Fabio Sterpone

List of Publications by Year
in descending order

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86	5,151	136740	88477
papers	citations	32 h-index	70 g-index

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

#	Article	IF	Citations
1	Water Determines the Structure and Dynamics of Proteins. Chemical Reviews, 2016, 116, 7673-7697.	23.0	645
2	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	23.0	530
3	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
4	Reorientation and Allied Dynamics in Water and Aqueous Solutions. Annual Review of Physical Chemistry, 2011, 62, 395-416.	4.8	310
5	Water Rotational Relaxation and Diffusion in Hydrated Lysozyme. Journal of the American Chemical Society, 2002, 124, 6787-6791.	6.6	232
6	How Protein Surfaces Induce Anomalous Dynamics of Hydration Water. Journal of Physical Chemistry B, 2007, 111, 7584-7590.	1.2	221
7	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
8	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
9	Magnitude and Molecular Origin of Water Slowdown Next to a Protein. Journal of the American Chemical Society, 2012, 134, 4116-4119.	6.6	171
10	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
11	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
12	Biomolecular hydration dynamics: a jump model perspective. Chemical Society Reviews, 2013, 42, 5672.	18.7	100
13	Water Jump Reorientation: From Theoretical Prediction to Experimental Observation. Accounts of Chemical Research, 2012, 45, 53-62.	7.6	90
14	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
15	Dynamics of hydration in hen egg white lysozyme. Journal of Molecular Biology, 2001, 311, 409-419.	2.0	78
16	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
17	Thermophilic proteins: insight and perspective from in silico experiments. Chemical Society Reviews, 2012, 41, 1665-1676.	18.7	68
18	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

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19	Stability Effect of Quinary Interactions Reversed by Single Point Mutations. Journal of the American Chemical Society, 2019, 141, 4660-4669.	6.6	61
20	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
21	Molecular Dynamics Study of Temperature Dehydration of a C12E6Spherical Micelle. Langmuir, 2004, 20, 4311-4314.	1.6	50
22	Dissecting the Hydrogen Bond: A Quantum Monte Carlo Approach. Journal of Chemical Theory and Computation, 2008, 4, 1428-1434.	2.3	46
23	Key Role of Proximal Water in Regulating Thermostable Proteins. Journal of Physical Chemistry B, 2009, 113, 131-137.	1.2	46
24	Hydrodynamic effects on Î²-amyloid (16-22) peptide aggregation. Journal of Chemical Physics, 2016, 145, 035102.	1.2	44
25	Nonadiabatic Simulations of Exciton Dissociation in Poly-p-phenylenevinylene Oligomers. Journal of Physical Chemistry A, 2010, 114, 7661-7670.	1.1	43
26	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
27	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
28	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
29	Structural and Spectroscopic Properties of Water around Small Hydrophobic Solutes. Journal of Physical Chemistry B, 2012, 116, 11695-11700.	1.2	39
30	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
31	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
32	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
33	How Conformational Flexibility Stabilizes the Hyperthermophilic Elongation Factor G-Domain. Journal of Physical Chemistry B, 2013, 117, 13775-13785.	1.2	34
34	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
35	Water permeation across artificial I-quartet membrane channels: from structure to disorder. Faraday Discussions, 2018, 209, 125-148.	1.6	29
36	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

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37	Mechanics of Protein Adaptation to High Temperatures. Journal of Physical Chemistry Letters, 2017, 8, 5884-5890.	2.1	28
38	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
39	Hydroxy Channelsâ€“Adaptive Pathways for Selective Water Cluster Permeation. Journal of the American Chemical Society, 2021, 143, 4224-4233.	6.6	27
40	Multi-scale simulations of biological systems using the OPEP coarse-grained model. Biochemical and Biophysical Research Communications, 2018, 498, 296-304.	1.0	26
41	Sphere versus Cylinder: The Effect of Packing on the Structure of Nonionic C₁₂E₆ Micelles. Langmuir, 2009, 25, 8960-8967.	1.6	25
42	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
43	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
44	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
45	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
46	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
47	Multiscale simulation of molecular processes in cellular environments. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160225.	1.6	22
48	Modelling lipid systems in fluid with Lattice Boltzmann Molecular Dynamics simulations and hydrodynamics. Scientific Reports, 2019, 9, 16450.	1.6	22
49	Nonadiabatic Mixed Quantumâ^'Classical Dynamic Simulation of Ï€-Stacked Oligophenylenevinylenes. Journal of Physical Chemistry A, 2009, 113, 3427-3430.	1.1	21
50	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
51	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
52	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
53	Thermal activation of â€˜allosteric-likeâ€™ large-scale motions in a eukaryotic Lactate Dehydrogenase. Scientific Reports, 2017, 7, 41092.	1.6	19
54	Aggregation of disease-related peptides. Progress in Molecular Biology and Translational Science, 2020, 170, 435-460.	0.9	19

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55	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
56	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
57	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
58	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
59	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
60	Water around thermophilic proteins: the role of charged and apolar atoms. Journal of Physics Condensed Matter, 2010, 22, 284113.	0.7	14
61	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
62	Energy landscape of polymorphic amyloid generation of Î²2-microglobulin revealed by calorimetry. Chemical Communications, 2018, 54, 7995-7998.	2.2	14
63	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
64	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
65	Small Oligomers of AÎ²42 Protein in the Bulk Solution with AlphaFold2. ACS Chemical Neuroscience, 2022, 13, 711-713.	1.7	14
66	Protein thermal stability. Progress in Molecular Biology and Translational Science, 2020, 170, 239-272.	0.9	11
67	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
68	Interface Matters: The Stiffness Route to Stability of a Thermophilic Tetrameric Malate Dehydrogenase. PLoS ONE, 2014, 9, e113895.	1.1	11
69	Exposure of Von Willebrand Factor Cleavage Site in A1A2A3-Fragment under Extreme Hydrodynamic Shear. Polymers, 2021, 13, 3912.	2.0	10
70	Configurational Disorder of Water Hydrogen-Bond Network at the Protein Dynamical Transition. Journal of Physical Chemistry B, 2017, 121, 6792-6798.	1.2	9
71	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
72	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

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73	Pressure-Induced Core Packing and Interfacial Dehydration in Nonionic C12E6 Micelle in Aqueous Solution. Langmuir, 2008, 24, 6067-6071.	1.6	7
74	Specific Interactions and Environment Flexibility Tune Protein Stability under Extreme Crowding. Journal of Physical Chemistry B, 2021, 125, 6103-6111.	1.2	7
75	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
76	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
77	Mesoscale biosimulations within a unified framework: from proteins to plasmids. Molecular Simulation, 2021, 47, 101-112.	0.9	2
78	Using Computer Simulations and Virtual Reality to Understand, Design and Optimize Artificial Water Channels. Lecture Notes in Bioengineering, 2020, , 78-99.	0.3	2
79	Hydrodynamic Effects on Amyloid-Î² Aggregation. Biophysical Journal, 2016, 110, 219a.	0.2	1
80	In-silico analysis of airflow dynamics and particle transport within a human nasal cavity. Journal of Computational Science, 2021, 54, 101411.	1.5	1
81	Computational Insights into the Unfolding of a Destabilized Superoxide Dismutase 1 Mutant. Biology, 2021, 10, 1240.	1.3	1
82	Protein Flexibility and Stability: Thermophiles Know Best. Biophysical Journal, 2014, 106, 256a-257a.	0.2	0
83	Advancing Multi-Scale Simulation Methods for Biological Membrane Systems. Biophysical Journal, 2019, 116, 373a-374a.	0.2	0
84	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
85	Three-stage multiscale modelling of the NMDA neuroreceptor. Molecular Physics, 0, , e1928312.	0.8	0
86	Tribute to Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10591-10593.	1.2	0