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	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
2	A generalized Flory-Stockmayer kinetic theory of connectivity percolation and rigidity percolation of cytoskeletal networks. PLoS Computational Biology, 2022, 18, e1010105.	1.5	4
3	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
4	Calmodulin, Models of. , 2022, , 670-673.		0
5	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
6	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
7	The Zero-Order Loop in Apoazurin Modulates Folding Mechanism In Silico. Journal of Physical Chemistry B, 2021, 125, 3501-3509.	1.2	3
8	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
9	Coarse-Grained Modeling and Molecular Dynamics Simulations of Ca2+-Calmodulin. Frontiers in Molecular Biosciences, 2021, 8, 661322.	1.6	5
10	Understanding protein-complex assembly through grand canonical maximum entropy modeling. Physical Review Research, 2021, 3, .	1.3	2
11	Forecasting Avalanches in Branched Actomyosin Networks with Network Science and Machine Learning. Journal of Physical Chemistry B, 2021, 125, 11591-11605.	1.2	3
12	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
13	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
14	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
15	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
16	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
17	Molecular Dynamics Ensemble Refinement of Intrinsically Disordered Peptides According to Deconvoluted Spectra from Circular Dichroism. Biophysical Journal, 2020, 118, 1665-1678.	0.2	18
18	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

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19	Towards a portable hierarchical view of distributed shared memory systems. , 2020, , .		1
20	Insights from graph theory on the morphologies of actomyosin networks with multilinkers. Physical Review E, 2020, 102, 062420.	0.8	6
21	Editorial: RMP: Looking Forward. Reviews of Modern Physics, 2019, 91, .	16.4	0
22	pointerchain: Tracing pointers to their roots â€“ A case study in molecular dynamics simulations. Parallel Computing, 2019, 85, 190-203.	1.3	0
23	Gecko. , 2019, , .		2
24	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
25	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
26	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
27	Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein. Physical Review X, 2019, 9, .	2.8	16
28	Impact of hydrodynamic interactions on protein folding rates depends on temperature. Physical Review E, 2018, 97, 032402.	0.8	7
29	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
30	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
31	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
32	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
33	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
34	Towards developing principles of protein folding and dynamics in the cell. Physical Biology, 2018, 15, 063001.	0.8	16
35	Path forward for softwarization to tackle evolving hardware. , 2018, , .		0
36	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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37	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
38	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
39	Correlation between Gene Variants, Signaling Pathways, and Efficacy of Chemotherapy Drugs against Colon Cancers. Cancer Informatics, 2016, 15, CIN.S34506.	0.9	13
40	Electrostatics, structure prediction, and the energy landscapes for protein folding and binding. Protein Science, 2016, 25, 255-269.	3.1	71
41	Lessons in Protein Design from Combined Evolution and Conformational Dynamics. Scientific Reports, 2015, 5, 14259.	1.6	13
42	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
43	Conformational frustration in calmodulinâ€“target recognition. Journal of Molecular Recognition, 2015, 28, 74-86.	1.1	19
44	Relative Cosolute Size Influences the Kinetics of Protein-Protein Interactions. Biophysical Journal, 2015, 109, 510-520.	0.2	11
45	Effects of macromolecular crowding agents on protein folding in vitro and in silico. Biophysical Reviews, 2013, 5, 137-145.	1.5	69
46	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
47	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
48	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
49	An Execution Environment for Robust Parallel Computing on Volunteer PC Grids. , 2012, , .		3
50	Effects of Macromolecular Crowding on Burst Phase Kinetics of Cytochrome c Folding. Biochemistry, 2012, 51, 9836-9845.	1.2	43
51	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
52	Multiscale Simulation on a Light-Harvesting Molecular Triad. Journal of Physical Chemistry B, 2012, 116, 8460-8473.	1.2	16
53	A Physics-Based Approach of Coarse-Graining the Cytoplasm of Escherichia coli (CGCYTO). Biophysical Journal, 2012, 102, 2353-2361.	0.2	30
54	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

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55	A Robust Communication Framework for Parallel Execution on Volunteer PC Grids. , 2011, , .		5
56	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
57	The Effect of Macromolecular Crowding, Ionic Strength and Calcium Binding on Calmodulin Dynamics. PLoS Computational Biology, 2011, 7, e1002114.	1.5	60
58	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
59	Multiscale investigation of chemical interference in proteins. Journal of Chemical Physics, 2010, 132, 175101.	1.2	34
60	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
61	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
62	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
63	Crowding Effects on the Structural Transitions in a Flexible Helical Homopolymer. Physical Review Letters, 2009, 102, 118101.	2.9	32
64	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
65	Hydrophobic Interactions of Hexane in Nanosized Water Droplets. Journal of Physical Chemistry B, 2009, 113, 12337-12342.	1.2	2
66	Modulation of Calmodulin Plasticity by the Effect of Macromolecular Crowding. Journal of Molecular Biology, 2009, 391, 933-943.	2.0	52
67	Macromolecular Crowding Modulates Folding Mechanism of Î±/Î² Protein Apoflavodoxin. Biophysical Journal, 2009, 96, 671-680.	0.2	77
68	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
69	Manipulating Biopolymer Dynamics by Anisotropic Nanoconfinement. Nano Letters, 2007, 7, 3438-3442.	4.5	31
70	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
71	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
72	Cysteine-Cysteine Contact Preference Leads to Target-Focusing in Protein Folding. Biophysical Journal, 2007, 93, 938-951.	0.2	12

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73	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
74	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
75	Computational Studies of the Reversible Domain Swapping of p13suc1. Biophysical Journal, 2005, 89, 2693-2700.	0.2	8
76	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
77	The energy landscape for protein folding and possible connections to function. Polymer, 2004, 45, 547-555.	1.8	45
78	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
79	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
80	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
81	Mechanisms of cooperativity underlying sequence-independent Î²-sheet formation. Journal of Chemical Physics, 2002, 116, 4353-4365.	1.2	31
82	Pathways of Electron Transfer in Escherichia coli DNA Photolyase:Trp306 to FADH. Biophysical Journal, 1999, 76, 1241-1249.	0.2	77