Charles L Brooks Iii

List of Publications by Year
in descending order

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124 papers	15,957 citations	41258 49 h-index	21474 114 g-index
130 all docs	130 docs citations	130 times ranked	14751 citing authors

#	Article	IF	Citations
1	Optimizing Multisite Î»-Dynamics Throughput with Charge Renormalization. Journal of Chemical Information and Modeling, 2022, 62, 1479-1488.	2.5	8
2	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. Journal of Chemical Information and Modeling, 2022, 62, 1458-1470.	2.5	8
3	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states. PLoS Computational Biology, 2022, 18, e1009977.	1.5	3
4	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. Journal of Computational Chemistry, 2021, 42, 1088-1094.	1.5	12
5	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. Journal of Chemical Information and Modeling, 2021, 61, 5535-5549.	2.5	13
6	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. Journal of Chemical Theory and Computation, 2021, 17, 6799-6807.	2.3	23
7	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.	1.5	9
8	Automated, Accurate, and Scalable Relative Proteinâ€“Ligand Binding Free-Energy Calculations Using Lambda Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 7895-7914.	2.3	43
9	Exploring pH Dependent Host/Guest Binding Affinities. Journal of Physical Chemistry B, 2020, 124, 6520-6528.	1.2	6
10	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. Journal of Physical Chemistry Letters, 2020, 11, 864-868.	2.1	13
11	Overcoming Challenging Substituent Perturbations with Multisite Î»-Dynamics: A Case Study Targeting Î²-Secretase 1. Journal of Physical Chemistry Letters, 2019, 10, 4875-4880.	2.1	17
12	Computational Studies of Catalytic Loop Dynamics in Yersinia Protein Tyrosine Phosphatase Using Pathway Optimization Methods. Journal of Physical Chemistry B, 2019, 123, 7840-7851.	1.2	4
13	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. Journal of Physical Chemistry B, 2019, 123, 8065-8073.	1.2	12
14	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. Journal of Physical Chemistry Letters, 2019, 10, 5963-5968.	2.1	9
15	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. Journal of the American Chemical Society, 2019, 141, 9980-9988.	6.6	28
16	Structural Basis for Selectivity in Flavin-Dependent Monooxygenase-Catalyzed Oxidative Dearomatization. ACS Catalysis, 2019, 9, 3633-3640.	5.5	28
17	Deciphering protein evolution and fitness landscapes with latent space models. Nature Communications, 2019, 10, 5644.	5.8	64
18	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. Journal of the American Chemical Society, 2018, 140, 16560-16569.	6.6	51

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19	Approaching protein design with multisite Î» dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. Protein Science, 2018, 27, 1910-1922.	3.1	26
20	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite Î» Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 3328-3332.	2.1	28
21	Molecular Interactions between Graphene and Biological Molecules. Journal of the American Chemical Society, 2017, 139, 1928-1936.	6.6	96
22	Exploring Proteinâ€“Nanoparticle Interactions with Coarseâ€Grained Protein Folding Models. Small, 2017, 13, 1603748.	5.2	29
23	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886.	1.5	311
24	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. Journal of Physical Chemistry C, 2016, 120, 19078-19086.	1.5	12
25	Efficient implementation of constant pH molecular dynamics on modern graphics processors. Journal of Computational Chemistry, 2016, 37, 2171-2180.	1.5	22
26	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.	1.5	23
27	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.	1.5	88
28	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.	1.5	42
29	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1319-1331.	1.5	99
30	PCASSO: A fast and efficient CÎ±â€based method for accurately assigning protein secondary structure elements. Journal of Computational Chemistry, 2014, 35, 1757-1761.	1.5	28
31	Assessing the quality of absolute hydration free energies among CHARMMâ€compatible ligand parameterization schemes. Journal of Computational Chemistry, 2013, 34, 893-903.	1.5	32
32	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.	3.1	18
33	MATCH: An atomâ€typing toolset for molecular mechanics force fields. Journal of Computational Chemistry, 2012, 33, 189-202.	1.5	140
34	Predicting extreme pK_a shifts in staphylococcal nuclease mutants with constant pH molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3276-3286.	1.5	43
35	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. Molecular Informatics, 2011, 30, 896-906.	1.4	19
36	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. Journal of Computational Chemistry, 2011, 32, 2909-2923.	1.5	63

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37	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. Journal of Computational Chemistry, 2011, 32, 3423-3432.	1.5	39
38	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.	1.5	4
39	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.	1.5	33
40	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.	1.5	11
41	Î»â€Dynamics free energy simulation methods. Journal of Computational Chemistry, 2009, 30, 1692-1700.	1.5	164
42	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. Proteins: Structure, Function and Bioinformatics, 2009, 77, 448-453.	1.5	11
43	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.	6.6	56
44	Insights from Coarse-Grained GÅ•Models for Protein Folding and Dynamics. International Journal of Molecular Sciences, 2009, 10, 889-905.	1.8	228
45	The origins of asymmetry in the folding transition states of protein L and protein G. Protein Science, 2009, 11, 2351-2361.	3.1	352
46	Improved model building and assessment of the Calciumâ€sensing receptor transmembrane domain. Proteins: Structure, Function and Bioinformatics, 2008, 71, 215-226.	1.5	28
47	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. Journal of Computational Chemistry, 2008, 29, 820-831.	1.5	40
48	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. Physical Chemistry Chemical Physics, 2008, 10, 471-481.	1.3	130
49	Thermodynamic Aspects. Advances in Chemical Physics, 2007, , 175-190.	0.3	0
50	Experimental Comparisons and Analysis. Advances in Chemical Physics, 2007, , 191-224.	0.3	0
51	Protein Structure and Dynamics-An Overview. Advances in Chemical Physics, 2007, , 7-21.	0.3	9
52	Potential Functions. Advances in Chemical Physics, 2007, , 23-31.	0.3	1
53	Dynamical Simulation Methods. Advances in Chemical Physics, 2007, , 33-58.	0.3	4
54	Thermodynamic Methods. Advances in Chemical Physics, 2007, , 59-74.	0.3	0

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55	Atom and Sidechain Motions. Advances in Chemical Physics, 2007, , 75-116.	0.3	0
56	Rigid-Body Motions. Advances in Chemical Physics, 2007, , 117-126.	0.3	2
57	Larger-Scale Motions. Advances in Chemical Physics, 2007, , 127-136.	0.3	0
58	Solvent Influence on Protein Dynamics. Advances in Chemical Physics, 2007, , 137-174.	0.3	2
59	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. Proteins: Structure, Function and Bioinformatics, 2007, 67, 922-930.	1.5	124
60	Conformational change of the methionine 20 loop ofEscherichia colidihydrofolate reductase modulates pKaof the bound dihydrofolate. Protein Science, 2007, 16, 1087-1100.	3.1	34
61	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. Molecular Simulation, 2006, 32, 231-249.	0.9	116
62	Revisiting the hexane-water interface via molecular dynamics simulations using nonadditive alkane-water potentials. Journal of Chemical Physics, 2006, 124, 204706.	1.2	58
63	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.	3.1	22
64	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. Journal of Chemical Physics, 2006, 125, 174108.	1.2	42
65	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.	1.2	8
66	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.	1.2	66
67	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.	1.5	30
68	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. Journal of Computational Chemistry, 2005, 26, 1565-1578.	1.5	67
69	Exploring Assembly Energetics of the 30S Ribosomal Subunit Using an Implicit Solvent Approach. Journal of the American Chemical Society, 2005, 127, 11125-11133.	6.6	25
70	Structure, thermodynamics, and liquid-vapor equilibrium of ethanol from molecular-dynamics simulations using nonadditive interactions. Journal of Chemical Physics, 2005, 123, 164502.	1.2	63
71	A modified TIP3P water potential for simulation with Ewald summation. Journal of Chemical Physics, 2004, 121, 10096-10103.	1.2	1,063
72	Constant-pH molecular dynamics using continuous titration coordinates. Proteins: Structure, Function and Bioinformatics, 2004, 56, 738-752.	1.5	316

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73	An electrostatic basis for the stability of thermophilic proteins. Proteins: Structure, Function and Bioinformatics, 2004, 57, 128-141.	1.5	122
74	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. Proteins: Structure, Function and Bioinformatics, 2004, 57, 444-457.	1.5	50
75	Receptor rigidity and ligand mobility in trypsin-ligand complexes. Proteins: Structure, Function and Bioinformatics, 2004, 58, 407-417.	1.5	22
76	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. Journal of Computational Chemistry, 2004, 25, 1-16.	1.5	457
77	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.	1.5	523
78	Efficient approximate all-atom solvent accessible surface area method parameterized for folded and denatured protein conformations. Journal of Computational Chemistry, 2004, 25, 1005-1014.	1.5	23
79	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.	1.5	3,145
80	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.	1.5	410
81	Implicit solvation based on generalized Born theory in different dielectric environments. Journal of Chemical Physics, 2004, 120, 903-911.	1.2	136
82	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.	1.3	230
83	Comparative study of several algorithms for flexible ligand docking. Journal of Computer-Aided Molecular Design, 2003, 17, 755-763.	1.3	297
84	Temperature-Dependent Behavior of Protein-Chromophore Interactions: A Theoretical Study of a Blue Fluorescent Antibody. ChemPhysChem, 2003, 4, 848-855.	1.0	5
85	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. Journal of Computational Chemistry, 2003, 24, 1348-1356.	1.5	474
86	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.	1.5	1,299
87	Generalized born model with a simple smoothing function. Journal of Computational Chemistry, 2003, 24, 1691-1702.	1.5	642
88	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.	1.5	33
89	Effect of gatekeepers on the early folding kinetics of a model Î²-barrel protein. Journal of Chemical Physics, 2003, 119, 5722-5729.	1.2	21
90	Novel generalized Born methods. Journal of Chemical Physics, 2002, 116, 10606-10614.	1.2	416

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91	Modern protein force fields behave comparably in molecular dynamics simulations. Journal of Computational Chemistry, 2002, 23, 1045-1057.	1.5	99
92	Evaluating CASP4 predictions with physical energy functions. Proteins: Structure, Function and Bioinformatics, 2002, 49, 232-245.	1.5	78
93	FROMFOLDINGTHEORIES TOFOLDINGPROTEINS: A Review and Assessment of Simulation Studies of Protein Folding and Unfolding. Annual Review of Physical Chemistry, 2001, 52, 499-535.	4.8	483
94	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. Proteins: Structure, Function and Bioinformatics, 2000, 41, 86-97.	1.5	85
95	Energetic frustration and the nature of the transition state in protein folding. Journal of Chemical Physics, 2000, 113, 7663-7671.	1.2	84
96	Free energy screening of small ligands binding to an artificial protein cavity. Journal of Chemical Physics, 2000, 113, 3423-3433.	1.2	22
97	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.	1.5	30
98	Assessing energy functions for flexible docking. Journal of Computational Chemistry, 1998, 19, 1612-1622.	1.5	144
99	Assessing search strategies for flexible docking. Journal of Computational Chemistry, 1998, 19, 1623-1631.	1.5	112
100	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.	1.2	92
101	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.	1.2	65
102	Curious structure in â€œcanonicalâ€•alanine-based peptides. , 1997, 28, 59-71.		58
103	A molecular dynamics simulation study of segment B1 of protein G. , 1997, 29, 193-202.		40
104	Thermodynamics of protein folding: A statistical mechanical study of a small all-Î² protein. , 1997, 42, 745-757.		106
105	Î»â€dynamics: A new approach to free energy calculations. Journal of Chemical Physics, 1996, 105, 2414-2423.	1.2	324
106	A Microscopic View of Helix Propagation: N and C-terminal Helix Growth in Alanine Helices. Journal of Molecular Biology, 1996, 259, 560-572.	2.0	117
107	Dynamic load balancing algorithms for replicated data molecular dynamics. Journal of Computational Chemistry, 1995, 16, 715-722.	1.5	7
108	Prediction of Quaternary Structure of Coiled Coils. Application to Mutants of the GCN4 Leucine Zipper. Journal of Molecular Biology, 1995, 251, 448-467.	2.0	45

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109	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.	1.5	5
110	Cluster structure determination using Gaussian density distribution global minimization methods. Journal of Chemical Physics, 1994, 101, 6405-6411.	1.2	32
111	The Stability of Protein Secondary Structures in Aqueous Solution. AIP Conference Proceedings, 1991, , .	0.3	4
112	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. Journal of Computational Chemistry, 1991, 12, 1270-1277.	1.5	40
113	Virtual rigid body dynamics. Biopolymers, 1991, 31, 77-100.	1.2	28
114	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. Journal of Chemical Physics, 1991, 95, 7612-7625.	1.2	63
115	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.	1.5	40
116	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.	1.2	62
117	Thermodynamic calculations on biological molecules. International Journal of Quantum Chemistry, 1988, 34, 221-234.	1.0	16
118	Molecular dynamics with internal coordinate constraints. Journal of Chemical Physics, 1988, 89, 5115-5127.	1.2	90
119	An ab initio study of hydrated chloride ion complexes: Evidence of polarization effects and nonadditivity. Journal of Chemical Physics, 1987, 87, 5892-5894.	1.2	35
120	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. Journal of Chemical Physics, 1987, 87, 3029-3037.	1.2	127
121	The influence of longâ€range force truncation on the thermodynamics of aqueous ionic solutions. Journal of Chemical Physics, 1987, 86, 5156-5162.	1.2	78
122	Structural and energetic effects of truncating long ranged interactions in ionic and polar fluids. Journal of Chemical Physics, 1985, 83, 5897-5908.	1.2	290
123	Implicit Solvent Force-Field Optimization. , 0, , 167-190.		1
124	Exploring the Functional Landscape of Biomolecular Machines via Elastic Network Normal Mode Analysis. , 0, , 59-77.		3