Peter Minary

List of Publications by Year
in descending order

27 papers	1,246 citations	430874 18 h-index	526287 27 g-index
28 all docs	28 docs citations	28 times ranked	1589 citing authors

#	Article	IF	Citations
1	Ab initio molecular dynamics: Concepts, recent developments, and future trends. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6654-6659.	7.1	232
2	On the use of the adiabatic molecular dynamics technique in the calculation of free energy profiles. Journal of Chemical Physics, 2002, 116, 4389-4402.	3.0	203
3	Tuning Cytokine Receptor Signaling by Re-orienting Dimer Geometry with Surrogate Ligands. Cell, 2015, 160, 1196-1208.	28.9	138
4	Algorithms and novel applications based on the isokinetic ensemble. I. Biophysical and path integral molecular dynamics. Journal of Chemical Physics, 2003, 118, 2510.	3.0	89
5	Modeling nucleic acids. Current Opinion in Structural Biology, 2012, 22, 273-278.	5.7	85
6	A new reciprocal space based treatment of long range interactions on surfaces. Journal of Chemical Physics, 2002, 116, 5351-5362.	3.0	73
7	Modeling and design by hierarchical natural moves. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2890-2895.	7.1	42
8	Non-linear response and hydrogen bond dynamics for electron solvation in methanol. Chemical Physics Letters, 2000, 316, 465-470.	2.6	36
9	Probing Protein Fold Space with a Simplified Model. Journal of Molecular Biology, 2008, 375, 920-933.	4.2	36
10	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. Journal of Chemical Physics, 1999, 110, 10953-10962.	3.0	35
11	Multiscale natural moves refine macromolecules using single-particle electron microscopy projection images. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9845-9850.	7.1	32
12	Reaction Mechanism of cis-1,3-Butadiene Addition to the Si(100)-2 Ã— 1 Surface. Journal of the American Chemical Society, 2005, 127, 1110-1111.	13.7	28
13	Reaction Pathway of the [4 + 2] Dielsâ"Alder Adduct Formation on Si(100)-2Ã—1. Journal of the American Chemical Society, 2004, 126, 13920-13921.	13.7	27
14	Training-free atomistic prediction of nucleosome occupancy. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6293-6298.	7.1	25
15	Long range interactions on wires: A reciprocal space based formalism. Journal of Chemical Physics, 2004, 121, 11949-11956.	3.0	24
16	Dynamical Spatial Warping: A Novel Method for the Conformational Sampling of Biophysical Structure. SIAM Journal of Scientific Computing, 2008, 30, 2055-2083.	2.8	23
17	Conformational Optimization with Natural Degrees of Freedom: A Novel Stochastic Chain Closure Algorithm. Journal of Computational Biology, 2010, 17, 993-1010.	1.6	23
18	Exploring peptide/MHC detachment processes using hierarchical natural move Monte Carlo. Bioinformatics, 2016, 32, 181-186.	4.1	21

#	Article	IF	Citations
19	Algorithms and novel applications based on the isokinetic ensemble. II. Ab initio molecular dynamics. Journal of Chemical Physics, 2003, 118, 2527.	3.0	19
20	crisprSQL: a novel database platform for CRISPR/Cas off-target cleavage assays. Nucleic Acids Research, 2021, 49, D855-D861.	14.5	16
21	Training-free measures based on algorithmic probability identify high nucleosome occupancy in DNA sequences. Nucleic Acids Research, 2019, 47, e129-e129.	14.5	9
22	Tertiary Element Interaction in HIV-1 TAR. Journal of Chemical Information and Modeling, 2016, 56, 1746-1754.	5.4	8
23	Modeling Functional Motions of Biological Systems by Customized Natural Moves. Biophysical Journal, 2016, 111, 710-721.	0.5	7
24	Hierarchical natural move Monte Carlo refines flexible RNA structures into cryo-EM densities. Rna, 2020, 26, 1755-1766.	3.5	6
25	In silico structural modeling of multiple epigenetic marks on DNA. Bioinformatics, 2018, 34, 41-48.	4.1	4
26	Discussion of â€œEqui-energy samplerâ€•by Kou, Zhou and Wong. Annals of Statistics, 2006, 34, .	2.6	3
27	HLA-DM Stabilizes the Empty MHCII Binding Groove: A Model Using Customized Natural Move Monte Carlo. Journal of Chemical Information and Modeling, 2019, 59, 2894-2899.	5.4	1