Fabio Sterpone

List of Publications by Year
in descending order

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86	5,151	136885	88593
papers	citations	32 h-index	70 g-index

87	87	87	5015
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Small Oligomers of AÎ²42 Protein in the Bulk Solution with AlphaFold2. ACS Chemical Neuroscience, 2022, 13, 711-713.	1.7	14
2	Mesoscale biosimulations within a unified framework: from proteins to plasmids. Molecular Simulation, 2021, 47, 101-112.	0.9	2
3	Hydroxy Channelsâ€“Adaptive Pathways for Selective Water Cluster Permeation. Journal of the American Chemical Society, 2021, 143, 4224-4233.	6.6	27
4	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	23.0	406
5	Stabilizing or Destabilizing: Simulations of Chymotrypsin Inhibitor 2 under Crowding Reveal Existence of a Crossover Temperature. Journal of Physical Chemistry Letters, 2021, 12, 1741-1746.	2.1	11
6	Multi-Scale Simulations and Neutron Scattering Experiments Reveal Dynamical Properties of the Bacterial Cytoplasm Near Cell-Death Temperature. Biophysical Journal, 2021, 120, 298a-299a.	0.2	0
7	Molecular dynamics simulations reveal statistics and microscopic mechanisms of water permeation in membrane-embedded artificial water channel nanoconstructs. Journal of Chemical Physics, 2021, 154, 184102.	1.2	5
8	Specific Interactions and Environment Flexibility Tune Protein Stability under Extreme Crowding. Journal of Physical Chemistry B, 2021, 125, 6103-6111.	1.2	7
9	Biochemical, structural and dynamical studies reveal strong differences in the thermal-dependent allosteric behavior of two extremophilic lactate dehydrogenases. Journal of Structural Biology, 2021, 213, 107769.	1.3	4
10	In-silico analysis of airflow dynamics and particle transport within a human nasal cavity. Journal of Computational Science, 2021, 54, 101411.	1.5	1
11	Computational Insights into the Unfolding of a Destabilized Superoxide Dismutase 1 Mutant. Biology, 2021, 10, 1240.	1.3	1
12	Sequestration of Proteins in Stress Granules Relies on the In-Cell but Not the In Vitro Folding Stability. Journal of the American Chemical Society, 2021, 143, 19909-19918.	6.6	14
13	Exposure of Von Willebrand Factor Cleavage Site in A1A2A3-Fragment under Extreme Hydrodynamic Shear. Polymers, 2021, 13, 3912.	2.0	10
14	Aggregation of disease-related peptides. Progress in Molecular Biology and Translational Science, 2020, 170, 435-460.	0.9	19
15	Differences in thermal structural changes and melting between mesophilic and thermophilic dihydrofolate reductase enzymes. Physical Chemistry Chemical Physics, 2020, 22, 18361-18373.	1.3	18
16	Thermal Adaptation of Enzymes: Impacts of Conformational Shifts on Catalytic Activation Energy and Optimum Temperature. Chemistry - A European Journal, 2020, 26, 10045-10056.	1.7	19
17	Protein thermal stability. Progress in Molecular Biology and Translational Science, 2020, 170, 239-272.	0.9	11
18	The Unfolding Journey of Superoxide Dismutase 1 Barrels under Crowding: Atomistic Simulations Shed Light on Intermediate States and Their Interactions with Crowders. Journal of Physical Chemistry Letters, 2020, 11, 4206-4212.	2.1	18

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19	Temperature Unmasks Allosteric Propensity in a Thermophilic Malate Dehydrogenase via Dewetting and Collapse. Journal of Physical Chemistry B, 2020, 124, 1001-1008.	1.2	9
20	Using Computer Simulations and Virtual Reality to Understand, Design and Optimize Artificial Water Channels. Lecture Notes in Bioengineering, 2020, , 78-99.	0.3	2
21	Tribute to Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10591-10593.	1.2	0
22	OPEP6: A New Constant-pH Molecular Dynamics Simulation Scheme with OPEP Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2019, 15, 3875-3888.	2.3	27
23	Multiscale Aggregation of the Amyloid AÎ²_{16â€“22} Peptide: From Disordered Coagulation and Lateral Branching to Amorphous Prefibrils. Journal of Physical Chemistry Letters, 2019, 10, 1594-1599.	2.1	29
24	Stability Effect of Quinary Interactions Reversed by Single Point Mutations. Journal of the American Chemical Society, 2019, 141, 4660-4669.	6.6	61
25	Amyloid-Î²(29â€“42) Dimeric Conformations in Membranes Rich in Omega-3 and Omega-6 Polyunsaturated Fatty Acids. Journal of Physical Chemistry B, 2019, 123, 2687-2696.	1.2	14
26	Advancing Multi-Scale Simulation Methods for Biological Membrane Systems. Biophysical Journal, 2019, 116, 373a-374a.	0.2	0
27	Modelling lipid systems in fluid with Lattice Boltzmann Molecular Dynamics simulations and hydrodynamics. Scientific Reports, 2019, 9, 16450.	1.6	22
28	Molecular Mechanism of Protein Unfolding under Shear: A Lattice Boltzmann Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 1573-1579.	1.2	23
29	Probing the quality control mechanism of the Escherichia coli twin-arginine translocase with folding variants of a de novoâ€“designed heme protein. Journal of Biological Chemistry, 2018, 293, 6672-6681.	1.6	17
30	Multi-scale simulations of biological systems using the OPEP coarse-grained model. Biochemical and Biophysical Research Communications, 2018, 498, 296-304.	1.0	26
31	Three Weaknesses for Three Perturbations: Comparing Protein Unfolding Under Shear, Force, and Thermal Stresses. Journal of Physical Chemistry B, 2018, 122, 11922-11930.	1.2	24
32	Energy landscape of polymorphic amyloid generation of Î²2-microglobulin revealed by calorimetry. Chemical Communications, 2018, 54, 7995-7998.	2.2	14
33	Water permeation across artificial I-quartet membrane channels: from structure to disorder. Faraday Discussions, 2018, 209, 125-148.	1.6	29
34	Configurational Disorder of Water Hydrogen-Bond Network at the Protein Dynamical Transition. Journal of Physical Chemistry B, 2017, 121, 6792-6798.	1.2	9
35	Why Is Research on Amyloid-Î² Failing to Give New Drugs for Alzheimerâ€™s Disease?. ACS Chemical Neuroscience, 2017, 8, 1435-1437.	1.7	201
36	Thermal activation of â€˜allosteric-likeâ€™ large-scale motions in a eukaryotic Lactate Dehydrogenase. Scientific Reports, 2017, 7, 41092.	1.6	19

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37	Critical structural fluctuations of proteins upon thermal unfolding challenge the Lindemann criterion. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9361-9366.	3.3	35
38	Mechanics of Protein Adaptation to High Temperatures. Journal of Physical Chemistry Letters, 2017, 8, 5884-5890.	2.1	28
39	Coarseâ€grained and Allâ€atom Simulations towards the Early and Late Steps of Amyloid Fibril Formation. Israel Journal of Chemistry, 2017, 57, 564-573.	1.0	23
40	Impact of the A2V Mutation on the Heterozygous and Homozygous AÎ²1â€“40 Dimer Structures from Atomistic Simulations. ACS Chemical Neuroscience, 2016, 7, 823-832.	1.7	51
41	Water Determines the Structure and Dynamics of Proteins. Chemical Reviews, 2016, 116, 7673-7697.	23.0	645
42	Multiscale simulation of molecular processes in cellular environments. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160225.	1.6	22
43	Dimerization Mechanism of Alzheimer AÎ²₄₀ Peptides: The High Content of Intrapeptide-Stabilized Conformations in A2V and A2T Heterozygous Dimers Retards Amyloid Fibril Formation. Journal of Physical Chemistry B, 2016, 120, 12111-12126.	1.2	38
44	Hydrodynamic effects on Î²-amyloid (16-22) peptide aggregation. Journal of Chemical Physics, 2016, 145, 035102.	1.2	44
45	Hydrodynamic Effects on Amyloid-Î² Aggregation. Biophysical Journal, 2016, 110, 219a.	0.2	1
46	Stability and Function at High Temperature. What Makes a Thermophilic GTPase Different from Its Mesophilic Homologue. Journal of Physical Chemistry B, 2016, 120, 2721-2730.	1.2	20
47	Recovering Protein Thermal Stability Using All-Atom Hamiltonian Replica-Exchange Simulations in Explicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 5573-5577.	2.3	40
48	Structures of the Alzheimerâ€™s Wild-Type AÎ²1-40 Dimer from Atomistic Simulations. Journal of Physical Chemistry B, 2015, 119, 10478-10487.	1.2	81
49	Protein Simulations in Fluids: Coupling the OPEP Coarse-Grained Force Field with Hydrodynamics. Journal of Chemical Theory and Computation, 2015, 11, 1843-1853.	2.3	61
50	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	23.0	530
51	Stay Wet, Stay Stable? How Internal Water Helps the Stability of Thermophilic Proteins. Journal of Physical Chemistry B, 2015, 119, 12760-12770.	1.2	21
52	Are coarse-grained models apt to detect protein thermal stability? The case of OPEP force field. Journal of Non-Crystalline Solids, 2015, 407, 494-501.	1.5	17
53	Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains. Journal of Physical Chemistry B, 2015, 119, 8939-8949.	1.2	21
54	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. Chemical Society Reviews, 2014, 43, 4871-4893.	18.7	147

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55	Protein Flexibility and Stability: Thermophiles Know Best. Biophysical Journal, 2014, 106, 256a-257a.	0.2	0
56	Interface Matters: The Stiffness Route to Stability of a Thermophilic Tetrameric Malate Dehydrogenase. PLoS ONE, 2014, 9, e113895.	1.1	11
57	How Conformational Flexibility Stabilizes the Hyperthermophilic Elongation Factor G-Domain. Journal of Physical Chemistry B, 2013, 117, 13775-13785.	1.2	34
58	Importance of the Ion-Pair Interactions in the OPEP Coarse-Grained Force Field: Parametrization and Validation. Journal of Chemical Theory and Computation, 2013, 9, 4574-4584.	2.3	38
59	Biomolecular hydration dynamics: a jump model perspective. Chemical Society Reviews, 2013, 42, 5672.	18.7	100
60	Water Jump Reorientation: From Theoretical Prediction to Experimental Observation. Accounts of Chemical Research, 2012, 45, 53-62.	7.6	90
61	Structural and Spectroscopic Properties of Water around Small Hydrophobic Solutes. Journal of Physical Chemistry B, 2012, 116, 11695-11700.	1.2	39
62	Early Stage of the Dehydrogenation of NaAlH₄ by Ab Initio Rare Event Simulations. Journal of Physical Chemistry C, 2012, 116, 19636-19643.	1.5	14
63	Magnitude and Molecular Origin of Water Slowdown Next to a Protein. Journal of the American Chemical Society, 2012, 134, 4116-4119.	6.6	171
64	Thermophilic proteins: insight and perspective from in silico experiments. Chemical Society Reviews, 2012, 41, 1665-1676.	18.7	68
65	Coherent Excitation Transfer Driven by Torsional Dynamics: a Model Hamiltonian for PPV Type Systems. Zeitschrift Fur Physikalische Chemie, 2011, 225, 541-551.	1.4	22
66	Dynamics of Water in Concentrated Solutions of Amphiphiles: Key Roles of Local Structure and Aggregation. Journal of Physical Chemistry B, 2011, 115, 3254-3262.	1.2	70
67	Reorientation and Allied Dynamics in Water and Aqueous Solutions. Annual Review of Physical Chemistry, 2011, 62, 395-416.	4.8	310
68	Water around thermophilic proteins: the role of charged and apolar atoms. Journal of Physics Condensed Matter, 2010, 22, 284113.	0.7	14
69	Nonadiabatic Simulations of Exciton Dissociation in Poly-p-phenylenevinylene Oligomers. Journal of Physical Chemistry A, 2010, 114, 7661-7670.	1.1	43
70	Water Hydrogen-Bond Dynamics around Amino Acids: The Key Role of Hydrophilic Hydrogen-Bond Acceptor Groups. Journal of Physical Chemistry B, 2010, 114, 2083-2089.	1.2	113
71	Nonadiabatic Mixed Quantumâ^'Classical Dynamic Simulation of Ï€-Stacked Oligophenylenevinylenes. Journal of Physical Chemistry A, 2009, 113, 3427-3430.	1.1	21
72	Key Role of Proximal Water in Regulating Thermostable Proteins. Journal of Physical Chemistry B, 2009, 113, 131-137.	1.2	46

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73	Sphere versus Cylinder: The Effect of Packing on the Structure of Nonionic C₁₂E₆ Micelles. Langmuir, 2009, 25, 8960-8967.	1.6	25
74	Molecular Modeling and Simulation of Conjugated Polymer Oligomers:â€‰ Ground and Excited State Chain Dynamics of PPV in the Gas Phase. Journal of Physical Chemistry B, 2008, 112, 4983-4993.	1.2	39
75	Dissecting the Hydrogen Bond: A Quantum Monte Carlo Approach. Journal of Chemical Theory and Computation, 2008, 4, 1428-1434.	2.3	46
76	Pressure-Induced Core Packing and Interfacial Dehydration in Nonionic C12E6 Micelle in Aqueous Solution. Langmuir, 2008, 24, 6067-6071.	1.6	7
77	How Protein Surfaces Induce Anomalous Dynamics of Hydration Water. Journal of Physical Chemistry B, 2007, 111, 7584-7590.	1.2	221
78	Molecular Modeling and Simulation of Water near Model Micelles:Â Diffusion, Rotational Relaxation and Structure at the Hydration Interface. Journal of Physical Chemistry B, 2006, 110, 11504-11510.	1.2	40
79	Structure and Dynamics of Hydrogen Bonds in the Interface of a C12E6Spherical Micelle in Water Solution:Â A MD Study at Various Temperatures. Journal of Physical Chemistry B, 2006, 110, 18254-18261.	1.2	8
80	Molecular Modeling and Simulations of AOTâ^'Water Reverse Micelles in Isooctane:Â Structural and Dynamic Properties. Journal of Physical Chemistry B, 2004, 108, 19458-19466.	1.2	209
81	Molecular Dynamics Study of Temperature Dehydration of a C12E6Spherical Micelle. Langmuir, 2004, 20, 4311-4314.	1.6	50
82	Linear Response and Electron Transfer in Complex Biomolecular Systems and a Reaction Center Protein. Journal of Physical Chemistry B, 2003, 107, 11208-11215.	1.2	22
83	Water Rotational Relaxation and Diffusion in Hydrated Lysozyme. Journal of the American Chemical Society, 2002, 124, 6787-6791.	6.6	232
84	Dynamics of hydration in hen egg white lysozyme. Journal of Molecular Biology, 2001, 311, 409-419.	2.0	78
85	Molecular Dynamics Study of Spherical Aggregates of Chain Molecules at Different Degrees of Hydrophilicity in Water Solution. Langmuir, 2001, 17, 5103-5110.	1.6	32
86	Three-stage multiscale modelling of the NMDA neuroreceptor. Molecular Physics, 0, , e1928312.	0.8	0