James C Gumbart

List of Publications by Year
in descending order

111 papers	21,616 citations	76196 40 h-index	25716 108 g-index
125 all docs	125 docs citations	125 times ranked	25597 citing authors

#	Article	IF	Citations
1	Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. Physical Chemistry Chemical Physics, 2022, 24, 3586-3597.	1.3	3
2	Adaptation of the periplasm to maintain spatial constraints essential for cell envelope processes and cell viability. ELife, 2022, 11, .	2.8	17
3	Resolving the Hydride Transfer Pathway in Oxidative Conversion of Proline to Pyrrole. Biochemistry, 2022, 61, 206-215.	1.2	5
4	Comprehensive structure and functional adaptations of the yeast nuclear pore complex. Cell, 2022, 185, 361-378.e25.	13.5	87
5	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
6	The Mechanism of Action of Hepatitis B Virus Capsid Assembly Modulators Can Be Predicted from Binding to Early Assembly Intermediates. Journal of Medicinal Chemistry, 2022, 65, 4854-4864.	2.9	8
7	Restoring and Enhancing the Potency of Existing Antibiotics against Drug-Resistant Gram-Negative Bacteria through the Development of Potent Small-Molecule Adjuvants. ACS Infectious Diseases, 2022, 8, 1491-1508.	1.8	10
8	Î²-Barrel proteins tether the outer membrane in many Gram-negative bacteria. Nature Microbiology, 2021, 6, 19-26.	5.9	46
9	A Novel Approach to Simulating the Gating Transitions of Mechanosensitive Channels. Biophysical Journal, 2021, 120, 185-186.	0.2	0
10	Molecular Machinery Responsible for Graphene Oxideâ€™s Distinct Inhibitory Effects toward Pseudomonas aeruginosa and Staphylococcus aureus Pathogens. ACS Applied Bio Materials, 2021, 4, 660-668.	2.3	6
11	Preparing Membrane Proteins for Simulation Using CHARMM-GUI. Methods in Molecular Biology, 2021, 2302, 237-251.	0.4	9
12	Stepwise gating of the Sec61 protein-conducting channel by Sec63 and Sec62. Nature Structural and Molecular Biology, 2021, 28, 162-172.	3.6	43
13	Bifunctional Janus Particles as Multivalent Synthetic Nanoparticle Antibodies (SNAbs) for Selective Depletion of Target Cells. Nano Letters, 2021, 21, 875-886.	4.5	24
14	Coarse-Grained Simulations of DNA Reveal Angular Dependence of Sticky-End Binding. Journal of Physical Chemistry B, 2021, 125, 4016-4024.	1.2	5
15	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. Journal of Physical Chemistry Letters, 2021, 12, 4195-4202.	2.1	19
16	Gatekeeping Ketosynthases Dictate Initiation of Assembly Line Biosynthesis of Pyrrolic Polyketides. Journal of the American Chemical Society, 2021, 143, 7617-7622.	6.6	10
17	Combinatorial phosphorylation modulates the structure and function of the G protein Î³ subunit in yeast. Science Signaling, 2021, 14, .	1.6	4
18	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. Journal of Physical Chemistry Letters, 2021, 12, 5494-5502.	2.1	44

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19	Quantifying arrhythmic long QT effects of hydroxychloroquine and azithromycin with whole-heart optical mapping and simulations. Heart Rhythm O2, 2021, 2, 394-404.	0.6	16
20	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. Biophysical Journal, 2021, 120, 3973-3982.	0.2	13
21	Inward-facing glycine residues create sharp turns in Î²-barrel membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183662.	1.4	7
22	ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV. Chemical Communications, 2021, 57, 5949-5952.	2.2	26
23	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
24	Folding and Insertion of Transmembrane Helices at the ER. International Journal of Molecular Sciences, 2021, 22, 12778.	1.8	5
25	Plasticity within the barrel domain of BamA mediates a hybrid-barrel mechanism by BAM. Nature Communications, 2021, 12, 7131.	5.8	34
26	Presence of substrate aids lateral gate separation in LptD. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183025.	1.4	17
27	A Minimal Membrane Metal Transport System: Dynamics and Energetics of mer Proteins. Journal of Computational Chemistry, 2020, 41, 528-537.	1.5	5
28	Parameterization of a drug molecule with a halogen Ï*f*-hole particle using ffTK: Implementation, testing, and comparison. Journal of Chemical Physics, 2020, 153, 164104.	1.2	11
29	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
30	Fatal arrhythmias: Another reason why doctors remain cautious about chloroquine/hydroxychloroquine for treating COVID-19. Heart Rhythm, 2020, 17, 1445-1451.	0.3	25
31	The Effect of (â^)-Epigallocatechin-3-Gallate on the Amyloid-Î² Secondary Structure. Biophysical Journal, 2020, 119, 349-359.	0.2	18
32	Synergistic Biophysical Techniques Reveal Structural Mechanisms of Engineered Cationic Antimicrobial Peptides in Lipid Model Membranes. Chemistry - A European Journal, 2020, 26, 6247-6256.	1.7	9
33	BamA is required for autotransporter secretion. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129581.	1.1	10
34	Outer membrane protein size and LPS O-antigen define protective antibody targeting to the Salmonella surface. Nature Communications, 2020, 11, 851.	5.8	49
35	Membrane thinning and lateral gating are consistent features of BamA across multiple species. PLoS Computational Biology, 2020, 16, e1008355.	1.5	22
36	Structural insight into toxin secretion by contact-dependent growth inhibition transporters. ELife, 2020, 9, .	2.8	14

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37	Tyrosine, cysteine, and proton coupled electron transfer in a ribonucleotide reductase-inspired beta hairpin maquette. Chemical Communications, 2019, 55, 9399-9402.	2.2	9
38	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. Journal of Chemical Theory and Computation, 2019, 15, 4673-4686.	2.3	85
39	Stable calcium-free myocilin olfactomedin domain variants reveal challenges in differentiating between benign and glaucoma-causing mutations. Journal of Biological Chemistry, 2019, 294, 12717-12728.	1.6	13
40	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. ACS Infectious Diseases, 2019, 5, 1926-1935.	1.8	21
41	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. Biophysical Journal, 2019, 116, 648-658.	0.2	27
42	A novel human IL2RB mutation results in T and NK cellâ€“driven immune dysregulation. Journal of Experimental Medicine, 2019, 216, 1255-1267.	4.2	64
43	Structure and Function of Tryptophanâ€“Tyrosine Dyads in Biomimetic Î² Hairpins. Journal of Physical Chemistry B, 2019, 123, 2780-2791.	1.2	6
44	ATP-Dependent Signaling in Simulations of a Revised Model of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). Journal of Physical Chemistry B, 2019, 123, 3177-3188.	1.2	4
45	Non-detergent isolation of a cyanobacterial photosystem I using styrene maleic acid alternating copolymers. RSC Advances, 2019, 9, 31781-31796.	1.7	19
46	Computed Free Energies of Peptide Insertion into Bilayers are Independent of Computational Method. Journal of Membrane Biology, 2018, 251, 345-356.	1.0	22
47	Diverse Protein-Folding Pathways and Functions of Î²-Hairpins and Î²-Sheets. , 2018, , 1-20.		0
48	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2018, 58, 556-560.	2.5	51
49	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2018, 14, 784-798.	2.3	20
50	Transmembrane but not soluble helices fold inside the ribosome tunnel. Nature Communications, 2018, 9, 5246.	5.8	36
51	Distribution of mechanical stress in the Escherichia coli cell envelope. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2566-2575.	1.4	66
52	Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. Environmental Science: Nano, 2018, 5, 2117-2128.	2.2	22
53	C-terminal kink formation is required for lateral gating in BamA. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7942-E7949.	3.3	42
54	Folding free energy landscapes of Î²-sheets with non-polarizable and polarizable CHARMM force fields. Journal of Chemical Physics, 2018, 149, 072317.	1.2	28

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55	The Î²-barrel assembly machinery in motion. Nature Reviews Microbiology, 2017, 15, 197-204.	13.6	174
56	Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired Î²-Hairpin Maquette Determined through Spectroscopy and Simulation. Journal of Physical Chemistry B, 2017, 121, 3536-3545.	1.2	15
57	Toward the rational design of macrolide antibiotics to combat resistance. Chemical Biology and Drug Design, 2017, 90, 641-652.	1.5	10
58	Structural basis for substrate selection by the translocation and assembly module of the Î²â€barrel assembly machinery. Molecular Microbiology, 2017, 106, 142-156.	1.2	29
59	Producing membrane proteins one simulation at a time. Journal of Biological Chemistry, 2017, 292, 19546-19547.	1.6	1
60	Structure and Misfolding of the Flexible Tripartite Coiled-Coil Domain of Glaucoma-Associated Myocilin. Structure, 2017, 25, 1697-1707.e5.	1.6	26
61	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	2.5	174
62	Membrane proteins: Where theory meets experiment. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1553-1555.	1.4	3
63	Structural and Functional Characterization of the LPS Transporter LptDE from Gram-Negative Pathogens. Structure, 2016, 24, 965-976.	1.6	110
64	Decrypting protein insertion through the translocon with free-energy calculations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1663-1671.	1.4	15
65	Transitions of Double-Stranded DNA Between the A- and B-Forms. Journal of Physical Chemistry B, 2016, 120, 8449-8456.	1.2	38
66	Role of the Native Outer-Membrane Environment on the Transporter BtuB. Biophysical Journal, 2016, 111, 1409-1417.	0.2	48
67	Accelerating the use of molecular modeling in the high school classroom with <scp>VMD</scp> Lite. Biochemistry and Molecular Biology Education, 2016, 44, 124-129.	0.5	5
68	DNA Scrunching in the Packaging of Viral Genomes. Journal of Physical Chemistry B, 2016, 120, 6200-6207.	1.2	10
69	Coarse-Grained Molecular Dynamics Simulations of the Bacterial Cell Wall. Methods in Molecular Biology, 2016, 1440, 247-270.	0.4	3
70	Living on the edge: Simulations of bacterial outer-membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1753-1759.	1.4	37
71	Parametrization of macrolide antibiotics using the force field toolkit. Journal of Computational Chemistry, 2015, 36, 2052-2063.	1.5	15
72	Conformational Changes of the Clamp of the Protein Translocation ATPase SecA. Journal of Molecular Biology, 2015, 427, 2348-2359.	2.0	26

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73	Coarse-grained simulations of bacterial cell wall growth reveal that local coordination alone can be sufficient to maintain rod shape. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3689-98.	3.3	50
74	Structural and biophysical characterization of an epitope-specific engineered Fab fragment and complexation with membrane proteins: implications for co-crystallization. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 896-906.	2.5	13
75	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. Journal of Physical Chemistry B, 2015, 119, 1129-1151.	1.2	351
76	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. PLoS Computational Biology, 2014, 10, e1003475.	1.5	92
77	Thermodynamics of Deca-alanine Folding in Water. Journal of Chemical Theory and Computation, 2014, 10, 2836-2844.	2.3	44
78	Structure of the SecY channel during initiation of protein translocation. Nature, 2014, 506, 102-106.	13.7	138
79	Lateral Opening and Exit Pore Formation Are Required for BamA Function. Structure, 2014, 22, 1055-1062.	1.6	166
80	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	3.0	115
81	Efficient Determination of Proteinâ€“Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	2.3	188
82	Structural insight into the biogenesis of Î²-barrel membrane proteins. Nature, 2013, 501, 385-390.	13.7	368
83	IcmQ in the Type 4b Secretion System Contains an NAD+ Binding Domain. Structure, 2013, 21, 1361-1373.	1.6	6
84	Reconciling the Roles of Kinetic and Thermodynamic Factors in Membraneâ€“Protein Insertion. Journal of the American Chemical Society, 2013, 135, 2291-2297.	6.6	41
85	Rapid parameterization of small molecules using the force field toolkit. Journal of Computational Chemistry, 2013, 34, 2757-2770.	1.5	403
86	The mobility of two kinase domains in the <scp>E</scp>scherichia coli chemoreceptor array varies with signalling state. Molecular Microbiology, 2013, 89, 831-841.	1.2	59
87	Architecture and assembly of the <scp>G</scp>ramâ€positive cell wall. Molecular Microbiology, 2013, 88, 664-672.	1.2	116
88	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	2.3	298
89	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. Journal of General Physiology, 2013, 142, 465-475.	0.9	51
90	Structural basis for iron piracy by pathogenic Neisseria. Nature, 2012, 483, 53-58.	13.7	239

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91	Molecular Basis for the Activation of a Catalytic Asparagine Residue in a Self-Cleaving Bacterial Autotransporter. Journal of Molecular Biology, 2012, 415, 128-142.	2.0	40
92	Determination of Membrane-Insertion Free Energies by Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 795-801.	0.2	49
93	Mechanisms of SecM-Mediated Stalling in the Ribosome. Biophysical Journal, 2012, 103, 331-341.	0.2	82
94	Free Energy of Nascent-Chain Folding in the Translocon. Journal of the American Chemical Society, 2011, 133, 7602-7607.	6.6	36
95	Applications of the molecular dynamics flexible fitting method. Journal of Structural Biology, 2011, 173, 420-427.	1.3	44
96	Cryo-EM structure of the ribosomeâ€“SecYE complex in the membrane environment. Nature Structural and Molecular Biology, 2011, 18, 614-621.	3.6	264
97	Symmetry-Restrained Flexible Fitting for Symmetric EM Maps. Structure, 2011, 19, 1211-1218.	1.6	66
98	Free-energy cost for translocon-assisted insertion of membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3596-3601.	3.3	74
99	Selfâ€Assembly of Photosynthetic Membranes. ChemPhysChem, 2010, 11, 1154-1159.	1.0	23
100	Regulation of the Protein-Conducting Channel by a Bound Ribosome. Structure, 2009, 17, 1453-1464.	1.6	107
101	Coupling of Calcium and Substrate Binding through Loop Alignment in the Outer-Membrane Transporter BtuB. Journal of Molecular Biology, 2009, 393, 1129-1142.	2.0	30
102	Protein-Induced Membrane Curvature Investigated through Molecular Dynamics Flexible Fitting. Biophysical Journal, 2009, 97, 321-329.	0.2	68
103	Membrane Curvature Induced by Aggregates of LH2s and Monomeric LH1s. Biophysical Journal, 2009, 97, 2978-2984.	0.2	28
104	Structure of Monomeric Yeast and Mammalian Sec61 Complexes Interacting with the Translating Ribosome. Science, 2009, 326, 1369-1373.	6.0	263
105	Intrinsic Curvature Properties of Photosynthetic Proteins in Chromatophores. Biophysical Journal, 2008, 95, 2822-2836.	0.2	73
106	The Roles of Pore Ring and Plug in the SecY Protein-conducting Channel. Journal of General Physiology, 2008, 132, 709-719.	0.9	36
107	Structural Determinants of Lateral Gate Opening in the Protein Translocon. Biochemistry, 2007, 46, 11147-11157.	1.2	59
108	Mechanics of Force Propagation in TonB-Dependent Outer Membrane Transport. Biophysical Journal, 2007, 93, 496-504.	0.2	98

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109	Molecular Dynamics Studies of the Archaeal Translocon. Biophysical Journal, 2006, 90, 2356-2367.	0.2	78
110	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	1.5	15,208
111	The Role of Extracellular Loops in the Folding of Outer Membrane Protein X (OmpX) of Escherichia coli. Frontiers in Molecular Biosciences, 0, 9, .	1.6	3