Brian K Radak

List of Publications by Year
in descending order

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25 papers	2,521 citations	567281 15 h-index	552781 26 g-index
28 all docs	28 docs citations	28 times ranked	3081 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.	5.4	177
3	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
4	Rigorous Free Energy Simulations in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4153-4169.	5.4	114
5	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 153-164.	5.3	76
6	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2â€²-O -transphosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13002-13007.	7.1	62
7	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	5.3	58
8	A Variational Linear-Scaling Framework to Build Practical, Efficient Next-Generation Orbital-Based Quantum Force Fields. Journal of Chemical Theory and Computation, 2013, 9, 1417-1427.	5.3	55
9	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	5.4	37
10	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	5.3	35
11	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	3.0	26
12	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. ACS Catalysis, 2016, 6, 1853-1869.	11.2	24
13	Accounting for the Central Role of Interfacial Water in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2020, 16, 7883-7894.	5.3	24
14	Molecular Simulations of RNA 2â€²-O-Transesterification Reaction Models in Solution. Journal of Physical Chemistry B, 2013, 117, 94-103.	2.6	21
15	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. Rna, 2015, 21, 1566-1577.	3.5	18
16	Multiscale Methods for Computational RNA Enzymology. Methods in Enzymology, 2015, 553, 335-374.	1.0	16
17	Fast Equilibration of Water between Buried Sites and the Bulk by Molecular Dynamics with Parallel Monte Carlo Water Moves on Graphical Processing Units. Journal of Chemical Theory and Computation, 2021, 17, 7366-7372.	5.3	16
18	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 134109.	3.0	15

#	Article	IF	Citations
19	Modeling Reactive Scattering of F(²P) at a Liquid Squalane Interface: A Hybrid QM/MM Molecular Dynamics Study. Journal of Physical Chemistry A, 2009, 113, 7218-7226.	2.5	13
20	A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3975-3984.	5.3	12
21	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	5.3	10
22	A generalized linear response framework for expanded ensemble and replica exchange simulations. Journal of Chemical Physics, 2018, 149, 072315.	3.0	7
23	Precise Binding Free Energy Calculations for Multiple Molecules Using an Optimal Measurement Network of Pairwise Differences. Journal of Chemical Theory and Computation, 2022, 18, 650-663.	5.3	7
24	Modeling Ion Channels Using Poissonâ€“Nernstâ€“Planck Theory as an Integrated Approach To Introducing Nanotechnology Concepts: The PNP Cyclic Peptide Ion Channel Model. Journal of Chemical Education, 2008, 85, 744.	2.3	2
25	Finite-sample bias in free energy bridge estimators. Journal of Chemical Physics, 2019, 151, 034105.	3.0	1