Charles L Brooks Iii

List of Publications by Year
in descending order

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124 papers	15,957 citations	41344 49 h-index	21540 114 g-index
130 all docs	130 docs citations	130 times ranked	14751 citing authors

#	Article	IF	Citations
1	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, 1400-1415.	3.3	3,145
2	Detailed analysis of grid-based molecular docking: A case study of CDOCKER?A CHARMm-based MD docking algorithm. Journal of Computational Chemistry, 2003, 24, 1549-1562.	3.3	1,299
3	A modified TIP3P water potential for simulation with Ewald summation. Journal of Chemical Physics, 2004, 121, 10096-10103.	3.0	1,063
4	Generalized born model with a simple smoothing function. Journal of Computational Chemistry, 2003, 24, 1691-1702.	3.3	642
5	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	3.3	523
6	FROMFOLDINGTHEORIES TOFOLDINGPROTEINS: A Review and Assessment of Simulation Studies of Protein Folding and Unfolding. Annual Review of Physical Chemistry, 2001, 52, 499-535.	10.8	483
7	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. Journal of Computational Chemistry, 2003, 24, 1348-1356.	3.3	474
8	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. Journal of Computational Chemistry, 2004, 25, 1-16.	3.3	457
9	Novel generalized Born methods. Journal of Chemical Physics, 2002, 116, 10606-10614.	3.0	416
10	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, 1504-1514.	3.3	410
11	The origins of asymmetry in the folding transition states of protein L and protein G. Protein Science, 2009, 11, 2351-2361.	7.6	352
12	Î»â€dynamics: A new approach to free energy calculations. Journal of Chemical Physics, 1996, 105, 2414-2423.	3.0	324
13	Constant-pH molecular dynamics using continuous titration coordinates. Proteins: Structure, Function and Bioinformatics, 2004, 56, 738-752.	2.6	316
14	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886.	3.3	311
15	Comparative study of several algorithms for flexible ligand docking. Journal of Computer-Aided Molecular Design, 2003, 17, 755-763.	2.9	297
16	Structural and energetic effects of truncating long ranged interactions in ionic and polar fluids. Journal of Chemical Physics, 1985, 83, 5897-5908.	3.0	290
17	Normal mode based flexible fitting of high-resolution structure into low-resolution experimental data from cryo-EM. Journal of Structural Biology, 2004, 147, 315-326.	2.8	230
18	Insights from Coarse-Grained GÅ•Models for Protein Folding and Dynamics. International Journal of Molecular Sciences, 2009, 10, 889-905.	4.1	228

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19	Î»â€Ðynamics free energy simulation methods. Journal of Computational Chemistry, 2009, 30, 1692-1700.	3.3	164
20	Assessing energy functions for flexible docking. Journal of Computational Chemistry, 1998, 19, 1612-1622.	3.3	144
21	MATCH: An atomâ€typing toolset for molecular mechanics force fields. Journal of Computational Chemistry, 2012, 33, 189-202.	3.3	140
22	Implicit solvation based on generalized Born theory in different dielectric environments. Journal of Chemical Physics, 2004, 120, 903-911.	3.0	136
23	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. Physical Chemistry Chemical Physics, 2008, 10, 471-481.	2.8	130
24	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. Journal of Chemical Physics, 1987, 87, 3029-3037.	3.0	127
25	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. Proteins: Structure, Function and Bioinformatics, 2007, 67, 922-930.	2.6	124
26	An electrostatic basis for the stability of thermophilic proteins. Proteins: Structure, Function and Bioinformatics, 2004, 57, 128-141.	2.6	122
27	A Microscopic View of Helix Propagation: N and C-terminal Helix Growth in Alanine Helices. Journal of Molecular Biology, 1996, 259, 560-572.	4.2	117
28	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. Molecular Simulation, 2006, 32, 231-249.	2.0	116
29	Assessing search strategies for flexible docking. Journal of Computational Chemistry, 1998, 19, 1623-1631.	3.3	112
30	Thermodynamics of protein folding: A statistical mechanical study of a small all-Î² protein. , 1997, 42, 745-757.		106
31	Modern protein force fields behave comparably in molecular dynamics simulations. Journal of Computational Chemistry, 2002, 23, 1045-1057.	3.3	99
32	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1319-1331.	2.6	99
33	Molecular Interactions between Graphene and Biological Molecules. Journal of the American Chemical Society, 2017, 139, 1928-1936.	13.7	96
34	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist Î²-barrel model. Journal of Chemical Physics, 1998, 109, 2895-2903.	3.0	92
35	Molecular dynamics with internal coordinate constraints. Journal of Chemical Physics, 1988, 89, 5115-5127.	3.0	90
36	Flexible <scp>CDOCKER</scp>: Development and application of a pseudoâ€explicit structureâ€based docking method within <scp>CHARMM</scp>. Journal of Computational Chemistry, 2016, 37, 753-762.	3.3	88

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37	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. Proteins: Structure, Function and Bioinformatics, 2000, 41, 86-97.	2.6	85
38	Energetic frustration and the nature of the transition state in protein folding. Journal of Chemical Physics, 2000, 113, 7663-7671.	3.0	84
39	The influence of longâ€•range force truncation on the thermodynamics of aqueous ionic solutions. Journal of Chemical Physics, 1987, 86, 5156-5162.	3.0	78
40	Evaluating CASP4 predictions with physical energy functions. Proteins: Structure, Function and Bioinformatics, 2002, 49, 232-245.	2.6	78
41	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. Journal of Computational Chemistry, 2005, 26, 1565-1578.	3.3	67
42	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.	3.0	66
43	A reexamination of the hydrophobic effect: Exploring the role of the solvent model in computing the methaneâ€“methane potential of mean force. Journal of Chemical Physics, 1997, 106, 9265-9269.	3.0	65
44	Deciphering protein evolution and fitness landscapes with latent space models. Nature Communications, 2019, 10, 5644.	12.8	64
45	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. Journal of Chemical Physics, 1991, 95, 7612-7625.	3.0	63
46	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. Journal of Chemical Physics, 2005, 123, 164502.	3.0	63
47	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. Journal of Computational Chemistry, 2011, 32, 2909-2923.	3.3	63
48	The thermodynamics of solvophobic effects: A molecularâ€dynamics study of nâ€butane in carbon tetrachloride and water. Journal of Chemical Physics, 1990, 92, 2582-2592.	3.0	62
49	Curious structure in â€œcanonicalâ€•alanine-based peptides. , 1997, 28, 59-71.		58
50	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. Journal of Chemical Physics, 2006, 124, 204706.	3.0	58
51	Functionally Important Conformations of the Met20 Loop in Dihydrofolate Reductase are Populated by Rapid Thermal Fluctuations. Journal of the American Chemical Society, 2009, 131, 5642-5647.	13.7	56
52	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. Journal of the American Chemical Society, 2018, 140, 16560-16569.	13.7	51
53	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. Proteins: Structure, Function and Bioinformatics, 2004, 57, 444-457.	2.6	50
54	Prediction of Quaternary Structure of Coiled Coils. Application to Mutants of the GCN4 Leucine Zipper. Journal of Molecular Biology, 1995, 251, 448-467.	4.2	45

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55	Predicting extreme pK_a shifts in staphylococcal nuclease mutants with constant pH molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3276-3286.	2.6	43
56	Automated, Accurate, and Scalable Relative Proteinâ€“Ligand Binding Free-Energy Calculations Using Lambda Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 7895-7914.	5.3	43
57	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. Journal of Chemical Physics, 2006, 125, 174108.	3.0	42
58	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.	2.6	42
59	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.	2.6	40
60	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. Journal of Computational Chemistry, 1991, 12, 1270-1277.	3.3	40
61	A molecular dynamics simulation study of segment B1 of protein G. , 1997, 29, 193-202.		40
62	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. Journal of Computational Chemistry, 2008, 29, 820-831.	3.3	40
63	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. Journal of Computational Chemistry, 2011, 32, 3423-3432.	3.3	39
64	An ab initio study of hydrated chloride ion complexes: Evidence of polarization effects and nonadditivity. Journal of Chemical Physics, 1987, 87, 5892-5894.	3.0	35
65	Conformational change of the methionine 20 loop ofEscherichia colidihydrofolate reductase modulates pKaof the bound dihydrofolate. Protein Science, 2007, 16, 1087-1100.	7.6	34
66	The importance of explicit chain representation in protein folding models: An examination of ising-like models. Proteins: Structure, Function and Bioinformatics, 2003, 53, 740-747.	2.6	33
67	FoldGPCR: Structure prediction protocol for the transmembrane domain of G proteinâ€coupled receptors from class A. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2189-2201.	2.6	33
68	Cluster structure determination using Gaussian density distribution global minimization methods. Journal of Chemical Physics, 1994, 101, 6405-6411.	3.0	32
69	Assessing the quality of absolute hydration free energies among CHARMMâ€compatible ligand parameterization schemes. Journal of Computational Chemistry, 2013, 34, 893-903.	3.3	32
70	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.	2.6	30
71	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, 1529-1541.	3.3	30
72	Exploring Proteinâ€“Nanoparticle Interactions with Coarseâ€Grained Protein Folding Models. Small, 2017, 13, 1603748.	10.0	29

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73	Virtual rigid body dynamics. Biopolymers, 1991, 31, 77-100.	2.4	28
74	Improved model building and assessment of the Calciumâ€sensing receptor transmembrane domain. Proteins: Structure, Function and Bioinformatics, 2008, 71, 215-226.	2.6	28
75	PCASSO: A fast and efficient CÎ±â€based method for accurately assigning protein secondary structure elements. Journal of Computational Chemistry, 2014, 35, 1757-1761.	3.3	28
76	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite Î» Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 3328-3332.	4.6	28
77	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. Journal of the American Chemical Society, 2019, 141, 9980-9988.	13.7	28
78	Structural Basis for Selectivity in Flavin-Dependent Monooxygenase-Catalyzed Oxidative Dearomatization. ACS Catalysis, 2019, 9, 3633-3640.	11.2	28
79	Approaching protein design with multisite Î» dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. Protein Science, 2018, 27, 1910-1922.	7.6	26
80	Exploring Assembly Energetics of the 30S Ribosomal Subunit Using an Implicit Solvent Approach. Journal of the American Chemical Society, 2005, 127, 11125-11133.	13.7	25
81	Efficient approximate all-atom solvent accessible surface area method parameterized for folded and denatured protein conformations. Journal of Computational Chemistry, 2004, 25, 1005-1014.	3.3	23
82	Parallelization and improvements of the generalized born model with a simple s<scp>W</scp>itching function for modern graphics processors. Journal of Computational Chemistry, 2016, 37, 927-939.	3.3	23
83	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. Journal of Chemical Theory and Computation, 2021, 17, 6799-6807.	5.3	23
84	Free energy screening of small ligands binding to an artificial protein cavity. Journal of Chemical Physics, 2000, 113, 3423-3433.	3.0	22
85	Receptor rigidity and ligand mobility in trypsin-ligand complexes. Proteins: Structure, Function and Bioinformatics, 2004, 58, 407-417.	2.6	22
86	Model of the toxic complex of anthrax: Responsive conformational changes in both the lethal factor and the protective antigen heptamer. Protein Science, 2006, 15, 2190-2200.	7.6	22
87	Efficient implementation of constant pH molecular dynamics on modern graphics processors. Journal of Computational Chemistry, 2016, 37, 2171-2180.	3.3	22
88	Effect of gatekeepers on the early folding kinetics of a model Î²-barrel protein. Journal of Chemical Physics, 2003, 119, 5722-5729.	3.0	21
89	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. Molecular Informatics, 2011, 30, 896-906.	2.5	19
90	pHâ€sensitive residues in the p19 RNA silencing suppressor protein from carnation Italian ringspot virus affect siRNA binding stability. Protein Science, 2013, 22, 595-604.	7.6	18

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91	Overcoming Challenging Substituent Perturbations with Multisite Î»-Dynamics: A Case Study Targeting Î²-Secretase 1. Journal of Physical Chemistry Letters, 2019, 10, 4875-4880.	4.6	17
92	Thermodynamic calculations on biological molecules. International Journal of Quantum Chemistry, 1988, 34, 221-234.	2.0	16
93	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. Journal of Physical Chemistry Letters, 2020, 11, 864-868.	4.6	13
94	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. Journal of Chemical Information and Modeling, 2021, 61, 5535-5549.	5.4	13
95	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. Journal of Physical Chemistry C, 2016, 120, 19078-19086.	3.1	12
96	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. Journal of Physical Chemistry B, 2019, 123, 8065-8073.	2.6	12
97	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. Journal of Computational Chemistry, 2021, 42, 1088-1094.	3.3	12
98	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. Proteins: Structure, Function and Bioinformatics, 2009, 77, 448-453.	2.6	11
99	The flexible Câ€terminal arm of the Lassa arenavirus Zâ€protein mediates interactions with multiple binding partners. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2251-2264.	2.6	11
100	Protein Structure and Dynamics-An Overview. Advances in Chemical Physics, 2007, , 7-21.	0.3	9
101	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. Journal of Physical Chemistry Letters, 2019, 10, 5963-5968.	4.6	9
102	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.	3.3	9
103	A line integral reaction path approximation for large systems via nonlinear constrained optimization: Application to alanine dipeptide and the Î² hairpin of protein G. Journal of Chemical Physics, 2006, 124, 194903.	3.0	8
104	Optimizing Multisite Î»-Dynamics Throughput with Charge Renormalization. Journal of Chemical Information and Modeling, 2022, 62, 1479-1488.	5.4	8
105	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. Journal of Chemical Information and Modeling, 2022, 62, 1458-1470.	5.4	8
106	Dynamic load balancing algorithms for replicated data molecular dynamics. Journal of Computational Chemistry, 1995, 16, 715-722.	3.3	7
107	Exploring pH Dependent Host/Guest Binding Affinities. Journal of Physical Chemistry B, 2020, 124, 6520-6528.	2.6	6
108	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.	3.3	5

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109	Temperature-Dependent Behavior of Protein-Chromophore Interactions: A Theoretical Study of a Blue Fluorescent Antibody. ChemPhysChem, 2003, 4, 848-855.	2.1	5
110	The Stability of Protein Secondary Structures in Aqueous Solution. AIP Conference Proceedings, 1991, , .	0.4	4
111	Dynamical Simulation Methods. Advances in Chemical Physics, 2007, , 33-58.	0.3	4
112	Steric and thermodynamic limits of design for the incorporation of large unnatural amino acids in aminoacylâ€tRNA synthetase enzymes. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1926-1938.	2.6	4
113	Computational Studies of Catalytic Loop Dynamics in Yersinia Protein Tyrosine Phosphatase Using Pathway Optimization Methods. Journal of Physical Chemistry B, 2019, 123, 7840-7851.	2.6	4
114	Exploring the Functional Landscape of Biomolecular Machines via Elastic Network Normal Mode Analysis. , 0, , 59-77.		3
115	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states. PLoS Computational Biology, 2022, 18, e1009977.	3.2	3
116	Rigid-Body Motions. Advances in Chemical Physics, 2007, , 117-126.	0.3	2
117	Solvent Influence on Protein Dynamics. Advances in Chemical Physics, 2007, , 137-174.	0.3	2
118	Potential Functions. Advances in Chemical Physics, 2007, , 23-31.	0.3	1
119	Implicit Solvent Force-Field Optimization. , 0, , 167-190.		1
120	Thermodynamic Aspects. Advances in Chemical Physics, 2007, , 175-190.	0.3	0
121	Experimental Comparisons and Analysis. Advances in Chemical Physics, 2007, , 191-224.	0.3	0
122	Thermodynamic Methods. Advances in Chemical Physics, 2007, , 59-74.	0.3	0
123	Atom and Sidechain Motions. Advances in Chemical Physics, 2007, , 75-116.	0.3	0
124	Larger-Scale Motions. Advances in Chemical Physics, 2007, , 127-136.	0.3	0