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	Peptide framework for screening the effects of amino acids on assembly. Science Advances, 2022, 8, eabj0305.	10.3	20
2	Natural language processing models that automate programming will transform chemistry research and teaching. , 2022, 1, 79-83.		19
3	Model agnostic generation of counterfactual explanations for molecules. Chemical Science, 2022, 13, 3697-3705.	7.4	47
4	Simulation-based inference with approximately correct parameters via maximum entropy. Machine Learning: Science and Technology, 2022, 3, 025006.	5.0	2
5	Iterative symbolic regression for learning transport equations. AICHE Journal, 2022, 68, .	3.6	3
6	Federated learning of molecular properties with graph neural networks in a heterogeneous setting. Patterns, 2022, 3, 100521.	5.9	9
7	Deep learning for molecules and materials. Living Journal of Computational Molecular Science, 2022, 3, .	6.4	11
8	Symmetric Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4077-4081.	5.3	1
9	Investigating Active Learning and Meta-Learning for Iterative Peptide Design. Journal of Chemical Information and Modeling, 2021, 61, 95-105.	5.4	11
10	Predicting chemical shifts with graph neural networks. Chemical Science, 2021, 12, 10802-10809.	7.4	25
11	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
12	Graph neural network based coarse-grained mapping prediction. Chemical Science, 2020, 11, 9524-9531.	7.4	32
13	Real-Time Interactive Simulation and Visualization of Organic Molecules. Journal of Chemical Education, 2020, 97, 4189-4195.	2.3	10
14	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
15	Reconstruction of the interatomic forces from dynamic scanning transmission electron microscopy data. Journal of Applied Physics, 2020, 127, 224301.	2.5	2
16	Is preservation of symmetry necessary for coarse-graining?. Physical Chemistry Chemical Physics, 2020, 22, 14998-15005.	2.8	19
17	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
18	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655

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19	Recent advances in maximum entropy biasing techniques for molecular dynamics. Molecular Simulation, 2019, 45, 1285-1294.	2.0	23
20	Combining enhanced sampling with experiment-directed simulation of the GYG peptide. Journal of Theoretical and Computational Chemistry, 2018, 17, 1840007.	1.8	10
21	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
22	Encoding and selecting coarse-grain mapping operators with hierarchical graphs. Journal of Chemical Physics, 2018, 149, 134106.	3.0	35
23	Classifying antimicrobial and multifunctional peptides with Bayesian network models. Peptide Science, 2018, 110, e24079.	1.8	15
24	Social and Tactile Mixed Reality Increases Student Engagement in Undergraduate Lab Activities. Journal of Chemical Education, 2018, 95, 1755-1762.	2.3	30
25	Communication: Improved ab initio molecular dynamics by minimally biasing with experimental data. Journal of Chemical Physics, 2017, 146, 041102.	3.0	20
26	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
27	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
28	Designing Free Energy Surfaces That Match Experimental Data with Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 2451-2460.	5.3	49
29	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
30	Chemical insights into dodecylamine spore lethal germination. Chemical Science, 2014, 5, 3320-3324.	7.4	5
31	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. Journal of Chemical Theory and Computation, 2014, 10, 3023-3030.	5.3	90
32	Biologically Inspired Stealth Peptide-Capped Gold Nanoparticles. Langmuir, 2014, 30, 1864-1870.	3.5	73
33	Directly Functionalizable Surface Platform for Protein Arrays in Undiluted Human Blood Plasma. Analytical Chemistry, 2013, 85, 1447-1453.	6.5	41
34	Free Energy of Solvated Salt Bridges: A Simulation and Experimental Study. Journal of Physical Chemistry B, 2013, 117, 7254-7259.	2.6	40
35	Screening nonspecific interactions of peptides without background interference. Biomaterials, 2013, 34, 1871-1877.	11.4	38
36	Standardizing and Simplifying Analysis of Peptide Library Data. Journal of Chemical Information and Modeling, 2013, 53, 493-499.	5.4	4

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37	Sequence, Structure, and Function of Peptide Self-Assembled Monolayers. Journal of the American Chemical Society, 2012, 134, 6000-6005.	13.7	254
38	Decoding nonspecific interactions from nature. Chemical Science, 2012, 3, 3488.	7.4	96
39	Role of Nonspecific Interactions in Molecular Chaperones through Model-Based Bioinformatics. Biophysical Journal, 2012, 103, 2484-2491.	0.5	11
40	Different effects of zwitterion and ethylene glycol on proteins. Journal of Chemical Physics, 2012, 136, 225101.	3.0	39
41	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
42	Difference in Hydration between Carboxybetaine and Sulfobetaine. Journal of Physical Chemistry B, 2010, 114, 16625-16631.	2.6	198
43	Functionalizable and ultra stable nanoparticles coated with zwitterionic poly(carboxybetaine) in undiluted blood serum. Biomaterials, 2009, 30, 5617-5621.	11.4	216