

Charles L Brooks Iii

List of Publications by Citations

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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. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1549-62	3.5	1032
121	A modified TIP3P water potential for simulation with Ewald summation. <i>Journal of Chemical Physics</i> , 2004 , 121, 10096-103	3.9	715
120	Generalized born model with a simple smoothing function. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Computational Chemistry</i> , 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. <i>Annual Review of Physical Chemistry</i> , 2001 , 52, 499-535	15.7	447
117	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1348-56	3.5	435
116	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1-15	3.5	414
115	Novel generalized Born methods. <i>Journal of Chemical Physics</i> , 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. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1504-14	3.5	371
113	The origins of asymmetry in the folding transition states of protein L and protein G. <i>Protein Science</i> , 2002 , 11, 2351-61	6.3	313
112	Structural and energetic effects of truncating long ranged interactions in ionic and polar fluids. <i>Journal of Chemical Physics</i> , 1985 , 83, 5897-5908	3.9	274
111	Constant-pH molecular dynamics using continuous titration coordinates. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 56, 738-52	4.2	267
110	Edynamics: A new approach to free energy calculations. <i>Journal of Chemical Physics</i> , 1996 , 105, 2414-2423	3.9	267
109	Comparative study of several algorithms for flexible ligand docking. <i>Journal of Computer-Aided Molecular Design</i> , 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. <i>Journal of Structural Biology</i> , 2004 , 147, 315-26	3.4	202
107	Insights from coarse-grained Gō models for protein folding and dynamics. <i>International Journal of Molecular Sciences</i> , 2009 , 10, 889-905	6.3	198

106	Lambda-dynamics free energy simulation methods. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1692-700	3.9	138
105	Assessing energy functions for flexible docking. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1612-1623	3.5	132
104	Implicit solvation based on generalized Born theory in different dielectric environments. <i>Journal of Chemical Physics</i> , 2004 , 120, 903-11	3.9	124
103	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. <i>Journal of Chemical Physics</i> , 1987 , 87, 3029-3037	3.9	118
102	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 67, 922-30	4.2	116
101	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 471-81	3.6	116
100	MATCH: an atom-typing toolset for molecular mechanics force fields. <i>Journal of Computational Chemistry</i> , 2012 , 33, 189-202	3.5	115
99	A microscopic view of helix propagation: N and C-terminal helix growth in alanine helices. <i>Journal of Molecular Biology</i> , 1996 , 259, 560-72	6.5	109
98	An electrostatic basis for the stability of thermophilic proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 57, 128-41	4.2	108
97	Thermodynamics of protein folding: a statistical mechanical study of a small all-beta protein. <i>Biopolymers</i> , 1997 , 42, 745-57	2.2	103
96	Assessing search strategies for flexible docking. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1623-1633	3.5	102
95	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. <i>Molecular Simulation</i> , 2006 , 32, 231-249	2	101
94	Modern protein force fields behave comparably in molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2002 , 23, 1045-57	3.5	92
93	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist E-barrel model. <i>Journal of Chemical Physics</i> , 1998 , 109, 2895-2903	3.9	89
92	Molecular dynamics with internal coordinate constraints. <i>Journal of Chemical Physics</i> , 1988 , 89, 5115-5123	3.9	81
91	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000 , 41, 86-97	4.2	80
90	Molecular Interactions between Graphene and Biological Molecules. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1928-1936	16.4	77
89	Evaluating CASP4 predictions with physical energy functions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002 , 49, 232-45	4.2	75

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

70	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. <i>Journal of Computational Chemistry</i> , 2008 , 29, 820-31	3.5	37
69	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. <i>Journal of Chemical Physics</i> , 2006 , 125, 174108	3.9	37
68	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. <i>Journal of Computational Chemistry</i> , 1991 , 12, 1270-1277	3.5	36
67	An ab initio study of hydrated chloride ion complexes: Evidence of polarization effects and nonadditivity. <i>Journal of Chemical Physics</i> , 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. <i>Protein Science</i> , 2007 , 16, 1087-100	6.3	34
65	Protein-drug interactions: characterization of inhibitor binding in complexes of DHFR with trimethoprim and related derivatives. <i>Proteins: Structure, Function and Bioinformatics</i> , 1990 , 7, 52-61	4.2	34
64	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16560-16569	16.4	33
63	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. <i>Journal of Computational Chemistry</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015 , 83, 403-410	4.2	31
61	FoldGPCR: structure prediction protocol for the transmembrane domain of G protein-coupled receptors from class A. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 2189-201	4.2	31
60	Assessing the quality of absolute hydration free energies among CHARMM-compatible ligand parameterization schemes. <i>Journal of Computational Chemistry</i> , 2013 , 34, 893-903	3.5	30
59	The importance of explicit chain representation in protein folding models: an examination of Ising-like models. <i>Proteins: Structure, Function and Bioinformatics</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 35, 447-452	4.2	29
57	Cluster structure determination using Gaussian density distribution global minimization methods. <i>Journal of Chemical Physics</i> , 1994 , 101, 6405-6411	3.9	27
56	Improved model building and assessment of the Calcium-sensing receptor transmembrane domain. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 215-26	4.2	26
55	Exploring Protein-Nanoparticle Interactions with Coarse-Grained Protein Folding Models. <i>Small</i> , 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. <i>Journal of Computational Chemistry</i> , 2005 , 26, 1529-41	3.5	25
53	Virtual rigid body dynamics. <i>Biopolymers</i> , 1991 , 31, 77-100	2.2	25

52	Deciphering protein evolution and fitness landscapes with latent space models. <i>Nature Communications</i> , 2019 , 10, 5644	17.4	25
51	Exploring assembly energetics of the 30S ribosomal subunit using an implicit solvent approach. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of Computational Chemistry</i> , 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. <i>Protein Science</i> , 2006 , 15, 2190-200	6.3	21
48	Receptor rigidity and ligand mobility in trypsin-ligand complexes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 58, 407-17	4.2	21
47	Efficient approximate all-atom solvent accessible surface area method parameterized for folded and denatured protein conformations. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1005-14	3.5	21
46	Effect of gatekeepers on the early folding kinetics of a model β barrel protein. <i>Journal of Chemical Physics</i> , 2003 , 119, 5722-5729	3.9	20
45	PCASSO: a fast and efficient C α -based method for accurately assigning protein secondary structure elements. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1757-61	3.5	19
44	Free energy screening of small ligands binding to an artificial protein cavity. <i>Journal of Chemical Physics</i> , 2000 , 113, 3423-3433	3.9	19
43	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. <i>Journal of the American Chemical Society</i> , 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. <i>ACS Catalysis</i> , 2019 , 9, 3633-3640	13.1	17
40	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite π Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3328-3332	6.4	17
39	Automated, Accurate, and Scalable Relative Protein-Ligand Binding Free-Energy Calculations Using Lambda Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 7895-7914	6.4	16
38	Efficient implementation of constant pH molecular dynamics on modern graphics processors. <i>Journal of Computational Chemistry</i> , 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. <i>Protein Science</i> , 2013 , 22, 595-604	6.3	13
36	Thermodynamic calculations on biological molecules. <i>International Journal of Quantum Chemistry</i> , 1988 , 34, 221-234	2.1	12
35	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 19078-19086	3.8	11

34	Approaching protein design with multisite \bar{E} dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. <i>Protein Science</i> , 2018 , 27, 1910-1922	6.3	11
33	Overcoming Challenging Substituent Perturbations with Multisite \bar{E} Dynamics: A Case Study Targeting \bar{E} Secretase 1. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 4875-4880	6.4	10
32	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 77, 448-53	4.2	10
31	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. <i>Journal of Physical Chemistry Letters</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 2251-64	4.2	9
29	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 8065-8073	3.4	8
28	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. <i>Journal of Physical Chemistry Letters</i> , 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. <i>Journal of Chemical Physics</i> , 2006 , 124, 194903	3.9	8
26	Protein Structure and Dynamics An Overview. <i>Advances in Chemical Physics</i> , 2007 , 7-21		7
25	Dynamic load balancing algorithms for replicated data molecular dynamics. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Computational Chemistry</i> , 2020 , 41, 830-838	3.5	7
23	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. <i>Molecular Informatics</i> , 2011 , 30, 896-906	3.8	6
22	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. <i>ChemPhysChem</i> , 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. <i>Journal of Computational Chemistry</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 1926-38	4.2	3
19	The Stability of Protein Secondary Structures in Aqueous Solution. <i>AIP Conference Proceedings</i> , 1991 ,	0	3
18	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. <i>Journal of Computational Chemistry</i> , 2021 , 42, 1088-1094	3.5	3
17	Exploring pH Dependent Host/Guest Binding Affinities. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 6520-6528	6.5	2

16	Exploring the Functional Landscape of Biomolecular Machines via Elastic Network Normal Mode Analysis	59-77	2
15	Dynamical Simulation Methods. <i>Advances in Chemical Physics</i> , 2007 , 33-58		2
14	Computational Studies of Catalytic Loop Dynamics in Protein Tyrosine Phosphatase Using Pathway Optimization Methods. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 7840-7851		3-4 1
13	Implicit Solvent Force-Field Optimization	167-190	1
12	Potential Functions. <i>Advances in Chemical Physics</i> , 2007 , 23-31		1
11	Rigid-Body Motions. <i>Advances in Chemical Physics</i> , 2007 , 117-126		1
10	Solvent Influence on Protein Dynamics. <i>Advances in Chemical Physics</i> , 2007 , 137-174		1
9	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 5535-5549		6.1 1
8	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6799-6807		6.4 1
7	Optimizing Multisite Dynamics Throughput with Charge Renormalization.. <i>Journal of Chemical Information and Modeling</i> , 2022 , 62, 1479-1488		6.1 1
6	Thermodynamic Aspects. <i>Advances in Chemical Physics</i> , 2007 , 175-190		
5	Experimental Comparisons and Analysis. <i>Advances in Chemical Physics</i> , 2007 , 191-224		
4	Thermodynamic Methods. <i>Advances in Chemical Physics</i> , 2007 , 59-74		
3	Atom and Sidechain Motions. <i>Advances in Chemical Physics</i> , 2007 , 75-116		
2	Larger-Scale Motions. <i>Advances in Chemical Physics</i> , 2007 , 127-136		
1	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states.. <i>PLoS Computational Biology</i> , 2022 , 18, e1009977		5