John D Chodera

List of Publications by Year
in descending order

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		36303	25787
111	17,051	51	108
papers	citations	h-index	g-index

172	172	172	16860
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	3.2	1,561
2	Statistically optimal analysis of samples from multiple equilibrium states. Journal of Chemical Physics, 2008, 129, 124105.	3.0	1,328
3	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
4	Markov models of molecular kinetics: Generation and validation. Journal of Chemical Physics, 2011, 134, 174105.	3.0	968
5	Markov state models of biomolecular conformational dynamics. Current Opinion in Structural Biology, 2014, 25, 135-144.	5.7	628
6	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	5.3	583
7	Automatic discovery of metastable states for the construction of Markov models of macromolecular conformational dynamics. Journal of Chemical Physics, 2007, 126, 155101.	3.0	567
8	Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity. Cell, 2021, 184, 1171-1187.e20.	28.9	541
9	Alchemical free energy methods for drug discovery: progress and challenges. Current Opinion in Structural Biology, 2011, 21, 150-160.	5.7	468
10	Use of the Weighted Histogram Analysis Method for the Analysis of Simulated and Parallel Tempering Simulations. Journal of Chemical Theory and Computation, 2007, 3, 26-41.	5.3	416
11	Entropy-Enthalpy Compensation: Role and Ramifications in Biomolecular Ligand Recognition and Design. Annual Review of Biophysics, 2013, 42, 121-142.	10.0	416
12	SARS-CoV-2 RBD antibodies that maximize breadth and resistance to escape. Nature, 2021, 597, 97-102.	27.8	385
13	Hypoxia Induces Production of L-2-Hydroxyglutarate. Cell Metabolism, 2015, 22, 304-311.	16.2	374
14	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.5	318
15	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	2.6	279
16	Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. Journal of Molecular Biology, 2007, 371, 1118-1134.	4.2	269
17	The Ribosome Modulates Nascent Protein Folding. Science, 2011, 334, 1723-1727.	12.6	268
18	On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. Journal of Chemical Physics, 2006, 125, 084902.	3.0	253

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19	Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. Journal of Medicinal Chemistry, 2008, 51, 769-779.	6.4	248
20	Comparison of Charge Models for Fixed-Charge Force Fields:Â Small-Molecule Hydration Free Energies in Explicit Solvent. Journal of Physical Chemistry B, 2007, 111, 2242-2254.	2.6	245
21	Acquired resistance to IDH inhibition through trans or cis dimer-interface mutations. Nature, 2018, 559, 125-129.	27.8	223
22	On the Use of Experimental Observations to Bias Simulated Ensembles. Journal of Chemical Theory and Computation, 2012, 8, 3445-3451.	5.3	222
23	Longâ€Time Protein Folding Dynamics from Shortâ€Time Molecular Dynamics Simulations. Multiscale Modeling and Simulation, 2006, 5, 1214-1226.	1.6	204
24	L-2-Hydroxyglutarate production arises from noncanonical enzyme function at acidic pH. Nature Chemical Biology, 2017, 13, 494-500.	8.0	190
25	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. Nature Chemistry, 2021, 13, 651-659.	13.6	190
26	Accurate and Efficient Corrections for Missing Dispersion Interactions in Molecular Simulations. Journal of Physical Chemistry B, 2007, 111, 13052-13063.	2.6	181
27	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. Annual Reports in Computational Chemistry, 2007, 3, 41-59.	1.7	175
28	Confine-and-Release Method:â€‰ Obtaining Correct Binding Free Energies in the Presence of Protein Conformational Change. Journal of Chemical Theory and Computation, 2007, 3, 1231-1235.	5.3	168
29	Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database. Journal of Chemical & Engineering Data, 2017, 62, 1559-1569.	1.9	164
30	Protein folding by zipping and assembly. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 11987-11992.	7.1	141
31	Quantitative self-assembly prediction yields targeted nanomedicines. Nature Materials, 2018, 17, 361-368.	27.5	141
32	Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing. Journal of Chemical Physics, 2011, 135, 194110.	3.0	137
33	A Simple Method for Automated Equilibration Detection in Molecular Simulations. Journal of Chemical Theory and Computation, 2016, 12, 1799-1805.	5.3	133
34	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	125
35	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775.	5.3	120
36	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	5.3	110

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37	Treating Entropy and Conformational Changes in Implicit Solvent Simulations of Small Molecules. Journal of Physical Chemistry B, 2008, 112, 938-946.	2.6	106
38	Overview of the SAMPL6 hostâ€“guest binding affinity prediction challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 937-963.	2.9	106
39	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827.	7.1	105
40	Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. Journal of Computer-Aided Molecular Design, 2013, 27, 989-1007.	2.9	100
41	Small-molecule targeting of MUSASHI RNA-binding activity in acute myeloid leukemia. Nature Communications, 2019, 10, 2691.	12.8	93
42	Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1009-18.	7.1	91
43	Crowdsourcing drug discovery for pandemics. Nature Chemistry, 2020, 12, 581-581.	13.6	88
44	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
45	Mechanistically distinct cancer-associated mTOR activation clusters predict sensitivity to rapamycin. Journal of Clinical Investigation, 2016, 126, 3526-3540.	8.2	82
46	The molten globule state is unusually deformable under mechanical force. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3796-3801.	7.1	81
47	Development and Benchmarking of Open Force Field v1.0.0â€”the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
48	INK4 Tumor Suppressor Proteins Mediate Resistance to CDK4/6 Kinase Inhibitors. Cancer Discovery, 2022, 12, 356-371.	9.4	68
49	Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations. Communications Biology, 2018, 1, 70.	4.4	66
50	Systematic errors in isothermal titration calorimetry: Concentrations and baselines. Analytical Biochemistry, 2011, 414, 297-299.	2.4	64
51	Biomolecular Simulations under Realistic Macroscopic Salt Conditions. Journal of Physical Chemistry B, 2018, 122, 5466-5486.	2.6	63
52	A dynamic mechanism for allosteric activation of Aurora kinase A by activation loop phosphorylation. ELife, 2018, 7, .	6.0	62
53	What Makes a Kinase Promiscuous for Inhibitors?. Cell Chemical Biology, 2019, 26, 390-399.e5.	5.2	59
54	Time Step Rescaling Recovers Continuous-Time Dynamical Properties for Discrete-Time Langevin Integration of Nonequilibrium Systems. Journal of Physical Chemistry B, 2014, 118, 6466-6474.	2.6	56

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55	Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures. Journal of Chemical Physics, 2011, 134, 244107.	3.0	55
56	A water-mediated allosteric network governs activation of Aurora kinase A. Nature Chemical Biology, 2017, 13, 402-408.	8.0	53
57	Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes via Nonequilibrium Candidate Monte Carlo. Journal of Physical Chemistry B, 2018, 122, 5579-5598.	2.6	53
58	Bayesian comparison of Markov models of molecular dynamics with detailed balance constraint. Journal of Chemical Physics, 2009, 131, 045106.	3.0	52
59	Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages. Journal of Chemical Physics, 2009, 131, 134110.	3.0	48
60	Splitting Probabilities as a Test of Reaction Coordinate Choice in Single-Molecule Experiments. Physical Review Letters, 2011, 107, 098102.	7.8	46
61	Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. Journal of Chemical Physics, 2011, 134, 244108.	3.0	46
62	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. Journal of Chemical Theory and Computation, 2019, 15, 813-836.	5.3	45
63	Assessing the accuracy of octanolâ€“water partition coefficient predictions in the SAMPL6 Part II logÂP Challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 335-370.	2.9	44
64	Using Nonequilibrium Fluctuation Theorems to Understand and Correct Errors in Equilibrium and Nonequilibrium Simulations of Discrete Langevin Dynamics. Physical Review X, 2013, 3, .	8.9	43
65	Limitations of Constant-Force-Feedback Experiments. Biophysical Journal, 2012, 103, 1490-1499.	0.5	42
66	An Alternative Explanation for the Catalytic Proficiency of Orotidine 5â€˜-Phosphate Decarboxylase. Journal of the American Chemical Society, 2001, 123, 12837-12848.	13.7	41
67	Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 945-958.	2.9	41
68	Octanolâ€“water partition coefficient measurements for the SAMPL6 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 405-420.	2.9	40
69	pKaÂmeasurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments. Journal of Computer-Aided Molecular Design, 2018, 32, 1117-1138.	2.9	39
70	Probability distributions of molecular observables computed from Markov models. II. Uncertainties in observables and their time-evolution. Journal of Chemical Physics, 2010, 133, 105102.	3.0	38
71	The dynamic conformational landscape of the protein methyltransferase SETD8. ELife, 2019, 8, .	6.0	38
72	An Open Library of Human Kinase Domain Constructs for Automated Bacterial Expression. Biochemistry, 2018, 57, 4675-4689.	2.5	37

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73	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. Journal of Chemical Theory and Computation, 2019, 15, 837-856.	5.3	34
74	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. Journal of Chemical Theory and Computation, 2021, 17, 3119-3133.	5.3	32
75	Toward Automated Benchmarking of Atomistic Force Fields: Neat Liquid Densities and Static Dielectric Constants from the ThermoML Data Archive. Journal of Physical Chemistry B, 2015, 119, 12912-12920.	2.6	30
76	A Small-Molecule Pan-Id Antagonist Inhibits Pathologic Ocular Neovascularization. Cell Reports, 2019, 29, 62-75.e7.	6.4	30
77	Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423.	5.3	30
78	Discovery of SARS-CoV-2 main protease inhibitors using a synthesis-directed de novo design model. Chemical Communications, 2021, 57, 5909-5912.	4.1	30
79	Mutation in Abl kinase with altered drug-binding kinetics indicates a novel mechanism of imatinib resistance. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	30
80	Quantifying Configuration-Sampling Error in Langevin Simulations of Complex Molecular Systems. Entropy, 2018, 20, 318.	2.2	29
81	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	5.4	26
82	Is Structure-Based Drug Design Ready for Selectivity Optimization?. Journal of Chemical Information and Modeling, 2020, 60, 6211-6227.	5.4	25
83	A white-knuckle ride of open COVID drug discovery. Nature, 2021, 594, 330-332.	27.8	25
84	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224.	2.5	24
85	Ancestral reconstruction reveals mechanisms of ERK regulatory evolution. ELife, 2019, 8, .	6.0	24
86	Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. Journal of Computer-Aided Molecular Design, 2021, 35, 131-166.	2.9	23
87	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	30.2	22
88	Binding Thermodynamics of Hostâ€“Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. Journal of Chemical Theory and Computation, 2019, 15, 6225-6242.	5.3	21
89	Standard state free energies, not pKas, are ideal for describing small molecule protonation and tautomeric states. Journal of Computer-Aided Molecular Design, 2020, 34, 561-573.	2.9	20
90	Ensembler: Enabling High-Throughput Molecular Simulations at the Superfamily Scale. PLoS Computational Biology, 2016, 12, e1004728.	3.2	20

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91	The Mechanical Properties of PCNA: Implications for the Loading and Function of a DNA Sliding Clamp. Biophysical Journal, 2010, 98, 3062-3069.	0.5	19
92	GCN2 kinase activation by ATP-competitive kinase inhibitors. Nature Chemical Biology, 2022, 18, 207-215.	8.0	19
93	Open Force Field Evaluator: An Automated, Efficient, and Scalable Framework for the Estimation of Physical Properties from Molecular Simulation. Journal of Chemical Theory and Computation, 2022, 18, 3566-3576.	5.3	19
94	MOPED: Method for optimizing physical energy parameters using decoys. Journal of Computational Chemistry, 2003, 24, 89-97.	3.3	18
95	Spectral Rate Theory for Two-State Kinetics. Physical Review X, 2014, 4, .	8.9	16
96	Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: Theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments. Journal of Chemical Physics, 2011, 134, 024111.	3.0	15
97	Fitting quantum machine learning potentials to experimental free energy data: predicting tautomer ratios in solution. Chemical Science, 2021, 12, 11364-11381.	7.4	15
98	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
99	Modeling error in experimental assays using the bootstrap principle: understanding discrepancies between assays using different dispensing technologies. Journal of Computer-Aided Molecular Design, 2015, 29, 1073-1086.	2.9	12
100	The social network (of protein conformations). Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 12969-12970.	7.1	11
101	SAMPL7 protein-ligand challenge: A community-wide evaluation of computational methods against fragment screening and pose-prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 291-311.	2.9	10
102	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. Journal of Chemical Theory and Computation, 2022, 18, 3577-3592.	5.3	9
103	Automated high throughput pKa and distribution coefficient measurements of pharmaceutical compounds for the SAMPL8 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 1141-1155.	2.9	6
104	Bayesian-Inference-Driven Model Parametrization and Model Selection for 2CLJQ Fluid Models. Journal of Chemical Information and Modeling, 2022, , .	5.4	6
105	Estimation and Validation of Markov Models. Advances in Experimental Medicine and Biology, 2014, 797, 45-60.	1.6	3
106	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	6.4	3
107	Uncertainty Estimation. Advances in Experimental Medicine and Biology, 2014, 797, 61-74.	1.6	1
108	The Mechanical Properties of PCNA: Implications for the Loading and Function of Sliding Clamps. Biophysical Journal, 2010, 98, 630a.	0.5	0

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109	Systematic Improvement on the Classical Molecular Model of Water. Biophysical Journal, 2014, 106, 403a.	0.5	0
110	Introduction to the special issue: Data Part 2: Experimental Data. Journal of Computer-Aided Molecular Design, 2015, 29, 777-777.	2.9	0
111	Simulating mTOR Hyperactivating Mutations to Understand Functionally Significant Structural Rearrangements. Biophysical Journal, 2016, 110, 207a.	0.5	0