

John M Stubbs

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

24
papers

1,013
citations

13
h-index

24
g-index

24
ext. papers

1,083
ext. citations

4.4
avg, IF

4.29
L-index

#	Paper	IF	Citations
24	Monte Carlo molecular simulation of solution and surface-bound DNA hybridization of short oligomers at varying surface densities.. <i>Biophysical Chemistry</i> , 2022 , 284, 106784	3.5	0
23	The role of differing probe and target strand lengths in DNA microarrays investigated via Monte Carlo molecular simulation. <i>Chemical Physics Letters</i> , 2018 , 693, 127-131	2.5	1
22	Prediction of binary phase behavior for supercritical carbon dioxide + 1-pentanol, 2-pentanone, 1-octene or ethylbenzene via molecular simulation. <i>Journal of Molecular Liquids</i> , 2017 , 245, 91-96	6	1
21	Molecular simulations of supercritical fluid systems. <i>Journal of Supercritical Fluids</i> , 2016 , 108, 104-122	4.2	42
20	The effect of unequal strand length on short DNA duplex hybridization in a model microarray system: A Monte Carlo simulation study. <i>Chemical Physics Letters</i> , 2015 , 634, 230-235	2.5	2
19	Solute extraction via supercritical ethane from poly(ethylene glycol): A Monte Carlo simulation study. <i>Fluid Phase Equilibria</i> , 2013 , 360, 351-356	2.5	2
18	Conformational analysis of 6 μ and 6 κ altrexol and derivatives and relationship to opioid receptor affinity. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 391-5	6.1	2
17	The influence of carbon dioxide cosolvent on solubility in poly(ethylene glycol). <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	4
16	Effect of surface binding on heterogeneous DNA melting equilibria: a Monte Carlo simulation study. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1720-6	3.4	12
15	Monte Carlo simulation of solute extraction via supercritical carbon dioxide from poly(ethylene glycol). <i>Fluid Phase Equilibria</i> , 2011 , 305, 76-82	2.5	10
14	Application of a coarse-grained model for DNA to homo- and heterogeneous melting equilibria. <i>Chemical Physics Letters</i> , 2010 , 485, 354-359	2.5	8
13	Elucidating the vibrational spectra of hydrogen-bonded aggregates in solution: electronic structure calculations with implicit solvent and first-principles molecular dynamics simulations with explicit solvent for 1-hexanol in n-hexane. <i>Journal of the American Chemical Society</i> , 2005 , 127, 4722-9	16.4	51
12	Transferable potentials for phase equilibria. 7. Primary, secondary, and tertiary amines, nitroalkanes and nitrobenzene, nitriles, amides, pyridine, and pyrimidine. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 18974-82	3.4	188
11	Effects of conformational distributions on sigma profiles in COSMO theories. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 11285-94	2.8	22
10	Partial molar volume and solvation structure of naphthalene in supercritical carbon dioxide: a Monte Carlo simulation study. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19885-92	3.4	27
9	Simulating the vapour-liquid equilibria of large cyclic alkanes. <i>Molecular Physics</i> , 2005 , 103, 99-104	1.7	31
8	Aspects of glycosidic bond formation in aqueous solution: chemical bonding and the role of water. <i>Chemistry - A European Journal</i> , 2005 , 11, 2651-9	4.8	25

7	Binary phase behavior and aggregation of dilute methanol in supercritical carbon dioxide: a Monte Carlo simulation study. <i>Journal of Chemical Physics</i> , 2004 , 121, 1525-34	3.9	60
6	Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 17596-17605	3.4	355
5	Glycosidic bond formation in aqueous solution: on the oxocarbenium intermediate. <i>Journal of the American Chemical Society</i> , 2003 , 125, 10960-2	16.4	28
4	Fast anomalous diffusion of small hydrophobic species in water. <i>Physical Review Letters</i> , 2002 , 89, 21590	7.4	46
3	Aggregation in Dilute Solutions of 1-Hexanol in n-Hexane: A Monte Carlo Simulation Study. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 3968-3978	3.4	53
2	Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 301-309	2.5	40
1	A Cooperative Molecular Modeling Exercise: The Hypersurface as Classroom. <i>Journal of Chemical Education</i> , 2001 , 78, 1202	2.4	3