Margaret S Cheung

List of Publications by Year
in descending order

82 papers	3,752 citations	172207 29 h-index	128067 60 g-index
86 all docs	86 docs citations	86 times ranked	3335 citing authors

#	Article	IF	Citations
1	Molecular crowding enhances native state stability and refolding rates of globular proteins. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 4753-4758.	3.3	512
2	Protein folding mediated by solvation: Water expulsion and formation of the hydrophobic core occur after the structural collapse. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 685-690.	3.3	461
3	Structure, function, and folding of phosphoglycerate kinase are strongly perturbed by macromolecular crowding. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 17586-17591.	3.3	284
4	Molecular crowding enhances native structure and stability of Î±/Î² protein flavodoxin. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18976-18981.	3.3	245
5	Crowded, cell-like environment induces shape changes in aspherical protein. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11754-11759.	3.3	194
6	Domain swapping is a consequence of minimal frustration. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 13786-13791.	3.3	164
7	Factors Defining Effects of Macromolecular Crowding on Protein Stability: An in Vitro/in Silico Case Study Using Cytochrome c. Biochemistry, 2010, 49, 6519-6530.	1.2	137
8	Nanoporeâ€“Protein Interactions Dramatically Alter Stability and Yield of the Native State in Restricted Spaces. Journal of Molecular Biology, 2006, 357, 632-643.	2.0	85
9	Pathways of Electron Transfer in Escherichia coli DNA Photolyase:Trp306 to FADH. Biophysical Journal, 1999, 76, 1241-1249.	0.2	77
10	Macromolecular Crowding Modulates Folding Mechanism of Î±/Î² Protein Apoflavodoxin. Biophysical Journal, 2009, 96, 671-680.	0.2	77
11	Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2018, 14, 6287-6294.	2.3	76
12	Effects of Crowding and Confinement on the Structures of the Transition State Ensemble in Proteins. Journal of Physical Chemistry B, 2007, 111, 8250-8257.	1.2	71
13	Electrostatics, structure prediction, and the energy landscapes for protein folding and binding. Protein Science, 2016, 25, 255-269.	3.1	71
14	Effects of macromolecular crowding agents on protein folding in vitro and in silico. Biophysical Reviews, 2013, 5, 137-145.	1.5	69
15	Folding, Stability and Shape of Proteins in Crowded Environments: Experimental and Computational Approaches. International Journal of Molecular Sciences, 2009, 10, 572-588.	1.8	65
16	The Effect of Macromolecular Crowding, Ionic Strength and Calcium Binding on Calmodulin Dynamics. PLoS Computational Biology, 2011, 7, e1002114.	1.5	60
17	Exploring the Interplay between Topology and Secondary Structural Formation in the Protein Folding Problem. Journal of Physical Chemistry B, 2003, 107, 11193-11200.	1.2	59
18	Modulation of Calmodulin Plasticity by the Effect of Macromolecular Crowding. Journal of Molecular Biology, 2009, 391, 933-943.	2.0	52

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19	Protein recognition and selection through conformational and mutually induced fit. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20545-20550.	3.3	50
20	Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoidâ€“Porphyrinâ€“C₆₀ Molecular Triad. Journal of Physical Chemistry Letters, 2015, 6, 1231-1237.	2.1	48
21	The energy landscape for protein folding and possible connections to function. Polymer, 2004, 45, 547-555.	1.8	45
22	Effects of Macromolecular Crowding on Burst Phase Kinetics of Cytochrome c Folding. Biochemistry, 2012, 51, 9836-9845.	1.2	43
23	Folding dynamics of Trp-cage in the presence of chemical interference and macromolecular crowding. I. Journal of Chemical Physics, 2011, 135, 175101.	1.2	36
24	Multiscale investigation of chemical interference in proteins. Journal of Chemical Physics, 2010, 132, 175101.	1.2	34
25	Computational Study of Charge-Transfer Dynamics in the Carotenoidâ€“Porphyrinâ€“C₆₀ Molecular Triad Solvated in Explicit Tetrahydrofuran and Its Spectroscopic Signature. Journal of Physical Chemistry C, 2018, 122, 11288-11299.	1.5	34
26	Crowding Effects on the Structural Transitions in a Flexible Helical Homopolymer. Physical Review Letters, 2009, 102, 118101.	2.9	32
27	Molecular origin of the weak susceptibility of kinesin velocity to loads and its relation to the collective behavior of kinesins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8611-E8617.	3.3	32
28	Mechanisms of cooperativity underlying sequence-independent Î²-sheet formation. Journal of Chemical Physics, 2002, 116, 4353-4365.	1.2	31
29	Manipulating Biopolymer Dynamics by Anisotropic Nanoconfinement. Nano Letters, 2007, 7, 3438-3442.	4.5	31
30	Assemblies of calcium/calmodulin-dependent kinase II with actin and their dynamic regulation by calmodulin in dendritic spines. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18937-18942.	3.3	31
31	A Physics-Based Approach of Coarse-Graining the Cytoplasm of Escherichia coli (CGCYTO). Biophysical Journal, 2012, 102, 2353-2361.	0.2	30
32	A Structural Model of Polyglutamine Determined from a Host-Guest Method Combining Experiments and Landscape Theory. Biophysical Journal, 2004, 87, 1900-1918.	0.2	26
33	Comparison of chemical and thermal protein denaturation by combination of computational and experimental approaches. II. Journal of Chemical Physics, 2011, 135, 175102.	1.2	26
34	Crowding-Induced Elongated Conformation of Urea-Unfolded Apoazurin: Investigating the Role of Crowder Shape in Silico. Journal of Physical Chemistry B, 2019, 123, 3607-3617.	1.2	25
35	Charge transfer rate constants for the carotenoid-porphyrin-C60 molecular triad dissolved in tetrahydrofuran: The spin-boson model vs the linearized semiclassical approximation. Journal of Chemical Physics, 2020, 153, 044105.	1.2	25
36	Influence of the Shape of Crowding Particles on the Structural Transitions in a Polymer. Journal of Physical Chemistry B, 2012, 116, 8513-8522.	1.2	23

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37	The role of the Arp2/3 complex in shaping the dynamics and structures of branched actomyosin networks. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10825-10831.	3.3	22
38	Multiscale Simulation of the Ground and Photo-Induced Charge-Separated States of a Molecular Triad in Polar Organic Solvent: Exploring the Conformations, Fluctuations, and Free Energy Landscapes. Journal of Physical Chemistry B, 2013, 117, 12065-12075.	1.2	21
39	Where soft matter meets living matterâ€"protein structure, stability, and folding in the cell. Current Opinion in Structural Biology, 2013, 23, 212-217.	2.6	21
40	Biophysical Properties of Membrane-Active Peptides Based on Micelle Modeling: A Case Study of Cell-Penetrating and Antimicrobial Peptides. Journal of Physical Chemistry B, 2010, 114, 13726-13735.	1.2	19
41	Conformational frustration in calmodulinâ€"target recognition. Journal of Molecular Recognition, 2015, 28, 74-86.	1.1	19
42	Molecular Dynamics Ensemble Refinement of Intrinsically Disordered Peptides According to Deconvoluted Spectra from Circular Dichroism. Biophysical Journal, 2020, 118, 1665-1678.	0.2	18
43	Multiscale Simulation on a Light-Harvesting Molecular Triad. Journal of Physical Chemistry B, 2012, 116, 8460-8473.	1.2	16
44	Towards developing principles of protein folding and dynamics in the cell. Physical Biology, 2018, 15, 063001.	0.8	16
45	Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein. Physical Review X, 2019, 9, .	2.8	16
46	Molecular-Level Exploration of the Structure-Function Relations Underlying Interfacial Charge Transfer in the Subphthalocyanine/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math> Organic Photovoltaic System. Physical Review Applied, 2020, 13, .	1.5	14
47	Residue-Specific Analysis of Frustration in the Folding Landscape of Repeat Î²/Î± Protein Apoflavodoxin. Journal of Molecular Biology, 2010, 396, 75-89.	2.0	13
48	Lessons in Protein Design from Combined Evolution and Conformational Dynamics. Scientific Reports, 2015, 5, 14259.	1.6	13
49	Correlation between Gene Variants, Signaling Pathways, and Efficacy of Chemotherapy Drugs against Colon Cancers. Cancer Informatics, 2016, 15, CIN.S34506.	0.9	13
50	Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10052-10057.	3.3	13
51	Photoinduced Charge Transfer Dynamics in the Carotenoidâ€"Porphyrinâ€"C₆₀ Triad via the Linearized Semiclassical Nonequilibrium Fermiâ€™s Golden Rule. Journal of Physical Chemistry B, 2020, 124, 9579-9591.	1.2	13
52	Cysteine-Cysteine Contact Preference Leads to Target-Focusing in Protein Folding. Biophysical Journal, 2007, 93, 938-951.	0.2	12
53	Relative Cosolute Size Influences the Kinetics of Protein-Protein Interactions. Biophysical Journal, 2015, 109, 510-520.	0.2	11
54	Opposing Intermolecular Tuning of Ca2+ Affinity for Calmodulin by Neurogranin and CaMKII Peptides. Biophysical Journal, 2017, 112, 1105-1119.	0.2	11

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55	CATS: A Tool for Clustering the Ensemble of Intrinsically Disordered Peptides on a Flat Energy Landscape. Journal of Physical Chemistry B, 2018, 122, 11807-11816.	1.2	11
56	Induced polarization restricts the conformational distribution of a light-harvesting molecular triad in the ground state. Physical Chemistry Chemical Physics, 2017, 19, 22969-22980.	1.3	10
57	Computational Studies of the Reversible Domain Swapping of p13suc1. Biophysical Journal, 2005, 89, 2693-2700.	0.2	8
58	Impact of hydrodynamic interactions on protein folding rates depends on temperature. Physical Review E, 2018, 97, 032402.	0.8	7
59	Competition of individual domain folding with inter-domain interaction in WW domain engineered repeat proteins. Physical Chemistry Chemical Physics, 2019, 21, 24393-24405.	1.3	7
60	On the Interplay between Electronic Structure and Polarizable Force Fields When Calculating Solution-Phase Charge-Transfer Rates. Journal of Chemical Theory and Computation, 2020, 16, 6481-6490.	2.3	6
61	Determining the atomic charge of calcium ion requires the information of its coordination geometry in an EF-hand motif. Journal of Chemical Physics, 2021, 154, 124104.	1.2	6
62	Insights from graph theory on the morphologies of actomyosin networks with multilinkers. Physical Review E, 2020, 102, 062420.	0.8	6
63	A Robust Communication Framework for Parallel Execution on Volunteer PC Grids. , 2011, , .		5
64	Coarse-Grained Modeling and Molecular Dynamics Simulations of Ca2+-Calmodulin. Frontiers in Molecular Biosciences, 2021, 8, 661322.	1.6	5
65	A Tale of Two Desolvation Potentials: An Investigation of Protein Behavior under High Hydrostatic Pressure. Journal of Physical Chemistry B, 2020, 124, 1619-1627.	1.2	4
66	CTRAMER: An open-source software package for correlating interfacial charge transfer rate constants with donor/acceptor geometries in organic photovoltaic materials. Journal of Chemical Physics, 2021, 154, 214108.	1.2	4
67	Correlating Interfacial Charge Transfer Rates with Interfacial Molecular Structure in the Tetraphenyldibenzoperiflanthene/C₇₀ Organic Photovoltaic System. Journal of Physical Chemistry Letters, 2022, 13, 763-769.	2.1	4
68	A generalized Flory-Stockmayer kinetic theory of connectivity percolation and rigidity percolation of cytoskeletal networks. PLoS Computational Biology, 2022, 18, e1010105.	1.5	4
69	Effects of Protein Crowders and Charge on the Folding of Superoxide Dismutase 1 Variants: A Computational Study. Journal of Physical Chemistry B, 2022, 126, 4458-4471.	1.2	4
70	An Execution Environment for Robust Parallel Computing on Volunteer PC Grids. , 2012, , .		3
71	Theoretical Investigations of the Role of Mutations in Dynamics of Kinesin Motor Proteins. Journal of Physical Chemistry B, 2018, 122, 4653-4661.	1.2	3
72	The Zero-Order Loop in Apoazurin Modulates Folding Mechanism In Silico. Journal of Physical Chemistry B, 2021, 125, 3501-3509.	1.2	3

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73	Forecasting Avalanches in Branched Actomyosin Networks with Network Science and Machine Learning. Journal of Physical Chemistry B, 2021, 125, 11591-11605.	1.2	3
74	Hydrophobic Interactions of Hexane in Nanosized Water Droplets. Journal of Physical Chemistry B, 2009, 113, 12337-12342.	1.2	2
75	Gecko. , 2019, , .		2
76	Understanding protein-complex assembly through grand canonical maximum entropy modeling. Physical Review Research, 2021, 3, .	1.3	2
77	Towards a portable hierarchical view of distributed shared memory systems. , 2020, , .		1
78	Editorial: RMP: Looking Forward. Reviews of Modern Physics, 2019, 91, .	16.4	0
79	pointerchain: Tracing pointers to their roots â€“ A case study in molecular dynamics simulations. Parallel Computing, 2019, 85, 190-203.	1.3	0
80	Editorial overview: Protein folding and binding: from protein folding in vitro to hierarchical assembly in vivo. Current Opinion in Structural Biology, 2021, 66, vi-vii.	2.6	0
81	Path forward for softwarization to tackle evolving hardware. , 2018, , .		0
82	Calmodulin, Models of. , 2022, , 670-673.		0