Andrew D White

List of Publications by Year
in descending order

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43 papers	2,380 citations	304743 22 h-index	265206 42 g-index
60 all docs	60 docs citations	60 times ranked	3138 citing authors

#	Article	IF	Citations
1	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
2	Sequence, Structure, and Function of Peptide Self-Assembled Monolayers. Journal of the American Chemical Society, 2012, 134, 6000-6005.	13.7	254
3	Functionalizable and ultra stable nanoparticles coated with zwitterionic poly(carboxybetaine) in undiluted blood serum. Biomaterials, 2009, 30, 5617-5621.	11.4	216
4	Difference in Hydration between Carboxybetaine and Sulfobetaine. Journal of Physical Chemistry B, 2010, 114, 16625-16631.	2.6	198
5	Decoding nonspecific interactions from nature. Chemical Science, 2012, 3, 3488.	7.4	96
6	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. Journal of Chemical Theory and Computation, 2014, 10, 3023-3030.	5.3	90
7	Biologically Inspired Stealth Peptide-Capped Gold Nanoparticles. Langmuir, 2014, 30, 1864-1870.	3.5	73
8	Local and Bulk Hydration of Zwitterionic Glycine and its Analogues through Molecular Simulations. Journal of Physical Chemistry B, 2011, 115, 660-667.	2.6	63
9	Designing Free Energy Surfaces That Match Experimental Data with Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 2451-2460.	5.3	49
10	Model agnostic generation of counterfactual explanations for molecules. Chemical Science, 2022, 13, 3697-3705.	7.4	47
11	Can parked cars and carbon taxes create a profit? The economics of vehicle-to-grid energy storage for peak reduction. Energy Policy, 2017, 106, 183-190.	8.8	43
12	Directly Functionalizable Surface Platform for Protein Arrays in Undiluted Human Blood Plasma. Analytical Chemistry, 2013, 85, 1447-1453.	6.5	41
13	Free Energy of Solvated Salt Bridges: A Simulation and Experimental Study. Journal of Physical Chemistry B, 2013, 117, 7254-7259.	2.6	40
14	Different effects of zwitterion and ethylene glycol on proteins. Journal of Chemical Physics, 2012, 136, 225101.	3.0	39
15	Multiscale Kinetic Modeling Reveals an Ensemble of Cl^{â€“}/H⁺ Exchange Pathways in ClC-ec1 Antiporter. Journal of the American Chemical Society, 2018, 140, 1793-1804.	13.7	39
16	Screening nonspecific interactions of peptides without background interference. Biomaterials, 2013, 34, 1871-1877.	11.4	38
17	Encoding and selecting coarse-grain mapping operators with hierarchical graphs. Journal of Chemical Physics, 2018, 149, 134106.	3.0	35
18	Difference of Carboxybetaine and Oligo(ethylene glycol) Moieties in Altering Hydrophobic Interactions: A Molecular Simulation Study. Journal of Physical Chemistry B, 2014, 118, 189-194.	2.6	32

#	Article	IF	Citations
19	Graph neural network based coarse-grained mapping prediction. Chemical Science, 2020, 11, 9524-9531.	7.4	32
20	Social and Tactile Mixed Reality Increases Student Engagement in Undergraduate Lab Activities. Journal of Chemical Education, 2018, 95, 1755-1762.	2.3	30
21	A Direct Method for Incorporating Experimental Data into Multiscale Coarse-Grained Models. Journal of Chemical Theory and Computation, 2016, 12, 2144-2153.	5.3	29
22	Predicting chemical shifts with graph neural networks. Chemical Science, 2021, 12, 10802-10809.	7.4	25
23	Recent advances in maximum entropy biasing techniques for molecular dynamics. Molecular Simulation, 2019, 45, 1285-1294.	2.0	23
24	Communication: Improved ab initio molecular dynamics by minimally biasing with experimental data. Journal of Chemical Physics, 2017, 146, 041102.	3.0	20
25	Peptide framework for screening the effects of amino acids on assembly. Science Advances, 2022, 8, eabj0305.	10.3	20
26	Is preservation of symmetry necessary for coarse-graining?. Physical Chemistry Chemical Physics, 2020, 22, 14998-15005.	2.8	19
27	Natural language processing models that automate programming will transform chemistry research and teaching. , 2022, 1, 79-83.		19
28	Classifying antimicrobial and multifunctional peptides with Bayesian network models. Peptide Science, 2018, 110, e24079.	1.8	15
29	Role of Nonspecific Interactions in Molecular Chaperones through Model-Based Bioinformatics. Biophysical Journal, 2012, 103, 2484-2491.	0.5	11
30	Investigating Active Learning and Meta-Learning for Iterative Peptide Design. Journal of Chemical Information and Modeling, 2021, 61, 95-105.	5.4	11
31	Deep learning for molecules and materials. Living Journal of Computational Molecular Science, 2022, 3, .	6.4	11
32	Combining enhanced sampling with experiment-directed simulation of the GYG peptide. Journal of Theoretical and Computational Chemistry, 2018, 17, 1840007.	1.8	10
33	Real-Time Interactive Simulation and Visualization of Organic Molecules. Journal of Chemical Education, 2020, 97, 4189-4195.	2.3	10
34	Federated learning of molecular properties with graph neural networks in a heterogeneous setting. Patterns, 2022, 3, 100521.	5.9	9
35	Chemical insights into dodecylamine spore lethal germination. Chemical Science, 2014, 5, 3320-3324.	7.4	5
36	HOOMD-TF: GPU-Accelerated, Online Machine Learning in the HOOMD-blue Molecular Dynamics Engine. Journal of Open Source Software, 2020, 5, 2367.	4.6	5

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37	Standardizing and Simplifying Analysis of Peptide Library Data. Journal of Chemical Information and Modeling, 2013, 53, 493-499.	5.4	4
38	City-Wide Modeling of Vehicle-to-Grid Economics to Understand Effects of Battery Performance. ACS Sustainable Chemistry and Engineering, 2021, 9, 14975-14985.	6.7	4
39	Iterative symbolic regression for learning transport equations. AICHE Journal, 2022, 68, .	3.6	3
40	Experimentally Consistent Simulation of AÎ²_{21â€“30} Peptides with a Minimal NMR Bias. Journal of Physical Chemistry B, 2020, 124, 8266-8277.	2.6	2
41	Reconstruction of the interatomic forces from dynamic scanning transmission electron microscopy data. Journal of Applied Physics, 2020, 127, 224301.	2.5	2
42	Simulation-based inference with approximately correct parameters via maximum entropy. Machine Learning: Science and Technology, 2022, 3, 025006.	5.0	2
43	Symmetric Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4077-4081.	5.3	1