Kim A Sharp

List of Publications by Year in Descending Order

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	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
97	DNA Conformational Changes Play a Force-Generating Role during Bacteriophage Genome Packaging. *Biophysical Journal*, **2019**, 116, 2172-2180	2.9	11
96	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
95	Companion Simulations and Modeling to NMR-Based Dynamical Studies of Proteins. *Methods in Enzymology*, **2019**, 615, 1-41	1.7	4
94	Measuring Entropy in Molecular Recognition by Proteins. *Annual Review of Biophysics*, **2018**, 47, 41-61	21.1	45
93	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
92	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
91	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
90	Characterization of Cetyltrimethylammonium Bromide/Hexanol Reverse Micelles by Experimentally Benchmarked Molecular Dynamics Simulations. *Langmuir*, **2016**, 32, 1674-84	4	20
89	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
88	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
87	Regulation of brain glutamate metabolism by nitric oxide and S-nitrosylation. *Science Signaling*, **2015**, 8, ra68	8.8	84
86	A sharp thermal transition of fast aromatic-ring dynamics in ubiquitin. *Angewandte Chemie - International Edition*, **2015**, 54, 102-7	16.4	22
85	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
84	Biochemistry. Protein folding, interrupted. *Science*, **2014**, 343, 743-4	33.3	3
83	Banding of NMR-derived methyl order parameters: implications for protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2106-17	4.2	12
82	The remarkable hydration of the antifreeze protein Maxi: a computational study. *Journal of Chemical Physics*, **2014**, 141, 22D510	3.9	24

81	TCR triggering by pMHC ligands tethered on surfaces via poly(ethylene glycol) depends on polymer length. *PLoS ONE*, **2014**, 9, e112292	3.7	25
80	Microscopic insights into the NMR relaxation-based protein conformational entropy meter. *Journal of the American Chemical Society*, **2013**, 135, 15092-100	16.4	105
79	Calculation of Molecular Entropies Using Temperature Integration. *Journal of Chemical Theory and Computation*, **2013**, 9, 1164-72	6.4	8
78	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
77	Allostery in the lac operon: population selection or induced dissociation?. *Biophysical Chemistry*, **2011**, 159, 66-72	3.5	6
76	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
75	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
74	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
73	Protein pockets: inventory, shape, and comparison. *Journal of Chemical Information and Modeling*, **2010**, 50, 589-603	6.1	55
72	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
71	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
70	Shape and evolution of thermostable protein structure. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 420-33	4.2	14
69	Building alternate protein structures using the elastic network model. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 682-700	4.2	20
68	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
67	One is not enough. *Journal of Molecular Biology*, **2009**, 392, 1133-44	6.5	21
66	Finding and characterizing tunnels in macromolecules with application to ion channels and pores. *Biophysical Journal*, **2009**, 96, 632-45	2.9	38
65	The role of conformation in ion permeation in a K+ channel. *Journal of the American Chemical Society*, **2008**, 130, 3389-98	16.4	31
64	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

63	Surface-anchored monomeric agonist pMHCs alone trigger TCR with high sensitivity. *PLoS Biology*, **2008**, 6, e43	9.7	90
62	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
61	Temperature dependence of fast dynamics in proteins. *Biophysical Journal*, **2007**, 92, L43-5	2.9	35
60	MAPPING COMPLICATED SURFACES ONTO A SPHERE. *International Journal of Computational Geometry and Applications*, **2007**, 17, 305-329	0.3	10
59	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
58	Protein-solvent interactions. *Chemical Reviews*, **2006**, 106, 1616-23	68.1	119
57	Hydrogen bonding and the cryoprotective properties of glycerol/water mixtures. *Journal of Physical Chemistry B*, **2006**, 110, 13670-7	3.4	206
56	Travel depth, a new shape descriptor for macromolecules: application to ligand binding. *Journal of Molecular Biology*, **2006**, 362, 441-58	6.5	70
55	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
54	Heat capacity in proteins. *Annual Review of Physical Chemistry*, **2005**, 56, 521-48	15.7	336
53	Carbohydrate intramolecular hydrogen bonding cooperativity and its effect on water structure. *Journal of Physical Chemistry B*, **2005**, 109, 24152-9	3.4	114
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	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
50	The mechanism of the type III antifreeze protein action: a computational study. *Biophysical Chemistry*, **2004**, 109, 137-48	3.5	62
49	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
48	Analysis of thermal hysteresis protein hydration using the random network model. *Biophysical Chemistry*, **2003**, 105, 195-209	3.5	46
47	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
46	Accessibility of oxygen with respect to the heme pocket in horseradish peroxidase. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 656-66	4.2	23

45	A Density Functional Theory Study of Conformers in the Ferrous CO Complex of Horseradish Peroxidase with Distinct Fe□□O Configurations. *Journal of Physical Chemistry B*, **2003**, 107, 1884-1892	3.4	8
44	A new angle on heat capacity changes in hydrophobic solvation. *Journal of the American Chemical Society*, **2003**, 125, 9853-60	16.4	140
43	Stability of macromolecular complexes. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 645-53	4.2	74
42	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
41	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
40	Entropy-enthalpy compensation: fact or artifact?. *Protein Science*, **2001**, 10, 661-7	6.3	347
39	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
38	Hydration heat capacity of nucleic acid constituents determined from the random network model. *Biophysical Journal*, **2001**, 81, 1881-7	2.9	36
37	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
36	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
35	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
34	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. *Nature Structural Biology*, **1999**, 6, 1055-61		176
33	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
32	Exploration of the structural features defining the conduction properties of a synthetic ion channel. *Biophysical Journal*, **1999**, 76, 618-30	2.9	67
31	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
30	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
29	Electrostatic contributions to heat capacity changes of DNA-ligand binding. *Biophysical Journal*, **1998**, 75, 769-76	2.9	94
28	Calculation of electron transfer reorganization energies using the finite difference Poisson-Boltzmann model. *Biophysical Journal*, **1998**, 74, 1241-50	2.9	61

27	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
26	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
25	Hydrophobic Effect, Water Structure, and Heat Capacity Changes. *Journal of Physical Chemistry B*, **1997**, 101, 4343-4348	3.4	131
24	Energetics of cyclic dipeptide crystal packing and solvation. *Biophysical Journal*, **1997**, 72, 913-27	2.9	32
23	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
22	Empirical free energy calculations: a blind test and further improvements to the method. *Journal of Molecular Biology*, **1997**, 268, 401-11	6.5	73
21	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
20	On the decomposition of free energies. *Journal of Molecular Biology*, **1996**, 263, 123-5	6.5	31
19	Electrostatic interactions in hirudin-thrombin binding. *Biophysical Chemistry*, **1996**, 61, 37-49	3.5	46
18	Decomposition of interaction free energies in proteins and other complex systems. *Journal of Molecular Biology*, **1995**, 254, 77-85	6.5	81
17	A rapid method for calculating derivatives of solvent accessible surface areas of molecules. *Journal of Computational Chemistry*, **1995**, 16, 1038-1044	3.5	62
16	Correlating solvation free energies and surface tensions of hydrocarbon solutes. *Biophysical Chemistry*, **1994**, 51, 397-403; discussion 404-9	3.5	102
15	How much is a stabilizing bond worth?. *Trends in Biochemical Sciences*, **1994**, 19, 526-9	10.3	15
14	Salt effects on ligand-DNA binding. Minor groove binding antibiotics. *Journal of Molecular Biology*, **1994**, 238, 245-63	6.5	173
13	Salt effects on protein-DNA interactions. The lambda cI repressor and EcoRI endonuclease. *Journal of Molecular Biology*, **1994**, 238, 264-80	6.5	147
12	On the calculation of pKas in proteins. *Proteins: Structure, Function and Bioinformatics*, **1993**, 15, 252-65	4.2	489
11	Electrostatic fields in antibodies and antibody/antigen complexes. *Progress in Biophysics and Molecular Biology*, **1992**, 58, 203-24	4.7	83
10	Analysis of the heat capacity dependence of protein folding. *Journal of Molecular Biology*, **1992**, 227, 889-900	6.5	99

9	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
8	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
7	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
6	The electrostatic potential of B-DNA. *Biopolymers*, **1989**, 28, 975-93	2.2	250
5	Calculating the electrostatic potential of molecules in solution: Method and error assessment. *Journal of Computational Chemistry*, **1988**, 9, 327-335	3.5	948
4	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
3	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
2	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
1	Electrostatic and electrokinetic potentials in two polymer aqueous phase systems. *Journal of Colloid and Interface Science*, **1984**, 102, 1-13	9.3	78