Charles L Brooks Iii

List of Publications by Citations

123 papers	13,552 citations	51 h-index	116 g-index
130 ext. papers	14,791 ext. citations	4.9 avg, IF	6.64 L-index

#	Paper	IF	Citations
123	Extending the treatment of backbone energetics in protein force fields: limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. *Journal of Computational Chemistry*, **2004**, 25, 1400-15	3.5	2792
122	Detailed analysis of grid-based molecular docking: A case study of CDOCKER-A CHARMm-based MD docking algorithm. *Journal of Computational Chemistry*, **2003**, 24, 1549-62	3.5	1032
121	A modified TIP3P water potential for simulation with Ewald summation. *Journal of Chemical Physics*, **2004**, 121, 10096-103	3.9	715
120	Generalized born model with a simple smoothing function. *Journal of Computational Chemistry*, **2003**, 24, 1691-702	3.5	578
119	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
118	From folding theories to folding proteins: a review and assessment of simulation studies of protein folding and unfolding. *Annual Review of Physical Chemistry*, **2001**, 52, 499-535	15.7	447
117	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. *Journal of Computational Chemistry*, **2003**, 24, 1348-56	3.5	435
116	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. *Journal of Computational Chemistry*, **2004**, 25, 1-15	3.5	414
115	Novel generalized Born methods. *Journal of Chemical Physics*, **2002**, 116, 10606-10614	3.9	391
114	CHARMM fluctuating charge force field for proteins: II protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. *Journal of Computational Chemistry*, **2004**, 25, 1504-14	3.5	371
113	The origins of asymmetry in the folding transition states of protein L and protein G. *Protein Science*, **2002**, 11, 2351-61	6.3	313
112	Structural and energetic effects of truncating long ranged interactions in ionic and polar fluids. *Journal of Chemical Physics*, **1985**, 83, 5897-5908	3.9	274
111	Constant-pH molecular dynamics using continuous titration coordinates. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 738-52	4.2	267
110	λ-dynamics: A new approach to free energy calculations. *Journal of Chemical Physics*, **1996**, 105, 2414-2423	3.9	267
109	Comparative study of several algorithms for flexible ligand docking. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 755-63	4.2	245
108	Normal mode based flexible fitting of high-resolution structure into low-resolution experimental data from cryo-EM. *Journal of Structural Biology*, **2004**, 147, 315-26	3.4	202
107	Insights from coarse-grained Gō models for protein folding and dynamics. *International Journal of Molecular Sciences*, **2009**, 10, 889-905	6.3	198

88	Energetic frustration and the nature of the transition state in protein folding. *Journal of Chemical Physics*, **2000**, 113, 7663-7671	3.9	75
87	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1319-31	4.2	73
86	The influence of long-range force truncation on the thermodynamics of aqueous ionic solutions. *Journal of Chemical Physics*, **1987**, 86, 5156-5162	3.9	71
85	A reexamination of the hydrophobic effect: Exploring the role of the solvent model in computing the methane–methane potential of mean force. *Journal of Chemical Physics*, **1997**, 106, 9265-9269	3.9	64
84	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. *Journal of Computational Chemistry*, **2005**, 26, 1565-78	3.5	63
83	Flexible CDOCKER: Development and application of a pseudo-explicit structure-based docking method within CHARMM. *Journal of Computational Chemistry*, **2016**, 37, 753-62	3.5	61
82	A nonadditive methanol force field: bulk liquid and liquid-vapor interfacial properties via molecular dynamics simulations using a fluctuating charge model. *Journal of Chemical Physics*, **2005**, 122, 024508	3.9	61
81	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. *Journal of Chemical Physics*, **1991**, 95, 7612-7625	3.9	61
80	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. *Journal of Computational Chemistry*, **2011**, 32, 2909-23	3.5	58
79	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. *Journal of Chemical Physics*, **2005**, 123, 164502	3.9	58
78	The thermodynamics of solvophobic effects: A molecular-dynamics study of n-butane in carbon tetrachloride and water. *Journal of Chemical Physics*, **1990**, 92, 2582-2592	3.9	56
77	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. *Journal of Chemical Physics*, **2006**, 124, 204706	3.9	54
76	Curious structure in "canonical" alanine-based peptides. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 59-71	4.2	53
75	Functionally important conformations of the Met20 loop in dihydrofolate reductase are populated by rapid thermal fluctuations. *Journal of the American Chemical Society*, **2009**, 131, 5642-7	16.4	52
74	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 444-57	4.2	47
73	Prediction of quaternary structure of coiled coils. Application to mutants of the GCN4 leucine zipper. *Journal of Molecular Biology*, **1995**, 251, 448-67	6.5	44
72	Predicting extreme pKa shifts in staphylococcal nuclease mutants with constant pH molecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3276-86	4.2	39
71	A molecular dynamics simulation study of segment B1 of protein G. *Proteins: Structure, Function and Bioinformatics*, **1997**, 29, 193-202	4.2	39

70	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. *Journal of Computational Chemistry*, **2008**, 29, 820-31	3.5	37
69	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. *Journal of Chemical Physics*, **2006**, 125, 174108	3.9	37
68	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. *Journal of Computational Chemistry*, **1991**, 12, 1270-1277	3.5	36
67	An ab initio study of hydrated chloride ion complexes: Evidence of polarization effects and nonadditivity. *Journal of Chemical Physics*, **1987**, 87, 5892-5894	3.9	35
66	Conformational change of the methionine 20 loop of Escherichia coli dihydrofolate reductase modulates pKa of the bound dihydrofolate. *Protein Science*, **2007**, 16, 1087-100	6.3	34
65	Protein-drug interactions: characterization of inhibitor binding in complexes of DHFR with trimethoprim and related derivatives. *Proteins: Structure, Function and Bioinformatics*, **1990**, 7, 52-61	4.2	34
64	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. *Journal of the American Chemical Society*, **2018**, 140, 16560-16569	16.4	33
63	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. *Journal of Computational Chemistry*, **2011**, 32, 3423-32	3.5	32
62	Frequent side chain methyl carbon-oxygen hydrogen bonding in proteins revealed by computational and stereochemical analysis of neutron structures. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 403-410	4.2	31
61	FoldGPCR: structure prediction protocol for the transmembrane domain of G protein-coupled receptors from class A. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2189-201	4.2	31
60	Assessing the quality of absolute hydration free energies among CHARMM-compatible ligand parameterization schemes. *Journal of Computational Chemistry*, **2013**, 34, 893-903	3.5	30
59	The importance of explicit chain representation in protein folding models: an examination of Ising-like models. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 740-7	4.2	30
58	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. *Proteins: Structure, Function and Bioinformatics*, **1999**, 35, 447-452	4.2	29
57	Cluster structure determination using Gaussian density distribution global minimization methods. *Journal of Chemical Physics*, **1994**, 101, 6405-6411	3.9	27
56	Improved model building and assessment of the Calcium-sensing receptor transmembrane domain. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 215-26	4.2	26
55	Exploring Protein-Nanoparticle Interactions with Coarse-Grained Protein Folding Models. *Small*, **2017**, 13, 1603748	11	25
54	Detailed considerations for a balanced and broadly applicable force field: a study of substituted benzenes modeled with OPLS-AA. *Journal of Computational Chemistry*, **2005**, 26, 1529-41	3.5	25
53	Virtual rigid body dynamics. *Biopolymers*, **1991**, 31, 77-100	2.2	25

52	Deciphering protein evolution and fitness landscapes with latent space models. *Nature Communications*, **2019**, 10, 5644	17.4	25
51	Exploring assembly energetics of the 30S ribosomal subunit using an implicit solvent approach. *Journal of the American Chemical Society*, **2005**, 127, 11125-33	16.4	24
50	Parallelization and improvements of the generalized born model with a simple sWitching function for modern graphics processors. *Journal of Computational Chemistry*, **2016**, 37, 927-39	3.5	21
49	Model of the toxic complex of anthrax: responsive conformational changes in both the lethal factor and the protective antigen heptamer. *Protein Science*, **2006**, 15, 2190-200	6.3	21
48	Receptor rigidity and ligand mobility in trypsin-ligand complexes. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 407-17	4.2	21
47	Efficient approximate all-atom solvent accessible surface area method parameterized for folded and denatured protein conformations. *Journal of Computational Chemistry*, **2004**, 25, 1005-14	3.5	21
46	Effect of gatekeepers on the early folding kinetics of a model Ɛbarrel protein. *Journal of Chemical Physics*, **2003**, 119, 5722-5729	3.9	20
45	PCASSO: a fast and efficient CƐbased method for accurately assigning protein secondary structure elements. *Journal of Computational Chemistry*, **2014**, 35, 1757-61	3.5	19
44	Free energy screening of small ligands binding to an artificial protein cavity. *Journal of Chemical Physics*, **2000**, 113, 3423-3433	3.9	19
43	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. *Journal of the American Chemical Society*, **2019**, 141, 9980-9988	16.4	18
42	CHARMM: The Energy Function and Its Parameterization		18
41	Structural basis for selectivity in flavin-dependent monooxygenase-catalyzed oxidative dearomatization. *ACS Catalysis*, **2019**, 9, 3633-3640	13.1	17
40	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite Ⅎ Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 3328-3332	6.4	17
39	Automated, Accurate, and Scalable Relative Protein-Ligand Binding Free-Energy Calculations Using Lambda Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 7895-7914	6.4	16
38	Efficient implementation of constant pH molecular dynamics on modern graphics processors. *Journal of Computational Chemistry*, **2016**, 37, 2171-80	3.5	13
37	pH-sensitive residues in the p19 RNA silencing suppressor protein from carnation Italian ringspot virus affect siRNA binding stability. *Protein Science*, **2013**, 22, 595-604	6.3	13
36	Thermodynamic calculations on biological molecules. *International Journal of Quantum Chemistry*, **1988**, 34, 221-234	2.1	12
35	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 19078-19086	3.8	11

34	Approaching protein design with multisite λdynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. *Protein Science*, **2018**, 27, 1910-1922	6.3	11
33	Overcoming Challenging Substituent Perturbations with Multisite λDynamics: A Case Study Targeting βSecretase 1. *Journal of Physical Chemistry Letters*, **2019**, 10, 4875-4880	6.4	10
32	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 448-53	4.2	10
31	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. *Journal of Physical Chemistry Letters*, **2019**, 10, 5963-5968	6.4	9
30	The flexible C-terminal arm of the Lassa arenavirus Z-protein mediates interactions with multiple binding partners. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2251-64	4.2	9
29	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. *Journal of Physical Chemistry B*, **2019**, 123, 8065-8073	3.4	8
28	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. *Journal of Physical Chemistry Letters*, **2020**, 11, 864-868	6.4	8
27	A line integral reaction path approximation for large systems via nonlinear constrained optimization: application to alanine dipeptide and the beta hairpin of protein G. *Journal of Chemical Physics*, **2006**, 124, 194903	3.9	8
26	Protein Structure and Dynamics—An Overview. *Advances in Chemical Physics*, **2007**, 7-21		7
25	Dynamic load balancing algorithms for replicated data molecular dynamics. *Journal of Computational Chemistry*, **1995**, 16, 715-722	3.5	7
24	Accelerating the Generalized Born with Molecular Volume and Solvent Accessible Surface Area Implicit Solvent Model Using Graphics Processing Units. *Journal of Computational Chemistry*, **2020**, 41, 830-838	3.5	7
23	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. *Molecular Informatics*, **2011**, 30, 896-906	3.8	6
22	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. *ChemPhysChem*, **2003**, 4, 848-55	3.2	5
21	Implementation of a data parallel, logical domain decomposition method for interparticle interactions in molecular dynamics of structured molecular fluids. *Journal of Computational Chemistry*, **1994**, 15, 44-53	3.5	4
20	Steric and thermodynamic limits of design for the incorporation of large unnatural amino acids in aminoacyl-tRNA synthetase enzymes. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1926-38	4.2	3
19	The Stability of Protein Secondary Structures in Aqueous Solution. *AIP Conference Proceedings*, **1991**,	0	3
18	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. *Journal of Computational Chemistry*, **2021**, 42, 1088-1094	3.5	3
17	Exploring pH Dependent Host/Guest Binding Affinities. *Journal of Physical Chemistry B*, **2020**, 124, 6520-6528	3.4	2