Jed W Pitera

List of Publications by Year
in descending order

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24 papers	4,902 citations	331259 21 h-index	642321 23 g-index
24 all docs	24 docs citations	24 times ranked	5104 citing authors

#	Article	IF	Citations
1	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. Journal of Chemical Physics, 2004, 120, 9665-9678.	1.2	1,747
2	Extremely precise free energy calculations of amino acid side chain analogs: Comparison of common molecular mechanics force fields for proteins. Journal of Chemical Physics, 2003, 119, 5740-5761.	1.2	611
3	Use of the Weighted Histogram Analysis Method for the Analysis of Simulated and Parallel Tempering Simulations. Journal of Chemical Theory and Computation, 2007, 3, 26-41.	2.3	416
4	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 1. Theory. Journal of Physical Chemistry B, 2004, 108, 6571-6581.	1.2	391
5	Understanding folding and design: Replica-exchange simulations of "Trp-cage" miniproteins. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7587-7592.	3.3	331
6	Longâ€Time Protein Folding Dynamics from Shortâ€Time Molecular Dynamics Simulations. Multiscale Modeling and Simulation, 2006, 5, 1214-1226.	0.6	204
7	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a Î²-Hairpin Peptide. Journal of Physical Chemistry B, 2004, 108, 6582-6594.	1.2	171
8	Heterogeneous Folding of the trpzip Hairpin: Full Atom Simulation and Experiment. Journal of Molecular Biology, 2004, 336, 241-251.	2.0	165
9	Two-Dimensional Pattern Formation Using Graphoepitaxy of PS-‹i›b‹/i›-PMMA Block Copolymers for Advanced FinFET Device and Circuit Fabrication. ACS Nano, 2014, 8, 5227-5232.	7.3	143
10	A Comparison of Non-Bonded Scaling Approaches for Free Energy Calculations. Molecular Simulation, 2002, 28, 45-65.	0.9	109
11	Characterization of the TIP4P-Ew water model: Vapor pressure and boiling point. Journal of Chemical Physics, 2005, 123, 194504.	1.2	103
12	Simulations of the Estrogen Receptor Ligand-Binding Domain:â€‰ Affinity of Natural Ligands and Xenoestrogens. Journal of Medicinal Chemistry, 2000, 43, 4594-4605.	2.9	100
13	Soft Patchy Nanoparticles from Solution-Phase Self-Assembly of Binary Diblock Copolymers. Nano Letters, 2008, 8, 611-618.	4.5	88
14	One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes. Journal of Physical Chemistry B, 2001, 105, 11264-11274.	1.2	59
15	Enabling complex nanoscale pattern customization using directed self-assembly. Nature Communications, 2014, 5, 5805.	5.8	51
16	Absence of reptation in the high-temperature folding of the trpzip2 Î²-hairpin peptide. Journal of Chemical Physics, 2006, 124, 141102.	1.2	44
17	Pattern Placement Accuracy in Block Copolymer Directed Self-Assembly Based on Chemical Epitaxy. ACS Nano, 2013, 7, 276-285.	7.3	34
18	Observation of Noncooperative Folding Thermodynamics in Simulations of 1BBL. Biophysical Journal, 2008, 94, 4837-4846.	0.2	32

#	Article	IF	Citations
19	Comparison of computational approaches for predicting the effects of missense mutations on p53 function. Journal of Molecular Graphics and Modelling, 2009, 27, 978-982.	1.3	26
20	Orientation Control of Block Copolymers Using Surface Active, Phase-Preferential Additives. ACS Applied Materials & Interfaces, 2016, 8, 29808-29817.	4.0	23
21	Correlation of early orientational ordering of engineered Î»6â€“85 structure with kinetics and thermodynamics. Chemical Physics, 2006, 323, 45-53.	0.9	22
22	Kinetic Computational Alanine Scanning: Application to p53 Oligomerization. Journal of Molecular Biology, 2006, 357, 1039-1049.	2.0	17
23	Interfacial Fluctuations of Block Copolymers:â€‰ A Coarse-Grain Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 13734-13742.	1.2	14
24	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. , 0, .		1