Bernard R Brooks

List of Publications by Year in Descending Order

133 papers	26,205 citations	39 h-index	137 g-index
137 ext. papers	28,957 ext. citations	4.6 avg, IF	6.52 L-index

#	Paper	IF	Citations
133	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules.. *Journal of Chemical Physics*, **2022**, 156, 184103	3.9	2
132	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. *Journal of Chemical Physics*, **2021**, 155, 194108	3.9	3
131	Analytical Hessians for Ewald and particle mesh Ewald electrostatics. *Journal of Chemical Physics*, **2021**, 154, 104101	3.9	2
130	A replica exchange umbrella sampling (REUS) approach to predict host-guest binding free energies in SAMPL8 challenge. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 667-677	4.2	1
129	The Extended Eighth-Shell method for periodic boundary conditions with rotational symmetry. *Journal of Computational Chemistry*, **2021**, 42, 1373-1383	3.5	1
128	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. *Journal of Physical Chemistry B*, **2021**, 125, 5233-5242	3.4	1
127	Improving the speed of volumetric density map generation via cubic spline interpolation. *Journal of Molecular Graphics and Modelling*, **2021**, 104, 107832	2.8	1
126	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. *Journal of Chemical Theory and Computation*, **2021**, 17, 1086-1097	6.4	5
125	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. *Journal of Chemical Theory and Computation*, **2021**, 17, 1581-1595	6.4	8
124	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. *Journal of Chemical Theory and Computation*, **2021**, 17, 1562-1580	6.4	6
123	A compression strategy for particle mesh Ewald theory. *Journal of Chemical Physics*, **2021**, 154, 054112	3.9	2
122	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. *Biophysical Journal*, **2021**, 120, 2902-2913	2.9	9
121	Determinants of conductance of a bacterial voltage-gated sodium channel. *Biophysical Journal*, **2021**, 120, 3050-3069	2.9	0
120	Psi4 1.4: Open-source software for high-throughput quantum chemistry. *Journal of Chemical Physics* , **2020**, 152, 184108	3.9	158
119	A deep learning approach for the blind logP prediction in SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 535-542	4.2	10
118	Quantum chemical predictions of water-octanol partition coefficients applied to the SAMPL6 logP blind challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 485-493	4.2	6
117	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of water-octanol partition coefficients in the SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 471-483	4.2	5

116	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 495-510	4.2	7
115	Protonation state of the selectivity filter of bacterial voltage-gated sodium channels is modulated by ions. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 527-539	4.2	4
114	A protocol for preparing explicitly solvated systems for stable molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 054123	3.9	11
113	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 10034-10047	3.4	39
112	Reformulation of the self-guided molecular simulation method. *Journal of Chemical Physics*, **2020**, 153, 094112	3.9	1
111	Membrane permeability of small molecules from unbiased molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 124107	3.9	15
110	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	1
109	Albumin-chaperoned cyanine dye yields superbright NIR-II fluorophore with enhanced pharmacokinetics. *Science Advances*, **2019**, 5, eaaw0672	14.3	93
108	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 3854-3867	6.4	19
107	The homogeneity condition: A simple way to derive isotropic periodic sum potentials for efficient calculation of long-range interactions in molecular simulation. *Journal of Chemical Physics*, **2019**, 150, 214109	3.9	3
106	A double exponential potential for van der Waals interaction. *AIP Advances*, **2019**, 9, 065304	1.5	5
105	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. *Journal of Physical Chemistry B*, **2018**, 122, 5657-5665	3.4	10
104	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 948-958	6.4	31
103	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. *Journal of Chemical Physics*, **2018**, 149, 072323	3.9	7
102	Prediction of CB[8] host-guest binding free energies in SAMPL6 using the double-decoupling method. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1059-1073	4.2	10
101	Absolute and relative pK predictions via a DFT approach applied to the SAMPL6 blind challenge. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1179-1189	4.2	14
100	On the convergence of multi-scale free energy simulations. *Molecular Simulation*, **2018**, 44, 1062-1081	2	30
99	Comparison of the umbrella sampling and the double decoupling method in binding free energy predictions for SAMPL6 octa-acid host-guest challenges. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1075-1086	4.2	14

98	Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 983-999	4.2	15
97	An explicit-solvent hybrid QM and MM approach for predicting pKa of small molecules in SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1191-1201	4.2	15
96	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. *Molecules*, **2018**, 23,	4.8	23
95	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimer's Aβ Protofilaments. *Journal of Physical Chemistry B*, **2018**, 122, 11535-11545	3.4	6
94	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. *Journal of Physical Chemistry B*, **2018**, 122, 6215-6223	3.4	5
93	Reservoir pH replica exchange. *Journal of Chemical Physics*, **2018**, 149, 072321	3.9	13
92	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 679-695	6.4	14
91	Absolute binding free energies for octa-acids and guests in SAMPL5 : Evaluating binding free energies for octa-acid and guest complexes in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 107-118	4.2	15
90	Finding multiple reaction pathways via global optimization of action. *Nature Communications*, **2017**, 8, 15443	17.4	24
89	Inverse Resolution Limit of Partition Density and Detecting Overlapping Communities by Link-Surprise. *Scientific Reports*, **2017**, 7, 12399	4.9	6
88	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. *PLoS Computational Biology*, **2017**, 13, e1005659	5	686
87	Global organization of a binding site network gives insight into evolution and structure-function relationships of proteins. *Scientific Reports*, **2017**, 7, 11652	4.9	4
86	Efficient Strategy for the Calculation of Solvation Free Energies in Water and Chloroform at the Quantum Mechanical/Molecular Mechanical Level. *Journal of Chemical Information and Modeling*, **2017**, 57, 2476-2489	6.1	23
85	Machine Learning Force Field Parameters from Ab Initio Data. *Journal of Chemical Theory and Computation*, **2017**, 13, 4492-4503	6.4	73
84	Mapping the Drude polarizable force field onto a multipole and induced dipole model. *Journal of Chemical Physics*, **2017**, 147, 161702	3.9	32
83	Origin of pK Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. *Journal of Physical Chemistry B*, **2017**, 121, 3318-3330	3.4	16
82	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 71-85	4.2	9
81	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4988-4997	3.4	14

80	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 989-1006	4.2	20
79	Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases. *Journal of the American Chemical Society*, **2016**, 138, 15035-15045	16.4	20
78	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. *Journal of Chemical Theory and Computation*, **2016**, 12, 499-511	6.4	70
77	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. *Human Molecular Genetics*, **2016**, 25, 1328-44	5.6	36
76	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. *Journal of Chemical Theory and Computation*, **2016**, 12, 1466-80	6.4	36
75	Molecular Multipole Potential Energy Functions for Water. *Journal of Physical Chemistry B*, **2016**, 120, 1833-42	3.4	9
74	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 332-44	6.4	36
73	An empirical extrapolation scheme for efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2016**, 145, 164101	3.9	24
72	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. *Journal of Chemical Physics*, **2016**, 145, 164110	3.9	5
71	Self-guided Langevin dynamics via generalized Langevin equation. *Journal of Computational Chemistry*, **2016**, 37, 595-601	3.5	40
70	Computational scheme for pH-dependent binding free energy calculation with explicit solvent. *Protein Science*, **2016**, 25, 231-43	6.3	25
69	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK corrections. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 1087-1100	4.2	24
68	The Atomistic Mechanism of Conformational Transition of Adenylate Kinase Investigated by Lorentzian Structure-Based Potential. *Journal of Chemical Theory and Computation*, **2015**, 11, 3211-24	6.4	12
67	Numerical study on the partitioning of the molecular polarizability into fluctuating charge and induced atomic dipole contributions. *Journal of Physical Chemistry A*, **2015**, 119, 5865-82	2.8	36
66	Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. *Journal of Chemical Theory and Computation*, **2015**, 11, 2560-74	6.4	28
65	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. *Journal of Chemical Physics*, **2015**, 142, 064501	3.9	25
64	Sigma-RF: prediction of the variability of spatial restraints in template-based modeling by random forest. *BMC Bioinformatics*, **2015**, 16, 94	3.6	16
63	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. *Journal of Chemical Information and Modeling*, **2015**, 55, 2308-14	6.1	43

62	Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 932-943	4	35
61	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. *Biophysical Chemistry*, **2015**, 196, 16-24	3.5	32
60	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
59	Efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2015**, 143, 074115	3.9	34
58	Protein structure determination by conformational space annealing using NMR geometric restraints. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 2251-62	4.2	13
57	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. *ACS Catalysis*, **2015**, 5, 3225-3237	13.1	22
56	Modulation of Alzheimer's A protofilament-membrane interactions by lipid headgroups. *ACS Chemical Neuroscience*, **2015**, 6, 446-55	5.7	42
55	A Virtual Mixture Approach to the Study of Multistate Equilibrium: Application to Constant pH Simulation in Explicit Water. *PLoS Computational Biology*, **2015**, 11, e1004480	5	13
54	Predicting hydration free energies with a hybrid QM/MM approach: an evaluation of implicit and explicit solvation models in SAMPL4. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 245-57	4.2	53
53	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. *Journal of Chemical Theory and Computation*, **2014**, 10, 2738-2750	6.4	54
52	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. *Journal of Chemical Theory and Computation*, **2014**, 10, 4198-4207	6.4	13
51	Web-based computational chemistry education with CHARMMing II: Coarse-grained protein folding. *PLoS Computational Biology*, **2014**, 10, e1003738	5	5
50	Web-based computational chemistry education with CHARMMing III: Reduction potentials of electron transfer proteins. *PLoS Computational Biology*, **2014**, 10, e1003739	5	5
49	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. *Journal of Chemical Physics*, **2014**, 140, 184101	3.9	41
48	Phosphoproteomic analysis reveals regulatory mechanisms at the kidney filtration barrier. *Journal of the American Society of Nephrology: JASN*, **2014**, 25, 1509-22	12.7	34
47	Accurate high-throughput structure mapping and prediction with transition metal ion FRET. *Structure*, **2013**, 21, 9-19	5.2	21
46	Targeted conformational search with map-restrained self-guided Langevin dynamics: application to flexible fitting into electron microscopic density maps. *Journal of Structural Biology*, **2013**, 183, 429-440	3.4	35
45	Protein-Protein Docking Using EMAP in CHARMM and Support Vector Machine: Application to Ab/Ag Complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 4186-94	6.4	2

44	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennett's Acceptance Ratio and Enveloping Distribution Sampling Methods. *Journal of Chemical Theory and Computation*, **2012**, 8, 3650-62	6.4	16
43	Efficient and Unbiased Sampling of Biomolecular Systems in the Canonical Ensemble: A Review of Self-Guided Langevin Dynamics. *Advances in Chemical Physics*, **2012**, 150, 255-326		29
42	Predicting binding affinities of host-guest systems in the SAMPL3 blind challenge: the performance of relative free energy calculations. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 543-50	4.2	25
41	Conformational relaxation and water penetration coupled to ionization of internal groups in proteins. *Journal of Physical Chemistry A*, **2011**, 115, 4042-53	2.8	32
40	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. *Journal of Chemical Physics*, **2011**, 134, 134108	3.9	33
39	Force-momentum-based self-guided Langevin dynamics: a rapid sampling method that approaches the canonical ensemble. *Journal of Chemical Physics*, **2011**, 135, 204101	3.9	18
38	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. *Journal of Chemical Theory and Computation*, **2011**, 7, 496-514	6.4	29
37	pH replica-exchange method based on discrete protonation states. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3420-36	4.2	89
36	Probing the periplasmic-open state of lactose permease in response to sugar binding and proton translocation. *Journal of Molecular Biology*, **2010**, 404, 506-21	6.5	28
35	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tamm-Dancoff approximation. *Molecular Physics*, **2010**, 108, 2791-2800	1.7	49
34	Isotropic periodic sum of electrostatic interactions for polar systems. *Journal of Chemical Physics*, **2009**, 131, 024107	3.9	35
33	Self-guided Langevin dynamics study of regulatory interactions in NtrC. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 1007-19	4.2	34
32	Backbone relaxation coupled to the ionization of internal groups in proteins: a self-guided Langevin dynamics study. *Biophysical Journal*, **2008**, 95, 4091-101	2.9	44
31	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. *Journal of Chemical Theory and Computation*, **2008**, 4, 107-15	6.4	10
30	Open science grid study of the coupling between conformation and water content in the interior of a protein. *Journal of Chemical Information and Modeling*, **2008**, 48, 2021-9	6.1	18
29	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. *Journal of Chemical Physics*, **2008**, 129, 154115	3.9	54
28	Isotropic periodic sum: a method for the calculation of long-range interactions. *Journal of Chemical Physics*, **2005**, 122, 44107	3.9	122
27	Pressure-Based Long-Range Correction for Lennard-Jones Interactions in Molecular Dynamics Simulations: Application to Alkanes and Interfaces. *Journal of Physical Chemistry B*, **2004**, 108, 363-368	3.4	90

26	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. *Theoretical Chemistry Accounts*, **2003**, 109, 140-148	1.9	93
25	Self-guided Langevin dynamics simulation method. *Chemical Physics Letters*, **2003**, 381, 512-518	2.5	329
24	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. *Journal of Chemical Physics*, **2002**, 117, 10534-10547	3.9	162
23	Direct observation of the folding and unfolding of a beta-hairpin in explicit water through computer simulation. *Journal of the American Chemical Society*, **2002**, 124, 5282-3	16.4	62
22	Simulations of membranes and other interfacial systems using P2(1) and Pc periodic boundary conditions. *Biophysical Journal*, **2002**, 82, 2317-25	2.9	51
21	Elastic molecular dynamics with self-consistent flexible constraints. *Journal of Chemical Physics*, **2000**, 112, 7919-7929	3.9	25
20	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. *Theoretical Chemistry Accounts*, **1998**, 99, 279-288	1.9	58
19	Molecular Dynamics of Staphylococcal Nuclease:Comparison of Simulation with15N and13C NMR Relaxation Data. *Journal of the American Chemical Society*, **1998**, 120, 5301-5311	16.4	114
18	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. *The Journal of Physical Chemistry*, **1996**, 100, 17011-17020		351
17	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. *International Journal of Quantum Chemistry*, **1996**, 60, 1189-1200	2.1	172
16	Constant pressure molecular dynamics simulation: The Langevin piston method. *Journal of Chemical Physics*, **1995**, 103, 4613-4621	3.9	3093
15	Harmonic analysis of large systems. I. Methodology. *Journal of Computational Chemistry*, **1995**, 16, 1522-1542	3.5	430
14	Harmonic analysis of large systems. II. Comparison of different protein models. *Journal of Computational Chemistry*, **1995**, 16, 1543-1553	3.5	69
13	Harmonic analysis of large systems. III. Comparison with molecular dynamics. *Journal of Computational Chemistry*, **1995**, 16, 1554-1566	3.5	81
12	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. *Journal of Computational Chemistry*, **1994**, 15, 532-552	3.5	48
11	New spherical-cutoff methods for long-range forces in macromolecular simulation. *Journal of Computational Chemistry*, **1994**, 15, 667-683	3.5	865
10	Theoretical studies of relaxation of a monomeric subunit of HIV-1 protease in water using molecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **1993**, 15, 374-84	4.2	19
9	Langevin dynamics of peptides: the frictional dependence of isomerization rates of N-acetylalanyl-NTmethylamide. *Biopolymers*, **1992**, 32, 523-35	2.2	663

8	Conformational states of a TT mismatch from molecular dynamics simulation of duplex d (CGCGATTCGCG). *Biopolymers*, **1992**, 32, 783-94	2.2	11
7	Computer simulations of a tumor surface octapeptide epitope. *Biopolymers*, **1989**, 28, 525-30	2.2	11
6	The effects of truncating long-range forces on protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **1989**, 6, 32-45	4.2	224
5	An analysis of the accuracy of Langevin and molecular dynamics algorithms. *Molecular Physics*, **1988** , 65, 1409-1419	1.7	668
4	Applications of Molecular Dynamics for Structural Analysis of Proteins and Peptides. *ACS Symposium Series*, **1987**, 123-145	0.4	15
3	Absorption mode two-dimensional NOE spectroscopy of exchangeable protons in oligonucleotides. *FEBS Letters*, **1987**, 216, 249-52	3.8	58
2	CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. *Journal of Computational Chemistry*, **1983**, 4, 187-217	3.5	13044
1	Dynamics of DNA oligomers. *Journal of Biomolecular Structure and Dynamics*, **1983**, 1, 231-52	3.6	170