Jeffrey J Potoff

List of Publications by Year
in descending order

54	4,599	218662	168376
papers	citations	26 h-index	53 g-index

55	55	55	3417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Vaporâ€“liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. AICHE Journal, 2001, 47, 1676-1682.	3.6	1,560
2	Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols. Journal of Physical Chemistry B, 2001, 105, 3093-3104.	2.6	730
3	Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. Journal of Physical Chemistry B, 2004, 108, 17596-17605.	2.6	410
4	Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. Journal of Chemical Physics, 1998, 109, 10914-10920.	3.0	347
5	Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. Journal of Chemical Physics, 2000, 112, 6411-6415.	3.0	144
6	Transferable Potentials for Phase Equilibria. 8. United-Atom Description for Thiols, Sulfides, Disulfides, and Thiophene. Journal of Physical Chemistry B, 2005, 109, 24100-24107.	2.6	112
7	Mie Potentials for Phase Equilibria Calculations: Application to Alkanes and Perfluoroalkanes. Journal of Physical Chemistry B, 2009, 113, 14725-14731.	2.6	110
8	An Improved Force Field for the Prediction of the Vaporâ^'Liquid Equilibria for Carboxylic Acids. Journal of Physical Chemistry B, 2004, 108, 14130-14136.	2.6	82
9	Effect of partial charge parametrization on the fluid phase behavior of hydrogen sulfide. Journal of Chemical Physics, 2005, 123, 124505.	3.0	69
10	Adiabatic Nuclear and Electronic Sampling Monte Carlo Simulations in the Gibbs Ensemble:Â Application to Polarizable Force Fields for Water. Journal of Physical Chemistry B, 2000, 104, 2378-2390.	2.6	68
11	Molecular Modeling of Phase Behavior and Microstructure of Acetoneâ^'Chloroformâ^'Methanol Binary Mixtures. Journal of Physical Chemistry B, 2005, 109, 19463-19473.	2.6	67
12	Development of an Optimized Intermolecular Potential for Sulfur Dioxide. Journal of Physical Chemistry B, 2011, 115, 4949-4954.	2.6	65
13	Application of TraPPE-UA force field for determination of vaporâ€“liquid equilibria of carboxylate esters. Fluid Phase Equilibria, 2006, 240, 46-55.	2.5	51
14	Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. Fluid Phase Equilibria, 2001, 183-184, 301-309.	2.5	44
15	Direct calculation of 1-octanolâ€“water partition coefficients from adaptive biasing force molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 014502.	3.0	44
16	Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes. Journal of Chemical Physics, 2015, 143, 114504.	3.0	43
17	All-Atom Force Field for the Prediction of Vaporâ^'Liquid Equilibria and Interfacial Properties of HFA134a. Journal of Physical Chemistry B, 2009, 113, 178-187.	2.6	42
18	Ca²⁺â€“dimethylphosphate complex formation: Providing insight into Ca²⁺â€mediated local dehydration and membrane fusion in cells. Cell Biology International, 2008, 32, 361-366.	3.0	40

#	Article	IF	Citations
19	Extension of the Transferable Potentials for Phase Equilibria Force Field to Dimethylmethyl Phosphonate, Sarin, and Soman. Journal of Physical Chemistry B, 2009, 113, 10292-10297.	2.6	37
20	Effect of quadrupole moment on the phase behavior of binary mixtures containing ethene. Fluid Phase Equilibria, 2005, 234, 144-150.	2.5	33
21	GOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluids. SoftwareX, 2019, 9, 20-27.	2.6	32
22	Development of the TraPPE-UA force field for ethylene oxide. Fluid Phase Equilibria, 2008, 274, 44-49.	2.5	30
23	Mie Potentials for Phase Equilibria: Application to Alkenes. Journal of Chemical & Engineering Data, 2014, 59, 3144-3150.	1.9	30
24	Ca²⁺ Bridging of Apposed Phospholipid Bilayers. Journal of Physical Chemistry B, 2010, 114, 13249-13254.	2.6	29
25	Membraneâ€directed molecular assembly of the neuronal SNARE complex. Journal of Cellular and Molecular Medicine, 2011, 15, 31-37.	3.6	29
26	Computational prediction of ionic liquid 1-octanol/water partition coefficients. Physical Chemistry Chemical Physics, 2012, 14, 4339.	2.8	28
27	GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. Computer Physics Communications, 2013, 184, 2662-2669.	7.5	27
28	Monte Carlo predictions for the phase behavior of H2 S+n-alkane, H2 S+CO2, CO2+CH4 and H2 S+CO2+CH4 mixtures. Fluid Phase Equilibria, 2006, 246, 71-78.	2.5	24
29	Prediction of 1-octanolâ€“water and airâ€“water partition coefficients for nitro-aromatic compounds from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6467.	2.8	24
30	Optimized Mie Potentials for Phase Equilibria: Application to Branched Alkanes. Journal of Chemical & Engineering Data, 2017, 62, 1806-1818.	1.9	24
31	Study on Interfacial Interaction between Polymer and Nanoparticle in a Nanocoating Matrix: A MARTINI Coarse-Graining Method. Industrial & Engineering Chemistry Research, 2013, 52, 73-82.	3.7	22
32	Effect of partial charge parameterization on the phase equilibria of dimethyl ether. Molecular Simulation, 2007, 33, 769-776.	2.0	20
33	Vaporâ"Liquid Phase Equilibria for Linear and Branched Alkane Monolayers Physisorbed on Au(111). Langmuir, 2002, 18, 6088-6095.	3.5	17
34	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	3.6	16
35	Effect of Branching on the Fluid Phase Behavior of Alkane Monolayers. Physical Review Letters, 2000, 85, 3460-3463.	7.8	15
36	Biomolecular Simulations with the Transferable Potentials for Phase Equilibria: Extension to Phospholipids. Journal of Physical Chemistry B, 2013, 117, 9910-9921.	2.6	14

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37	Optimised Mie potentials for phase equilibria: application to alkynes. Molecular Physics, 2017, 115, 1378-1388.	1.7	14
38	Accurate determination of solvation free energies of neutral organic compounds from first principles. Nature Communications, 2022, 13, 414.	12.8	14
39	Prediction of Radon-222 Phase Behavior by Monte Carlo Simulation. Journal of Chemical & Engineering Data, 2016, 61, 1625-1631.	1.9	13
40	Effect of torsional potential on the predicted phase behavior of n-alkanes. Fluid Phase Equilibria, 2009, 279, 100-104.	2.5	10
41	py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. Journal of Chemical Theory and Computation, 2022, 18, 4983-4994.	5.3	10
42	Monte Carlo predictions of phase equilibria and structure for dimethyl ether + sulfur dioxide and dimethyl ether + carbon dioxide. Journal of Chemical Physics, 2012, 136, 044514.	3.0	9
43	Prediction of phase equilibria and Gibbs free energies of transfer using molecular exchange Monte Carlo in the Gibbs ensemble. Fluid Phase Equilibria, 2019, 486, 106-118.	2.5	8
44	Improving performance of GPU code using novel features of the NVIDIA kepler architecture. Concurrency Computation Practice and Experience, 2016, 28, 3586-3605.	2.2	7
45	Molecular exchange Monte Carlo: A generalized method for identity exchanges in grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2018, 149, 072318.	3.0	7
46	The effect of fluorination on the physical properties and the free energies of hydration of 1-alcohols. Fluid Phase Equilibria, 2016, 407, 314-321.	2.5	6
47	Histogram-Free Reweighting with Grand Canonical Monte Carlo: Post-simulation Optimization of Non-bonded Potentials for Phase Equilibria. Journal of Chemical & Engineering Data, 2019, 64, 3701-3717.	1.9	5
48	Update 2.70 to â€œGOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluidsâ€• SoftwareX, 2021, 13, 100627.	2.6	5
49	Parallel Monte Carlo simulation in the canonical ensemble on the graphics processing unit. International Journal of Parallel, Emergent and Distributed Systems, 2014, 29, 379-400.	1.0	4
50	Self-Assembly and Biogenesis of the Cellular Membrane are Dictated by Membrane Stretch and Composition. Journal of Physical Chemistry B, 2019, 123, 6997-7005.	2.6	3
51	Vaporâ^'Liquid Equilibria of Diethylamine + Methanol, Diethylamine + Acetone and Diethylamine + Acetonitrile:â€‰ Predictions of Atomistic Computer Simulations. Journal of Physical Chemistry C, 2007, 111, 1451-1458.	3.1	2
52	Effect of fluorination on the partitioning of alcohols. Molecular Physics, 2019, 117, 3827-3839.	1.7	2
53	Evaluation of Hybrid Parallel Cell List Algorithms for Monte Carlo Simulation. , 2015, , .		0
54	Mechanism of Membrane Biogenesis. FASEB Journal, 2018, 32, 671.11.	0.5	0