Charles L Brooks Iii

List of Publications by Year in Descending Order

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	Optimizing Multisite λ-Dynamics Throughput with Charge Renormalization.. *Journal of Chemical Information and Modeling*, **2022**, 62, 1479-1488	6.1	1
122	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states.. *PLoS Computational Biology*, **2022**, 18, e1009977	5	
121	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. *Journal of Chemical Information and Modeling*, **2021**, 61, 5535-5549	6.1	1
120	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6799-6807	6.4	1
119	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
118	Exploring pH Dependent Host/Guest Binding Affinities. *Journal of Physical Chemistry B*, **2020**, 124, 6520-6528	3.4	2
117	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. *Journal of Physical Chemistry Letters*, **2020**, 11, 864-868	6.4	8
116	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
115	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
114	Computational Studies of Catalytic Loop Dynamics in Protein Tyrosine Phosphatase Using Pathway Optimization Methods. *Journal of Physical Chemistry B*, **2019**, 123, 7840-7851	3.4	1
113	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. *Journal of Physical Chemistry B*, **2019**, 123, 8065-8073	3.4	8
112	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. *Journal of Physical Chemistry Letters*, **2019**, 10, 5963-5968	6.4	9
111	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
110	Structural basis for selectivity in flavin-dependent monooxygenase-catalyzed oxidative dearomatization. *ACS Catalysis*, **2019**, 9, 3633-3640	13.1	17
109	Overcoming Challenging Substituent Perturbations with Multisite λ-Dynamics: A Case Study Targeting β-Secretase 1. *Journal of Physical Chemistry Letters*, **2019**, 10, 4875-4880	6.4	10
108	Deciphering protein evolution and fitness landscapes with latent space models. *Nature Communications*, **2019**, 10, 5644	17.4	25
107	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

106	Approaching protein design with multisite λ-dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. *Protein Science*, **2018**, 27, 1910-1922	6.3	11
105	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite λ Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 3328-3332	6.4	17
104	Molecular Interactions between Graphene and Biological Molecules. *Journal of the American Chemical Society*, **2017**, 139, 1928-1936	16.4	77
103	Exploring Protein-Nanoparticle Interactions with Coarse-Grained Protein Folding Models. *Small*, **2017**, 13, 1603748	11	25
102	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
101	Efficient implementation of constant pH molecular dynamics on modern graphics processors. *Journal of Computational Chemistry*, **2016**, 37, 2171-80	3.5	13
100	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
99	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
98	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
97	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1319-31	4.2	73
96	PCASSO: a fast and efficient Cα-based method for accurately assigning protein secondary structure elements. *Journal of Computational Chemistry*, **2014**, 35, 1757-61	3.5	19
95	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
94	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
93	MATCH: an atom-typing toolset for molecular mechanics force fields. *Journal of Computational Chemistry*, **2012**, 33, 189-202	3.5	115
92	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
91	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. *Molecular Informatics*, **2011**, 30, 896-906	3.8	6
90	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. *Journal of Computational Chemistry*, **2011**, 32, 2909-23	3.5	58
89	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. *Journal of Computational Chemistry*, **2011**, 32, 3423-32	3.5	32

88	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
87	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
86	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
85	Lambda-dynamics free energy simulation methods. *Journal of Computational Chemistry*, **2009**, 30, 1692-700	3.5	138
84	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 448-53	4.2	10
83	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
82	Insights from coarse-grained G models for protein folding and dynamics. *International Journal of Molecular Sciences*, **2009**, 10, 889-905	6.3	198
81	Improved model building and assessment of the Calcium-sensing receptor transmembrane domain. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 215-26	4.2	26
80	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
79	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. *Physical Chemistry Chemical Physics*, **2008**, 10, 471-81	3.6	116
78	Thermodynamic Aspects. *Advances in Chemical Physics*, **2007**, 175-190		
77	Experimental Comparisons and Analysis. *Advances in Chemical Physics*, **2007**, 191-224		
76	Protein Structure and Dynamics: An Overview. *Advances in Chemical Physics*, **2007**, 7-21		7
75	Potential Functions. *Advances in Chemical Physics*, **2007**, 23-31		1
74	Dynamical Simulation Methods. *Advances in Chemical Physics*, **2007**, 33-58		2
73	Thermodynamic Methods. *Advances in Chemical Physics*, **2007**, 59-74		
72	Atom and Sidechain Motions. *Advances in Chemical Physics*, **2007**, 75-116		
71	Rigid-Body Motions. *Advances in Chemical Physics*, **2007**, 117-126		1

70	Larger-Scale Motions. *Advances in Chemical Physics*, **2007**, 127-136		
69	Solvent Influence on Protein Dynamics. *Advances in Chemical Physics*, **2007**, 137-174		1
68	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 922-30	4.2	116
67	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
66	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. *Journal of Chemical Physics*, **2006**, 125, 174108	3.9	37
65	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
64	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. *Molecular Simulation*, **2006**, 32, 231-249	2	101
63	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. *Journal of Chemical Physics*, **2006**, 124, 204706	3.9	54
62	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
61	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
60	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
59	Receptor rigidity and ligand mobility in trypsin-ligand complexes. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 407-17	4.2	21
58	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
57	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
56	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. *Journal of Computational Chemistry*, **2005**, 26, 1565-78	3.5	63
55	A modified TIP3P water potential for simulation with Ewald summation. *Journal of Chemical Physics* , **2004**, 121, 10096-103	3.9	715
54	Constant-pH molecular dynamics using continuous titration coordinates. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 738-52	4.2	267
53	An electrostatic basis for the stability of thermophilic proteins. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 128-41	4.2	108

52	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 444-57	4.2	47
51	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
50	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
49	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
48	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
47	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
46	Implicit solvation based on generalized Born theory in different dielectric environments. *Journal of Chemical Physics*, **2004**, 120, 903-11	3.9	124
45	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
44	Comparative study of several algorithms for flexible ligand docking. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 755-63	4.2	245
43	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. *ChemPhysChem*, **2003**, 4, 848-55	3.2	5
42	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
41	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
40	Generalized born model with a simple smoothing function. *Journal of Computational Chemistry*, **2003**, 24, 1691-702	3.5	578
39	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
38	Effect of gatekeepers on the early folding kinetics of a model β-barrel protein. *Journal of Chemical Physics*, **2003**, 119, 5722-5729	3.9	20
37	The origins of asymmetry in the folding transition states of protein L and protein G. *Protein Science*, **2002**, 11, 2351-61	6.3	313
36	Modern protein force fields behave comparably in molecular dynamics simulations. *Journal of Computational Chemistry*, **2002**, 23, 1045-57	3.5	92
35	Evaluating CASP4 predictions with physical energy functions. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 232-45	4.2	75

34	Novel generalized Born methods. *Journal of Chemical Physics*, **2002**, 116, 10606-10614	3.9	391
33	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
32	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 86-97	4.2	80
31	Energetic frustration and the nature of the transition state in protein folding. *Journal of Chemical Physics*, **2000**, 113, 7663-7671	3.9	75
30	Free energy screening of small ligands binding to an artificial protein cavity. *Journal of Chemical Physics*, **2000**, 113, 3423-3433	3.9	19
29	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
28	Assessing energy functions for flexible docking. *Journal of Computational Chemistry*, **1998**, 19, 1612-1622	3.5	132
27	Assessing search strategies for flexible docking. *Journal of Computational Chemistry*, **1998**, 19, 1623-1631	3.5	102
26	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist □barrel model. *Journal of Chemical Physics*, **1998**, 109, 2895-2903	3.9	89
25	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
24	Curious structure in "canonical" alanine-based peptides. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 59-71	4.2	53
23	A molecular dynamics simulation study of segment B1 of protein G. *Proteins: Structure, Function and Bioinformatics*, **1997**, 29, 193-202	4.2	39
22	Thermodynamics of protein folding: a statistical mechanical study of a small all-beta protein. *Biopolymers*, **1997**, 42, 745-57	2.2	103
21	□dynamics: A new approach to free energy calculations. *Journal of Chemical Physics*, **1996**, 105, 2414-2423	3.9	267
20	A microscopic view of helix propagation: N and C-terminal helix growth in alanine helices. *Journal of Molecular Biology*, **1996**, 259, 560-72	6.5	109
19	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
18	Dynamic load balancing algorithms for replicated data molecular dynamics. *Journal of Computational Chemistry*, **1995**, 16, 715-722	3.5	7
17	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

16	Cluster structure determination using Gaussian density distribution global minimization methods. *Journal of Chemical Physics*, **1994**, 101, 6405-6411	3.9	27
15	The Stability of Protein Secondary Structures in Aqueous Solution. *AIP Conference Proceedings*, **1991**,	0	3
14	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
13	Virtual rigid body dynamics. *Biopolymers*, **1991**, 31, 77-100	2.2	25
12	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. *Journal of Chemical Physics*, **1991**, 95, 7612-7625	3.9	61
11	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
10	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
9	Thermodynamic calculations on biological molecules. *International Journal of Quantum Chemistry*, **1988**, 34, 221-234	2.1	12
8	Molecular dynamics with internal coordinate constraints. *Journal of Chemical Physics*, **1988**, 89, 5115-5127	3.9	81
7	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
6	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. *Journal of Chemical Physics*, **1987**, 87, 3029-3037	3.9	118
5	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
4	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
3	Exploring the Functional Landscape of Biomolecular Machines via Elastic Network Normal Mode Analysis	59-77	2
2	Implicit Solvent Force-Field Optimization	167-190	1
1	CHARMM: The Energy Function and Its Parameterization		18