Kim A Sharp

List of Publications by Year
in descending order

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99	16,590	31976	33894
papers	citations	53 h-index	99 g-index

101	101	101	15792
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Protein folding and association: Insights from the interfacial and thermodynamic properties of hydrocarbons. Proteins: Structure, Function and Bioinformatics, 1991, 11, 281-296.	2.6	5,360
2	The Common Feature of Leukemia-Associated IDH1 and IDH2 Mutations Is a Neomorphic Enzyme Activity Converting Î±-Ketoglutarate to 2-Hydroxyglutarate. Cancer Cell, 2010, 17, 225-234.	16.8	1,754
3	Calculating the electrostatic potential of molecules in solution: Method and error assessment. Journal of Computational Chemistry, 1988, 9, 327-335.	3.3	1,017
4	Focusing of electric fields in the active site of Cu-Zn superoxide dismutase: Effects of ionic strength and amino-acid modification. Proteins: Structure, Function and Bioinformatics, 1986, 1, 47-59.	2.6	730
5	On the calculation of pKas in proteins. Proteins: Structure, Function and Bioinformatics, 1993, 15, 252-265.	2.6	514
6	Entropy–enthalpy compensation: Fact or artifact?. Protein Science, 2001, 10, 661-667.	7.6	384
7	HEAT CAPACITY IN PROTEINS. Annual Review of Physical Chemistry, 2005, 56, 521-548.	10.8	384
8	The electrostatic potential of B-DNA. Biopolymers, 1989, 28, 975-993.	2.4	267
9	Hydrogen Bonding and the Cryoprotective Properties of Glycerol/Water Mixtures. Journal of Physical Chemistry B, 2006, 110, 13670-13677.	2.6	250
10	Effect of the Protein Denaturants Urea and Guanidinium on Water Structure:â€‰ A Structural and Thermodynamic Study. Journal of the American Chemical Society, 1998, 120, 10748-10753.	13.7	226
11	Water structure changes induced by hydrophobic and polar solutes revealed by simulations and infrared spectroscopy. Journal of Chemical Physics, 2001, 114, 1791-1796.	3.0	202
12	Electrostatic contributions to solvation energies: comparison of free energy perturbation and continuum calculations. Journal of the American Chemical Society, 1991, 113, 1454-1455.	13.7	197
13	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. Nature Structural Biology, 1999, 6, 1055-1061.	9.7	196
14	Salt Effects on Ligand-DNA Binding. Journal of Molecular Biology, 1994, 238, 245-263.	4.2	184
15	Salt Effects on Protein-DNA Interactions. Journal of Molecular Biology, 1994, 238, 264-280.	4.2	160
16	A New Angle on Heat Capacity Changes in Hydrophobic Solvation. Journal of the American Chemical Society, 2003, 125, 9853-9860.	13.7	152
17	On the calculation of absolute macromolecular binding free energies. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10399-10404.	7.1	145
18	Hydrophobic Effect, Water Structure, and Heat Capacity Changes. Journal of Physical Chemistry B, 1997, 101, 4343-4348.	2.6	141

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19	Entropy in molecular recognition by proteins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6563-6568.	7.1	139
20	Proteinâ˜Solvent Interactions. Chemical Reviews, 2006, 106, 1616-1623.	47.7	137
21	Analysis of the size dependence of macromolecular crowding shows that smaller is better. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7990-7995.	7.1	133
22	Carbohydrate Intramolecular Hydrogen Bonding Cooperativity and Its Effect on Water Structure. Journal of Physical Chemistry B, 2005, 109, 24152-24159.	2.6	128
23	Incorporating solvent and ion screening into molecular dynamics using the finite-difference Poisson-Boltzmann method. Journal of Computational Chemistry, 1991, 12, 454-468.	3.3	124
24	Microscopic Insights into the NMR Relaxation-Based Protein Conformational Entropy Meter. Journal of the American Chemical Society, 2013, 135, 15092-15100.	13.7	123
25	The role of protonation and metal chelation preferences in defining the properties of mercury-binding coiled coils 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1998, 280, 897-912.	4.2	121
26	Electrostatic Contributions to Heat Capacity Changes of DNA-Ligand Binding. Biophysical Journal, 1998, 75, 769-776.	0.5	120
27	Calculation of the Electrophoretic Mobility of a Particle Bearing Bound Polyelectrolyte Using the Nonlinear Poisson-Boltzmann Equation. Biophysical Journal, 1985, 47, 563-566.	0.5	117
28	Correlating solvation free energies and surface tensions of hydrocarbon solutes. Biophysical Chemistry, 1994, 51, 397-409.	2.8	109
29	Analysis of the heat capacity dependence of protein folding. Journal of Molecular Biology, 1992, 227, 889-900.	4.2	108
30	Regulation of brain glutamate metabolism by nitric oxide and S-nitrosylation. Science Signaling, 2015, 8, ra68.	3.6	108
31	Surface-Anchored Monomeric Agonist pMHCs Alone Trigger TCR with High Sensitivity. PLoS Biology, 2008, 6, e43.	5.6	100
32	Pump-probe molecular dynamics as a tool for studying protein motion and long range coupling. Proteins: Structure, Function and Bioinformatics, 2006, 65, 347-361.	2.6	96
33	Electrostatic fields in antibodies and antibody/antigen complexes. Progress in Biophysics and Molecular Biology, 1992, 58, 203-224.	2.9	92
34	Electrostatic and electrokinetic potentials in two polymer aqueous phase systems. Journal of Colloid and Interface Science, 1984, 102, 1-13.	9.4	90
35	Synthesis and application of a poly(ethylene glycol)-antibody affinity ligand for cell separations in aqueous polymer two-phase systems. Analytical Biochemistry, 1986, 154, 110-117.	2.4	88
36	Decomposition of Interaction Free Energies in Proteins and Other Complex Systems. Journal of Molecular Biology, 1995, 254, 77-85.	4.2	85

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37	Stability of macromolecular complexes. Proteins: Structure, Function and Bioinformatics, 2002, 48, 645-653.	2.6	85
38	Travel Depth, a New Shape Descriptor for Macromolecules: Application to Ligand Binding. Journal of Molecular Biology, 2006, 362, 441-458.	4.2	78
39	Measuring Entropy in Molecular Recognition by Proteins. Annual Review of Biophysics, 2018, 47, 41-61.	10.0	77
40	Empirical free energy calculations: a blind test and further improvements to the method 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1997, 268, 401-411.	4.2	76
41	Translation of Ludwig Boltzmannâ€™s Paper â€œOn the Relationship between the Second Fundamental Theorem of the Mechanical Theory of Heat and Probability Calculations Regarding the Conditions for Thermal Equilibriumâ€•Sitzungberichte der Kaiserlichen Akademie der Wissenschaften. Mathematisch-Naturwissen Classe. Abt. II, LXXVI 1877, pp 373-435 (Wien. Ber. 1877, 76:373-435). Reprinted in Wiss. Abhandlungen, Vol. II, reprint 42, p. 164-223, Barth, Leipzig, 1909. Entropy, 2015, 17, 1971-2009.	2.2	74
42	Water in the Half Shell: Structure of Water, Focusing on Angular Structure and Solvation. Accounts of Chemical Research, 2010, 43, 231-239.	15.6	73
43	Exploration of the Structural Features Defining the Conduction Properties of a Synthetic Ion Channel. Biophysical Journal, 1999, 76, 618-630.	0.5	72
44	Implementation and testing of stable, fast implicit solvation in molecular dynamics using the smooth-permittivity finite difference Poisson-Boltzmann method. Journal of Computational Chemistry, 2004, 25, 2049-2064.	3.3	71
45	Finite difference Poisson-Boltzmann electrostatic calculations: Increased accuracy achieved by harmonic dielectric smoothing and charge antialiasing. Journal of Computational Chemistry, 1997, 18, 268-276.	3.3	70
46	A rapid method for calculating derivatives of solvent accessible surface areas of molecules. Journal of Computational Chemistry, 1995, 16, 1038-1044.	3.3	67
47	Protein Pockets: Inventory, Shape, and Comparison. Journal of Chemical Information and Modeling, 2010, 50, 589-603.	5.4	67
48	The mechanism of the type III antifreeze protein action: a computational study. Biophysical Chemistry, 2004, 109, 137-148.	2.8	65
49	Calculation of Electron Transfer Reorganization Energies Using the Finite Difference Poisson-Boltzmann Model. Biophysical Journal, 1998, 74, 1241-1250.	0.5	64
50	Hydrophobic tendency of polar group hydration as a major force in type I antifreeze protein recognition. Proteins: Structure, Function and Bioinformatics, 2005, 59, 266-274.	2.6	62
51	On the relationship between NMR-derived amide order parameters and protein backbone entropy changes. Proteins: Structure, Function and Bioinformatics, 2015, 83, 922-930.	2.6	60
52	Molecular Origin of Hydration Heat Capacity Changes of Hydrophobic Solutes:Â Perturbation of Water Structure around Alkanes. Journal of Physical Chemistry B, 1997, 101, 11237-11242.	2.6	59
53	Calculation of Configurational Entropy with a Boltzmannâ€“Quasiharmonic Model: The Origin of High-Affinity Proteinâ€“Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 9461-9472.	2.6	55
54	Vibrational Stark Effects on Carbonyl, Nitrile, and Nitrosyl Compounds Including Heme Ligands, CO, CN, and NO, Studied with Density Functional Theory. Journal of Physical Chemistry B, 2004, 108, 6450-6457.	2.6	53

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55	A peek at ice binding by antifreeze proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7281-7282.	7.1	52
56	Analysis of thermal hysteresis protein hydration using the random network model. Biophysical Chemistry, 2003, 105, 195-209.	2.8	50
57	Electrostatic interactions in hirudin-thrombin binding. Biophysical Chemistry, 1996, 61, 37-49.	2.8	48
58	Changes in water structure induced by a hydrophobic solute probed by simulation of the water hydrogen bond angle and radial distribution functions. Biophysical Chemistry, 1999, 78, 33-41.	2.8	46
59	TCR Triggering by pMHC Ligands Tethered on Surfaces via Poly(Ethylene Glycol) Depends on Polymer Length. PLoS ONE, 2014, 9, e112292.	2.5	46
60	The Effects of Protein Environment on the Low Temperature Electronic Spectroscopy of Cytochrome c and Microperoxidase-11. Journal of Physical Chemistry B, 1999, 103, 6334-6348.	2.6	44
61	Finding and Characterizing Tunnels in Macromolecules with Application to Ion Channels and Pores. Biophysical Journal, 2009, 96, 632-645.	0.5	43
62	Hydration Heat Capacity of Nucleic Acid Constituents Determined from the Random Network Model. Biophysical Journal, 2001, 81, 1881-1887.	0.5	41
63	The Influence of Protein Environment on the Low Temperature Electronic Spectroscopy of Zn-Substituted Cytochromec. Journal of Physical Chemistry B, 2000, 104, 6932-6941.	2.6	39
64	Temperature Dependence of Fast Dynamics in Proteins. Biophysical Journal, 2007, 92, L43-L45.	0.5	38
65	Explicit ion, implicit water solvation for molecular dynamics of nucleic acids and highly charged molecules. Journal of Computational Chemistry, 2008, 29, 1113-1130.	3.3	38
66	On the Decomposition of Free Energies. Journal of Molecular Biology, 1996, 263, 123-125.	4.2	35
67	Energetics of Cyclic Dipeptide Crystal Packing and Solvation. Biophysical Journal, 1997, 72, 913-927.	0.5	33
68	The Role of Conformation in Ion Permeation in a K⁺ Channel. Journal of the American Chemical Society, 2008, 130, 3389-3398.	13.7	32
69	A Sharp Thermal Transition of Fast Aromatic-Ring Dynamics in Ubiquitin. Angewandte Chemie - International Edition, 2015, 54, 102-107.	13.8	31
70	Intrinsic Linear Heterogeneity of Amyloid Î² Protein Fibrils Revealed by Higher Resolution Mass-per-length Determinations. Journal of Biological Chemistry, 2010, 285, 41843-41851.	3.4	29
71	Optical Spectra of Fe(II) Cytochrome c Interpreted Using Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2002, 106, 5561-5571.	2.6	27
72	The remarkable hydration of the antifreeze protein Maxi: A computational study. Journal of Chemical Physics, 2014, 141, 22D510.	3.0	27

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73	Accessibility of oxygen with respect to the heme pocket in horseradish peroxidase. Proteins: Structure, Function and Bioinformatics, 2003, 53, 656-666.	2.6	25
74	One Is Not Enough. Journal of Molecular Biology, 2009, 392, 1133-1144.	4.2	25
75	Re-Evaluation of the Model-Free Analysis of Fast Internal Motion in Proteins Using NMR Relaxation. Journal of Physical Chemistry B, 2008, 112, 12095-12103.	2.6	23
76	Characterization of Cetyltrimethylammonium Bromide/Hexanol Reverse Micelles by Experimentally Benchmarked Molecular Dynamics Simulations. Langmuir, 2016, 32, 1674-1684.	3.5	23
77	Spectral Analysis of Cytochromec:Â Effect of Heme Conformation, Axial Ligand, Peripheral Substituents, and Local Electric Fields. Journal of Physical Chemistry B, 2001, 105, 282-286.	2.6	22
78	On the ability of molecular dynamics force fields to recapitulate <scp>NMR</scp> derived protein side chain order parameters. Protein Science, 2016, 25, 1156-1160.	7.6	21
79	Building alternate protein structures using the elastic network model. Proteins: Structure, Function and Bioinformatics, 2009, 74, 682-700.	2.6	20
80	Unpacking the origins of in-cell crowding. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1684-1685.	7.1	19
81	How much is a stabilizing bond worth?. Trends in Biochemical Sciences, 1994, 19, 526-529.	7.5	18
82	Banding 2of NMR-derived methyl order parameters: Implications for protein dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2106-2117.	2.6	18
83	Shape and evolution of thermostable protein structure. Proteins: Structure, Function and Bioinformatics, 2010, 78, 420-433.	2.6	17
84	Atomic Charge Parameters for the Finite Difference Poissonâ˜Boltzmann Method Using Electronegativity Neutralization. Journal of Chemical Theory and Computation, 2006, 2, 1152-1167.	5.3	15
85	Solvent dependent and independent motions of COâ€“horseradish peroxidase examined by infrared spectroscopy and molecular dynamics calculations. Biophysical Chemistry, 2003, 106, 1-14.	2.8	14
86	Water loading driven size, shape, and composition of cetyltrimethylammonium/hexanol/pentane reverse micelles. Journal of Colloid and Interface Science, 2019, 540, 207-217.	9.4	14
87	Protein Electric Field Effects on the CO Stretch Frequency of Carbonmonoxycytochromescas a Function of Carbonyl Tilting and Bending Investigated with a Continuum Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 7364-7367.	2.6	13
88	DNA Conformational Changes Play a Force-Generating Role during Bacteriophage Genome Packaging. Biophysical Journal, 2019, 116, 2172-2180.	0.5	13
89	MAPPING COMPLICATED SURFACES ONTO A SPHERE. International Journal of Computational Geometry and Applications, 2007, 17, 305-329.	0.5	12
90	Effect of charge interactions on the carboxylate vibrational stretching frequency in c-type cytochromes investigated by continuum electrostatic calculations and FTIR spectroscopy. Biophysical Chemistry, 1998, 71, 9-20.	2.8	11

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91	Influence of surface groups of proteins on water studied by freezing/thawing hysteresis and infrared spectroscopy. Biophysical Chemistry, 2009, 141, 222-230.	2.8	11
92	Allostery in the lac operon: Population selection or induced dissociation?. Biophysical Chemistry, 2011, 159, 66-72.	2.8	9
93	Calculation of Molecular Entropies Using Temperature Integration. Journal of Chemical Theory and Computation, 2013, 9, 1164-1172.	5.3	9
94	A Density Functional Theory Study of Conformers in the Ferrous CO Complex of Horseradish Peroxidase with Distinct Feâ˜Câ˜O Configurations. Journal of Physical Chemistry B, 2003, 107, 1884-1892.	2.6	8
95	Improved method of preparation of supported planar lipid bilayers as artificial membranes for antigen presentation. Microscopy Research and Technique, 2011, 74, 1174-1185.	2.2	6
96	Protein Folding, Interrupted. Science, 2014, 343, 743-744.	12.6	4
97	Companion Simulations and Modeling to NMR-Based Dynamical Studies of Proteins. Methods in Enzymology, 2019, 615, 1-41.	1.0	4
98	Computational Graphics Software for Interactive Docking and Visualization of Ligandâ€“Protein Complementarity. Journal of Chemical Information and Modeling, 2021, 61, 1427-1443.	5.4	2
99	Thermophilic protein structure adaptation examined with Burial Depth and Travel Depth. Biophysical Journal, 2009, 96, 584a.	0.5	1