Kim A Sharp

List of Publications by Citations

98 papers	15,074 citations	50 h-index	101 g-index
101 ext. papers	15,833 ext. citations	6.6 avg, IF	6.49 L-index

#	Paper	IF	Citations
98	Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. *Proteins: Structure, Function and Bioinformatics*, **1991**, 11, 281-96	4.2	5087
97	The common feature of leukemia-associated IDH1 and IDH2 mutations is a neomorphic enzyme activity converting alpha-ketoglutarate to 2-hydroxyglutarate. *Cancer Cell*, **2010**, 17, 225-34	24.3	1473
96	Calculating the electrostatic potential of molecules in solution: Method and error assessment. *Journal of Computational Chemistry*, **1988**, 9, 327-335	3.5	948
95	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	4.2	681
94	On the calculation of pKas in proteins. *Proteins: Structure, Function and Bioinformatics*, **1993**, 15, 252-65	4.2	489
93	Entropy-enthalpy compensation: fact or artifact?. *Protein Science*, **2001**, 10, 661-7	6.3	347
92	Heat capacity in proteins. *Annual Review of Physical Chemistry*, **2005**, 56, 521-48	15.7	336
91	The electrostatic potential of B-DNA. *Biopolymers*, **1989**, 28, 975-93	2.2	250
90	Effect of the Protein Denaturants Urea and Guanidinium on Water Structure: A Structural and Thermodynamic Study. *Journal of the American Chemical Society*, **1998**, 120, 10748-10753	16.4	215
89	Hydrogen bonding and the cryoprotective properties of glycerol/water mixtures. *Journal of Physical Chemistry B*, **2006**, 110, 13670-7	3.4	206
88	Water structure changes induced by hydrophobic and polar solutes revealed by simulations and infrared spectroscopy. *Journal of Chemical Physics*, **2001**, 114, 1791-1796	3.9	185
87	Electrostatic contributions to solvation energies: comparison of free energy perturbation and continuum calculations. *Journal of the American Chemical Society*, **1991**, 113, 1454-1455	16.4	183
86	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. *Nature Structural Biology*, **1999**, 6, 1055-61		176
85	Salt effects on ligand-DNA binding. Minor groove binding antibiotics. *Journal of Molecular Biology*, **1994**, 238, 245-63	6.5	173
84	Salt effects on protein-DNA interactions. The lambda cI repressor and EcoRI endonuclease. *Journal of Molecular Biology*, **1994**, 238, 264-80	6.5	147
83	A new angle on heat capacity changes in hydrophobic solvation. *Journal of the American Chemical Society*, **2003**, 125, 9853-60	16.4	140
82	Hydrophobic Effect, Water Structure, and Heat Capacity Changes. *Journal of Physical Chemistry B*, **1997**, 101, 4343-4348	3.4	131

81	On the calculation of absolute macromolecular binding free energies. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 10399-404	11.5	128
80	Incorporating solvent and ion screening into molecular dynamics using the finite-difference PoissonBoltzmann method. *Journal of Computational Chemistry*, **1991**, 12, 454-468	3.5	120
79	Protein-solvent interactions. *Chemical Reviews*, **2006**, 106, 1616-23	68.1	119
78	The role of protonation and metal chelation preferences in defining the properties of mercury-binding coiled coils. *Journal of Molecular Biology*, **1998**, 280, 897-912	6.5	115
77	Carbohydrate intramolecular hydrogen bonding cooperativity and its effect on water structure. *Journal of Physical Chemistry B*, **2005**, 109, 24152-9	3.4	114
76	Calculation of the electrophoretic mobility of a particle bearing bound polyelectrolyte using the nonlinear poisson-boltzmann equation. *Biophysical Journal*, **1985**, 47, 563-6	2.9	112
75	Microscopic insights into the NMR relaxation-based protein conformational entropy meter. *Journal of the American Chemical Society*, **2013**, 135, 15092-100	16.4	105
74	Correlating solvation free energies and surface tensions of hydrocarbon solutes. *Biophysical Chemistry*, **1994**, 51, 397-403; discussion 404-9	3.5	102
73	Analysis of the heat capacity dependence of protein folding. *Journal of Molecular Biology*, **1992**, 227, 889-900	6.5	99
72	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, 7990-5	11.5	97
71	Entropy in molecular recognition by proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6563-6568	11.5	96
70	Electrostatic contributions to heat capacity changes of DNA-ligand binding. *Biophysical Journal*, **1998**, 75, 769-76	2.9	94
69	Surface-anchored monomeric agonist pMHCs alone trigger TCR with high sensitivity. *PLoS Biology*, **2008**, 6, e43	9.7	90
68	Pump-probe molecular dynamics as a tool for studying protein motion and long range coupling. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 347-61	4.2	89
67	Regulation of brain glutamate metabolism by nitric oxide and S-nitrosylation. *Science Signaling*, **2015**, 8, ra68	8.8	84
66	Electrostatic fields in antibodies and antibody/antigen complexes. *Progress in Biophysics and Molecular Biology*, **1992**, 58, 203-24	4.7	83
65	Decomposition of interaction free energies in proteins and other complex systems. *Journal of Molecular Biology*, **1995**, 254, 77-85	6.5	81
64	Synthesis and application of a poly(ethylene glycol)-antibody affinity ligand for cell separations in aqueous polymer two-phase systems. *Analytical Biochemistry*, **1986**, 154, 110-7	3.1	78

63	Electrostatic and electrokinetic potentials in two polymer aqueous phase systems. *Journal of Colloid and Interface Science*, **1984**, 102, 1-13	9.3	78
62	Stability of macromolecular complexes. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 645-53	4.2	74
61	Empirical free energy calculations: a blind test and further improvements to the method. *Journal of Molecular Biology*, **1997**, 268, 401-11	6.5	73
60	Travel depth, a new shape descriptor for macromolecules: application to ligand binding. *Journal of Molecular Biology*, **2006**, 362, 441-58	6.5	70
59	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, 2049-64	3.5	67
58	Exploration of the structural features defining the conduction properties of a synthetic ion channel. *Biophysical Journal*, **1999**, 76, 618-30	2.9	67
57	Water in the half shell: structure of water, focusing on angular structure and solvation. *Accounts of Chemical Research*, **2010**, 43, 231-9	24.3	64
56	The mechanism of the type III antifreeze protein action: a computational study. *Biophysical Chemistry*, **2004**, 109, 137-48	3.5	62
55	A rapid method for calculating derivatives of solvent accessible surface areas of molecules. *Journal of Computational Chemistry*, **1995**, 16, 1038-1044	3.5	62
54	Calculation of electron transfer reorganization energies using the finite difference Poisson-Boltzmann model. *Biophysical Journal*, **1998**, 74, 1241-50	2.9	61
53	Finite difference Poisson-Boltzmann electrostatic calculations: Increased accuracy achieved by harmonic dielectric smoothing and charge antialiasing. *Journal of Computational Chemistry*, **1997**, 18, 268-276	3.5	60
52	Hydrophobic tendency of polar group hydration as a major force in type I antifreeze protein recognition. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 266-74	4.2	60
51	Molecular Origin of Hydration Heat Capacity Changes of Hydrophobic Solutes: Perturbation of Water Structure around Alkanes. *Journal of Physical Chemistry B*, **1997**, 101, 11237-11242	3.4	56
50	Protein pockets: inventory, shape, and comparison. *Journal of Chemical Information and Modeling*, **2010**, 50, 589-603	6.1	55
49	Translation of Ludwig Boltzmann's Paper "On the Relationship between the Second Fundamental Theorem of the Mechanical Theory of Heat and Probability Calculations Regarding the Conditions for Thermal Equilibrium" Sitzungberichte der Kaiserlichen Akademie der Wissenschaften. Mathematisch-Naturwissen Classe. Abt. II, LXXVI 1877, pp 373-435 (Wien. Ber. 1877, 76:373-435).	2.8	53
48	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, 6450-7	3.4	50
47	Calculation of configurational entropy with a Boltzmann-quasiharmonic model: the origin of high-affinity protein-ligand binding. *Journal of Physical Chemistry B*, **2011**, 115, 9461-72	3.4	48
46	On the relationship between NMR-derived amide order parameters and protein backbone entropy changes. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 922-30	4.2	46

45	Analysis of thermal hysteresis protein hydration using the random network model. *Biophysical Chemistry*, **2003**, 105, 195-209	3.5	46
44	Electrostatic interactions in hirudin-thrombin binding. *Biophysical Chemistry*, **1996**, 61, 37-49	3.5	46
43	Measuring Entropy in Molecular Recognition by Proteins. *Annual Review of Biophysics*, **2018**, 47, 41-61	21.1	45
42	A peek at ice binding by antifreeze proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 7281-2	11.5	45
41	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	3.5	42
40	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	3.4	41
39	Finding and characterizing tunnels in macromolecules with application to ion channels and pores. *Biophysical Journal*, **2009**, 96, 632-45	2.9	38
38	Explicit ion, implicit water solvation for molecular dynamics of nucleic acids and highly charged molecules. *Journal of Computational Chemistry*, **2008**, 29, 1113-30	3.5	36
37	The Influence of Protein Environment on the Low Temperature Electronic Spectroscopy of Zn-Substituted Cytochrome c. *Journal of Physical Chemistry B*, **2000**, 104, 6932-6941	3.4	36
36	Hydration heat capacity of nucleic acid constituents determined from the random network model. *Biophysical Journal*, **2001**, 81, 1881-7	2.9	36
35	Temperature dependence of fast dynamics in proteins. *Biophysical Journal*, **2007**, 92, L43-5	2.9	35
34	Energetics of cyclic dipeptide crystal packing and solvation. *Biophysical Journal*, **1997**, 72, 913-27	2.9	32
33	The role of conformation in ion permeation in a K+ channel. *Journal of the American Chemical Society*, **2008**, 130, 3389-98	16.4	31
32	On the decomposition of free energies. *Journal of Molecular Biology*, **1996**, 263, 123-5	6.5	31
31	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	3.4	26
30	TCR triggering by pMHC ligands tethered on surfaces via poly(ethylene glycol) depends on polymer length. *PLoS ONE*, **2014**, 9, e112292	3.7	25
29	The remarkable hydration of the antifreeze protein Maxi: a computational study. *Journal of Chemical Physics*, **2014**, 141, 22D510	3.9	24
28	Intrinsic linear heterogeneity of amyloid protein fibrils revealed by higher resolution mass-per-length determinations. *Journal of Biological Chemistry*, **2010**, 285, 41843-51	5.4	24

27	Accessibility of oxygen with respect to the heme pocket in horseradish peroxidase. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 656-66	4.2	23
26	A sharp thermal transition of fast aromatic-ring dynamics in ubiquitin. *Angewandte Chemie - International Edition*, **2015**, 54, 102-7	16.4	22
25	One is not enough. *Journal of Molecular Biology*, **2009**, 392, 1133-44	6.5	21
24	On the ability of molecular dynamics force fields to recapitulate NMR derived protein side chain order parameters. *Protein Science*, **2016**, 25, 1156-60	6.3	20
23	Characterization of Cetyltrimethylammonium Bromide/Hexanol Reverse Micelles by Experimentally Benchmarked Molecular Dynamics Simulations. *Langmuir*, **2016**, 32, 1674-84	4	20
22	Building alternate protein structures using the elastic network model. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 682-700	4.2	20
21	Re-evaluation of the model-free analysis of fast internal motion in proteins using NMR relaxation. *Journal of Physical Chemistry B*, **2008**, 112, 12095-103	3.4	20
20	Spectral Analysis of Cytochromec:Effect of Heme Conformation, Axial Ligand, Peripheral Substituents, and Local Electric Fields. *Journal of Physical Chemistry B*, **2001**, 105, 282-286	3.4	19
19	Unpacking the origins of in-cell crowding. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 1684-5	11.5	17
18	Atomic Charge Parameters for the Finite Difference Poisson-Boltzmann Method Using Electronegativity Neutralization. *Journal of Chemical Theory and Computation*, **2006**, 2, 1152-67	6.4	15
17	How much is a stabilizing bond worth?. *Trends in Biochemical Sciences*, **1994**, 19, 526-9	10.3	15
16	Shape and evolution of thermostable protein structure. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 420-33	4.2	14
15	Protein Electric Field Effects on the CO Stretch Frequency of Carbonmonoxycytochromes c as a Function of Carbonyl Tilting and Bending Investigated with a Continuum Electrostatic Approach. *Journal of Physical Chemistry B*, **1997**, 101, 7364-7367	3.4	13
14	Solvent dependent and independent motions of CO-horseradish peroxidase examined by infrared spectroscopy and molecular dynamics calculations. *Biophysical Chemistry*, **2003**, 106, 1-14	3.5	13
13	Banding of NMR-derived methyl order parameters: implications for protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2106-17	4.2	12
12	DNA Conformational Changes Play a Force-Generating Role during Bacteriophage Genome Packaging. *Biophysical Journal*, **2019**, 116, 2172-2180	2.9	11
11	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	3.5	11
10	Influence of surface groups of proteins on water studied by freezing/thawing hysteresis and infrared spectroscopy. *Biophysical Chemistry*, **2009**, 141, 222-30	3.5	10

9	MAPPING COMPLICATED SURFACES ONTO A SPHERE. *International Journal of Computational Geometry and Applications*, **2007**, 17, 305-329	0.3	10
8	Water loading driven size, shape, and composition of cetyltrimethylammonium/hexanol/pentane reverse micelles. *Journal of Colloid and Interface Science*, **2019**, 540, 207-217	9.3	10
7	Calculation of Molecular Entropies Using Temperature Integration. *Journal of Chemical Theory and Computation*, **2013**, 9, 1164-72	6.4	8
6	A Density Functional Theory Study of Conformers in the Ferrous CO Complex of Horseradish Peroxidase with Distinct Fe□□ Configurations. *Journal of Physical Chemistry B*, **2003**, 107, 1884-1892	3.4	8
5	Allostery in the lac operon: population selection or induced dissociation?. *Biophysical Chemistry*, **2011**, 159, 66-72	3.5	6
4	Improved method of preparation of supported planar lipid bilayers as artificial membranes for antigen presentation. *Microscopy Research and Technique*, **2011**, 74, 1174-85	2.8	6
3	Companion Simulations and Modeling to NMR-Based Dynamical Studies of Proteins. *Methods in Enzymology*, **2019**, 615, 1-41	1.7	4
2	Biochemistry. Protein folding, interrupted. *Science*, **2014**, 343, 743-4	33.3	3
1	Computational Graphics Software for Interactive Docking and Visualization of Ligand-Protein Complementarity. *Journal of Chemical Information and Modeling*, **2021**, 61, 1427-1443	6.1	1