Joseph A Morrone

List of Publications by Year
in descending order

24 papers	1,300 citations	361413 20 h-index	610901 24 g-index
24 all docs	24 docs citations	24 times ranked	1670 citing authors

#	Article	IF	Citations
1	Ab initio molecular dynamics study of proton mobility in liquid methanol. Journal of Chemical Physics, 2002, 117, 4403-4413.	3.0	135
2	Advances in free-energy-based simulations of protein folding and ligand binding. Current Opinion in Structural Biology, 2016, 36, 25-31.	5.7	121
3	Ab Initio Molecular Dynamics Simulation of the Structure and Proton Transport Dynamics of Methanolâ^'Water Solutionsâ€. Journal of Physical Chemistry B, 2006, 110, 3712-3720.	2.6	101
4	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	16.7	84
5	Role of water and steric constraints in the kinetics of cavityâ€“ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019.	7.1	74
6	Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 870-876.	5.3	68
7	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	3.0	66
8	Tunneling and delocalization effects in hydrogen bonded systems: A study in position and momentum space. Journal of Chemical Physics, 2009, 130, 204511.	3.0	65
9	Combining Docking Pose Rank and Structure with Deep Learning Improves Proteinâ€“Ligand Binding Mode Prediction over a Baseline Docking Approach. Journal of Chemical Information and Modeling, 2020, 60, 4170-4179.	5.4	64
10	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804.	5.3	57
11	Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274.	10.3	57
12	Interplay between Hydrodynamics and the Free Energy Surface in the Assembly of Nanoscale Hydrophobes. Journal of Physical Chemistry B, 2012, 116, 378-389.	2.6	52
13	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	7.8	49
14	Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled Î±-Helical Peptides to MDM2 and MDMX. Journal of Chemical Theory and Computation, 2017, 13, 863-869.	5.3	49
15	Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384.	1.2	45
16	How hydrophobic drying forces impact the kinetics of molecular recognition. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13277-13282.	7.1	45
17	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. Journal of Physical Chemistry C, 2012, 116, 9582-9593.	3.1	38
18	Are Hydrodynamic Interactions Important in the Kinetics of Hydrophobic Collapse?. Journal of Physical Chemistry B, 2012, 116, 11537-11544.	2.6	29

#	Article	IF	Citations
19	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. Journal of Physical Chemistry B, 2018, 122, 1176-1184.	2.6	29
20	Long range interactions on wires: A reciprocal space based formalism. Journal of Chemical Physics, 2004, 121, 11949-11956.	3.0	24
21	A simple quantum mechanical/molecular mechanical (QM/MM) model for methanol. Chemical Physics Letters, 2003, 370, 406-411.	2.6	17
22	Accelerating physical simulations of proteins by leveraging external knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1309.	14.6	16
23	Simplified, interpretable graph convolutional neural networks for small molecule activity prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 391-404.	2.9	10
24	Analysis of Training and Seed Bias in Small Molecules Generated with a Conditional Graph-Based Variational Autoencoderâ”€Insights for Practical AI-Driven Molecule Generation. Journal of Chemical Information and Modeling, 2022, 62, 801-816.	5.4	5