binding of Oxidized Cellulose Oligomers to Cellulases. Journal of Physical Chemistry B, 2015, 119, 6129-6143.	2.6	87
27	A biophysical perspective on the cellulosome: new opportunities for biomass conversion. Current Opinion in Biotechnology, 2008, 19, 218-227.	6.6	86
28	Molecular modeling suggests induced fit of Family I carbohydrate-binding modules with a broken-chain cellulose surface. Protein Engineering, Design and Selection, 2007, 20, 179-187.	2.1	79
29	Glycoside Hydrolase Processivity Is Directly Related to Oligosaccharide Binding Free Energy. Journal of the American Chemical Society, 2013, 135, 18831-18839.	13.7	79
30	Advances in Multiscale Modeling of Lignocellulosic Biomass. ACS Sustainable Chemistry and Engineering, 2020, 8, 3512-3531.	6.7	79
31	CHAMBER: Comprehensive support for CHARMM force fields within the AMBER software. International Journal of Quantum Chemistry, 2009, 109, 3767-3772.	2.0	76
32	Binding Preferences, Surface Attachment, Diffusivity, and Orientation of a Family 1 Carbohydrate-binding Module on Cellulose. Journal of Biological Chemistry, 2012, 287, 20603-20612.	3.4	76
33	Distinct roles of N- and O-glycans in cellulase activity and stability. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13667-13672.	7.1	76
34	The Energy Landscape for the Interaction of the Family 1 Carbohydrate-Binding Module and the Cellulose Surface is Altered by Hydrolyzed Glycosidic Bonds. Journal of Physical Chemistry B, 2009, 113, 10994-11002.	2.6	75
35	New perspective on glycoside hydrolase binding to lignin from pretreated corn stover. Biotechnology for Biofuels, 2015, 8, 214.	6.2	75
36	Engineering enhanced cellobiohydrolase activity. Nature Communications, 2018, 9, 1186.	12.8	72

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37	Examination of the Î±-Chitin Structure and Decrystallization Thermodynamics at the Nanoscale. Journal of Physical Chemistry B, 2011, 115, 4516-4522.	2.6	71
38	Probing Carbohydrate Product Expulsion from a Processive Cellulase with Multiple Absolute Binding Free Energy Methods. Journal of Biological Chemistry, 2011, 286, 18161-18169.	3.4	69
39	3D Electron Tomography of Pretreated Biomass Informs Atomic Modeling of Cellulose Microfibrils. ACS Nano, 2013, 7, 8011-8019.	14.6	68
40	Biomass Particle Models with Realistic Morphology and Resolved Microstructure for Simulations of Intraparticle Transport Phenomena. Energy & Fuels, 2015, 29, 242-254.	5.1	66
41	Effects of Lytic Polysaccharide Monooxygenase Oxidation on Cellulose Structure and Binding of Oxidized Cellulose Oligomers to Cellulases. Biophysical Journal, 2013, 104, 113a.	0.5	65
42	Computational Investigation of Glycosylation Effects on a Family 1 Carbohydrate-binding Module. Journal of Biological Chemistry, 2012, 287, 3147-3155.	3.4	64
43	Message-passing neural networks for high-throughput polymer screening. Journal of Chemical Physics, 2019, 150, 234111.	3.0	63
44	The Structure of the Catalytic Domain of a Plant Cellulose Synthase and Its Assembly into Dimers. Plant Cell, 2014, 26, 2996-3009.	6.6	61
45	Tracking unstable periodic orbits in the Belousov-Zhabotinsky reaction. Physical Review Letters, 1994, 72, 2955-2958.	7.8	58
46	Decrystallization of Oligosaccharides from the Cellulose IÎ² Surface with Molecular Simulation. Journal of Physical Chemistry Letters, 2011, 2, 1546-1550.	4.6	58
47	Product Binding Varies Dramatically between Processive and Nonprocessive Cellulase Enzymes. Journal of Biological Chemistry, 2012, 287, 24807-24813.	3.4	57
48	Binding Site Dynamics and Aromaticâ€“Carbohydrate Interactions in Processive and Non-Processive Family 7 Glycoside Hydrolases. Journal of Physical Chemistry B, 2013, 117, 4924-4933.	2.6	57
49	Structural, mutagenic and inÂsilico studies of xyloglucan fucosylation in Arabidopsis thaliana suggest a waterâ€mediated mechanism. Plant Journal, 2017, 91, 931-949.	5.7	53
50	Radical Nature of C-Lignin. ACS Sustainable Chemistry and Engineering, 2016, 4, 5327-5335.	6.7	52
51	Systematic parameterization of lignin for the CHARMM force field. Green Chemistry, 2019, 21, 109-122.	9.0	51
52	The molecular origins of twist in cellulose I-beta. Carbohydrate Polymers, 2015, 125, 146-152.	10.2	50
53	Computational simulations of the Trichoderma reesei cellobiohydrolase I acting on microcrystalline cellulose IÎ²: the enzymeâ€“substrate complex. Carbohydrate Research, 2009, 344, 1984-1992.	2.3	49
54	Molecular Lignin Solubility and Structure in Organic Solvents. ACS Sustainable Chemistry and Engineering, 2020, 8, 17839-17850.	6.7	48

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55	Automated Transformation of Lignin Topologies into Atomic Structures with LigninBuilder. ACS Sustainable Chemistry and Engineering, 2019, 7, 3443-3453.	6.7	47
56	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose Iˆ². Cellulose, 2008, 15, 261-273.	4.9	46
57	Modeling of the metallo-?-lactamase fromB. fragilis: Structural and dynamic effects of inhibitor binding. Proteins: Structure, Function and Bioinformatics, 2001, 44, 448-459.	2.6	44
58	Modeling the Self-assembly of the Cellulosome Enzyme Complex. Journal of Biological Chemistry, 2011, 286, 5614-5623.	3.4	43
59	Enabling microbial syringol conversion through structure-guided protein engineering. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13970-13976.	7.1	41
60	The dissociation mechanism of processive cellulases. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23061-23067.	7.1	40
61	Nanomechanics of cellulose deformation reveal molecular defects that facilitate natural deconstruction. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9825-9830.	7.1	40
62	A Quantitative Molecular Atlas for Interactions Between Lignin and Cellulose. ACS Sustainable Chemistry and Engineering, 2019, 7, 19570-19583.	6.7	36
63	Structural and molecular dynamics studies of a C1â€oxidizing lytic polysaccharide monooxygenase from Heterobasidion irregulare reveal amino acids important for substrate recognition. FEBS Journal, 2018, 285, 2225-2242.	4.7	35
64	Initial Recognition of a Cellodextrin Chain in the Cellulose-Binding Tunnel May Affect Cellobiohydrolase Directional Specificity. Biophysical Journal, 2013, 104, 904-912.	0.5	33
65	Loop Motions Important to Product Expulsion in the Thermobifida fusca Glycoside Hydrolase Family 6 Cellobiohydrolase from Structural and Computational Studies. Journal of Biological Chemistry, 2013, 288, 33107-33117.	3.4	31
66	Computational Investigation of the pH Dependence of Loop Flexibility and Catalytic Function in Glycoside Hydrolases. Journal of Biological Chemistry, 2013, 288, 12175-12186.	3.4	31
67	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. Wiley Interdisciplinary Reviews: Energy and Environment, 2018, 7, e297.	4.1	30
68	Study of a highly accurate and fast protein-ligand docking method based on molecular dynamics. Concurrency Computation Practice and Experience, 2005, 17, 1627-1641.	2.2	29
69	Coarse-Grain Model for Glucose, Cellobiose, and Cellotetraose in Water. Journal of Chemical Theory and Computation, 2011, 7, 2137-2150.	5.3	28
70	Conversion of cellulose Iˆ± to Iˆ² via a high temperature intermediate (I-HT) and other cellulose phase transformations. Cellulose, 2012, 19, 297-306.	4.9	27
71	Who's on base? Revealing the catalytic mechanism of inverting family 6 glycoside hydrolases. Chemical Science, 2016, 7, 5955-5968.	7.4	27
72	Sugar-binding sites on the surface of the carbohydrate-binding module of CBH I from Trichoderma reesei. Carbohydrate Research, 2011, 346, 839-846.	2.3	24

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73	Membrane Permeability of Fatty Acyl Compounds Studied via Molecular Simulation. Journal of Physical Chemistry B, 2017, 121, 11311-11324.	2.6	23
74	The impact ofO-glycan chemistry on the stability of intrinsically disordered proteins. Chemical Science, 2018, 9, 3710-3715.	7.4	23
75	Studying protein folding on the grid: experiences using CHARMM on NPACI resources under Legion. , 0, , .		22
76	Protein Allostery at the Solidâ€“Liquid Interface: Endoglucanase Attachment to Cellulose Affects Glucan Clenching in the Binding Cleft. Journal of the American Chemical Society, 2011, 133, 16617-16624.	13.7	22
77	Membrane Permeability of Terpenoids Explored with Molecular Simulation. Journal of Physical Chemistry B, 2018, 122, 10349-10361.	2.6	21
78	Comparing Residue Clusters from Thermophilic and Mesophilic Enzymes Reveals Adaptive Mechanisms. PLoS ONE, 2016, 11, e0145848.	2.5	21
79	AN ADAPTIVE CONTROL ALGORITHM FOR TRACKING UNSTABLE PERIODIC ORBITS. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 1994, 04, 1311-1317.	1.7	19
80	Simulation analysis of the cellulase Cel7A carbohydrate binding module on the surface of the cellulose Iβ. Cellulose, 2014, 21, 951-971.	4.9	19
81	Glycosylation Is Vital for Industrial Performance of Hyperactive Cellulases. ACS Sustainable Chemistry and Engineering, 2019, 7, 4792-4800.	6.7	19
82	Oâ€glycosylation effects on family 1 carbohydrateâ€binding module solution structures. FEBS Journal, 2015, 282, 4341-4356.	4.7	18
83	Simulations of cellulose translocation in the bacterial cellulose synthase suggest a regulatory mechanism for the dimeric structure of cellulose. Chemical Science, 2016, 7, 3108-3116.	7.4	18
84	Iodineâ€Catalyzed Isomerization of Dimethyl Muconate. ChemSusChem, 2018, 11, 1768-1780.	6.8	18
85	Building a foundation for structureâ€based cellulosome design for cellulosic ethanol: Insight into cohesinâ€dockerin complexation from computer simulation. Protein Science, 2009, 18, 949-959.	7.6	17
86	Density Functional Theory Study of Spirodienone Stereoisomers in Lignin. ACS Sustainable Chemistry and Engineering, 2017, 5, 7188-7194.	6.7	16
87	The hydrolysis mechanism of a GH45 cellulase and its potential relation to lytic transglycosylase and expansin function. Journal of Biological Chemistry, 2020, 295, 4477-4487.	3.4	16
88	Electronic coupling through natural amino acids. Journal of Chemical Physics, 2015, 143, 225102.	3.0	15
89	Coupling and Reactions of 5-Hydroxyconiferyl Alcohol in Lignin Formation. Journal of Agricultural and Food Chemistry, 2016, 64, 4742-4750.	5.2	15
90	Endoglucanase Peripheral Loops Facilitate Complexation of Glucan Chains on Cellulose via Adaptive Coupling to the Emergent Substrate Structures. Journal of Physical Chemistry B, 2013, 117, 10750-10758.	2.6	14

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91	Molecular dynamics investigation of the MBE growth of Si on Si{110}. Surface Science, 1993, 284, 91-102.	1.9	12
92	Comparison of the simulations of cellulosic crystals with three carbohydrate force fields. Carbohydrate Research, 2016, 422, 17-23.	2.3	12
93	Coupling and Reactions of Lignols and New Lignin Monomers: A Density Functional Theory Study. ACS Sustainable Chemistry and Engineering, 2020, 8, 11033-11045.	6.7	12
94	Prediction of reaction knockouts to maximize succinate production by Actinobacillus succinogenes. PLoS ONE, 2018, 13, e0189144.	2.5	12
95	Diffraction pattern simulation of cellulose fibrils using distributed and quantized pair distances. Journal of Applied Crystallography, 2016, 49, 2244-2248.	4.5	11
96	Efficient estimation of the maximum metabolic productivity of batch systems. Biotechnology for Biofuels, 2017, 10, 28.	6.2	11
97	Transition Path Sampling Study of the Feruloyl Esterase Mechanism. Journal of Physical Chemistry B, 2021, 125, 2018-2030.	2.6	11
98	Studying protein folding on the Grid: experiences using CHARMM on NPACI resources under Legion. Concurrency Computation Practice and Experience, 2004, 16, 385-397.	2.2	10
99	Strategies to reduce endâ€product inhibition in family 48 glycoside hydrolases. Proteins: Structure, Function and Bioinformatics, 2016, 84, 295-304.	2.6	10
100	Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors. Scientific Reports, 2018, 8, 12826.	3.3	9
101	Catalytic Mechanism of Aryl-Ether Bond Cleavage in Lignin by LigF and LigG. Journal of Physical Chemistry B, 2019, 123, 10142-10151.	2.6	8
102	Controlling spatiotemporal dynamics of flame fronts. Journal of Chemical Physics, 1994, 101, 6606-6614.	3.0	7
103	Asymptotic solutions of a reduced Oregonator model of the Belousov-Zhabotinsky reaction. The Journal of Physical Chemistry, 1984, 88, 762-766.	2.9	6
104	Experimental and Modeling Studies of an Unusual Water-Filled Pore Structure with Possible Mechanistic Implications in Family 48 Cellulases. Journal of Physical Chemistry B, 2014, 118, 2306-2315.	2.6	6
105	Coupling of Flavonoid Initiation Sites with Monolignols Studied by Density Functional Theory. ACS Sustainable Chemistry and Engineering, 2021, 9, 1518-1528.	6.7	6
106	Electrically Coupled Belousov-Zhabotinsky Oscillators: A Potential Chaos Generator. Springer Series in Synergetics, 1981, , 147-153.	0.4	6
107	Mechanism and Reaction Energy Landscape for Apiose Cross-Linking by Boric Acid in Rhamnogalacturonan II. Journal of Physical Chemistry B, 2020, 124, 10117-10125.	2.6	5
108	Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes. ACS Symposium Series, 2010, , 55-73.	0.5	4

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109	Electrically Coupled Belousov-Zhabotinskii Oscillators: Experimental Observation of Chaos in a Chemical System and Identification of its Source in the Field-Noyes Equations. Lecture Notes in Biomathematics, 1986, , 68-97.	0.3	3
110	Developing improved MD codes for understanding processive cellulases. Journal of Physics: Conference Series, 2008, 125, 012049.	0.4	2
111	Computational Approaches to Study Cellulose Hydrolysis. , 0, , 306-330.		2
112	Stabilizing steady and periodic behavior in propagating flame fronts. Physica D: Nonlinear Phenomena, 1995, 84, 12-22.	2.8	1
113	Response to Comment on â€œRevealing Natureâ€™s Cellulase Diversity: The Digestion Mechanism of Caldicellulosiruptor bescii CelAâ€• Science, 2014, 344, 578-578.	12.6	1
114	A Molecular-MNIST Dataset for Machine Learning Study on Diffraction Imaging and Microscopy. , 2020, , .		1
115	Observation of a peculiar phenomenon in the cerium-ion-catalyzed Belousov-Zhabotinskii oscillator with acetylacetone in CSTR mode. Reaction Kinetics and Catalysis Letters, 1985, 28, 233-238.	0.6	0
116	Modeling the Cellulosome Using Multiscale Methods. ACS Symposium Series, 2010, , 75-98.	0.5	0
117	Estimation of the Maximum Theoretical Productivity of Fed-Batch Bioreactors * *This work was funded by the US Department of Energyâ€™s Bioen-ergy Technologies Office (DOE-BETO), Contract No. DE-AC36-08GO28308 with the National Renewable Energy Laboratory. IFAC-PapersOnLine, 2017, 50, 9883-9888.	0.9	0
118	Reply to Cosgrove: Non-enzymatic action of expansins. Journal of Biological Chemistry, 2020, 295, 6783.	3.4	0
119	Towards Elucidating Structureâ€“Spectra Relationships in Rhamnogalacturonan II: Computational Protocols for Accurate 13C and 1H Shifts for Apiose and Its Borate Esters. Frontiers in Molecular Biosciences, 2021, 8, 756219.	3.5	0