John M Stubbs

List of Publications by Citations

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	Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. *Journal of Physical Chemistry B*, **2004**, 108, 17596-17605	3.4	355
23	Transferable potentials for phase equilibria. 7. Primary, secondary, and tertiary amines, nitroalkanes and nitrobenzene, nitriles, amides, pyridine, and pyrimidine. *Journal of Physical Chemistry B*, **2005**, 109, 18974-82	3.4	188
22	Binary phase behavior and aggregation of dilute methanol in supercritical carbon dioxide: a Monte Carlo simulation study. *Journal of Chemical Physics*, **2004**, 121, 1525-34	3.9	60
21	Aggregation in Dilute Solutions of 1-Hexanol in n-Hexane: A Monte Carlo Simulation Study. *Journal of Physical Chemistry B*, **2002**, 106, 3968-3978	3.4	53
20	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. *Journal of the American Chemical Society*, **2005**, 127, 4722-9	16.4	51
19	Fast anomalous diffusion of small hydrophobic species in water. *Physical Review Letters*, **2002**, 89, 215901	7.4	46
18	Molecular simulations of supercritical fluid systems. *Journal of Supercritical Fluids*, **2016**, 108, 104-122	4.2	42
17	Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. *Fluid Phase Equilibria*, **2001**, 183-184, 301-309	2.5	40
16	Simulating the vapour□quid equilibria of large cyclic alkanes. *Molecular Physics*, **2005**, 103, 99-104	1.7	31
15	Glycosidic bond formation in aqueous solution: on the oxocarbenium intermediate. *Journal of the American Chemical Society*, **2003**, 125, 10960-2	16.4	28
14	Partial molar volume and solvation structure of naphthalene in supercritical carbon dioxide: a Monte Carlo simulation study. *Journal of Physical Chemistry B*, **2005**, 109, 19885-92	3.4	27
13	Aspects of glycosidic bond formation in aqueous solution: chemical bonding and the role of water. *Chemistry - A European Journal*, **2005**, 11, 2651-9	4.8	25
12	Effects of conformational distributions on sigma profiles in COSMO theories. *Journal of Physical Chemistry A*, **2005**, 109, 11285-94	2.8	22
11	Effect of surface binding on heterogeneous DNA melting equilibria: a Monte Carlo simulation study. *Journal of Physical Chemistry B*, **2011**, 115, 1720-6	3.4	12
10	Monte Carlo simulation of solute extraction via supercritical carbon dioxide from poly(ethylene glycol). *Fluid Phase Equilibria*, **2011**, 305, 76-82	2.5	10
9	Application of a coarse-grained model for DNA to homo- and heterogeneous melting equilibria. *Chemical Physics Letters*, **2010**, 485, 354-359	2.5	8
8	The influence of carbon dioxide cosolvent on solubility in poly(ethylene glycol). *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	4

7	A Cooperative Molecular Modeling Exercise The Hypersurface as Classroom. *Journal of Chemical Education*, **2001**, 78, 1202	2.4	3
6	Solute extraction via supercritical ethane from poly(ethylene glycol): A Monte Carlo simulation study. *Fluid Phase Equilibria*, **2013**, 360, 351-356	2.5	2
5	The effect of unequal strand length on short DNA duplex hybridization in a model microarray system: A Monte Carlo simulation study. *Chemical Physics Letters*, **2015**, 634, 230-235	2.5	2
4	Conformational analysis of 6 and 6 haltrexol and derivatives and relationship to opioid receptor affinity. *Journal of Chemical Information and Modeling*, **2012**, 52, 391-5	6.1	2
3	The role of differing probe and target strand lengths in DNA microarrays investigated via Monte Carlo molecular simulation. *Chemical Physics Letters*, **2018**, 693, 127-131	2.5	1
2	Prediction of binary phase behavior for supercritical carbon dioxide + 1-pentanol, 2-pentanone, 1-octene or ethylbenzene via molecular simulation. *Journal of Molecular Liquids*, **2017**, 245, 91-96	6	1
1	Monte Carlo molecular simulation of solution and surface-bound DNA hybridization of short oligomers at varying surface densities.. *Biophysical Chemistry*, **2022**, 284, 106784	3.5	0