Jeffrey J Potoff

List of Publications by Year
in descending order

54 papers	4,599 citations	249298 26 h-index	190340 53 g-index
55 all docs	55 docs citations	55 times ranked	3925 citing authors

#	Article	IF	Citations
1	Accurate determination of solvation free energies of neutral organic compounds from first principles. Nature Communications, 2022, 13, 414.	5.8	14
2	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.	2.3	10
3	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.	1.2	5
4	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
5	Self-Assembly and Biogenesis of the Cellular Membrane are Dictated by Membrane Stretch and Composition. Journal of Physical Chemistry B, 2019, 123, 6997-7005.	1.2	3
6	Effect of fluorination on the partitioning of alcohols. Molecular Physics, 2019, 117, 3827-3839.	0.8	2
7	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.	1.4	8
8	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.	1.0	5
9	GOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluids. SoftwareX, 2019, 9, 20-27.	1.2	32
10	Molecular exchange Monte Carlo: A generalized method for identity exchanges in grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2018, 149, 072318.	1.2	7
11	Mechanism of Membrane Biogenesis. FASEB Journal, 2018, 32, 671.11.	0.2	0
12	Optimized Mie Potentials for Phase Equilibria: Application to Branched Alkanes. Journal of Chemical & Engineering Data, 2017, 62, 1806-1818.	1.0	24
13	Optimised Mie potentials for phase equilibria: application to alkynes. Molecular Physics, 2017, 115, 1378-1388.	0.8	14
14	Improving performance of GPU code using novel features of the NVIDIA kepler architecture. Concurrency Computation Practice and Experience, 2016, 28, 3586-3605.	1.4	7
15	Prediction of Radon-222 Phase Behavior by Monte Carlo Simulation. Journal of Chemical & Engineering Data, 2016, 61, 1625-1631.	1.0	13
16	The effect of fluorination on the physical properties and the free energies of hydration of 1-alcohols. Fluid Phase Equilibria, 2016, 407, 314-321.	1.4	6
17	Evaluation of Hybrid Parallel Cell List Algorithms for Monte Carlo Simulation. , 2015, , .		0
18	Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes. Journal of Chemical Physics, 2015, 143, 114504.	1.2	43

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19	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.	0.7	4
20	Mie Potentials for Phase Equilibria: Application to Alkenes. Journal of Chemical & Engineering Data, 2014, 59, 3144-3150.	1.0	30
21	GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. Computer Physics Communications, 2013, 184, 2662-2669.	3.0	27
22	Biomolecular Simulations with the Transferable Potentials for Phase Equilibria: Extension to Phospholipids. Journal of Physical Chemistry B, 2013, 117, 9910-9921.	1.2	14
23	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.	1.8	22
24	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.	1.3	24
25	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.	1.2	9
26	Direct calculation of 1-octanolâ€“water partition coefficients from adaptive biasing force molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 014502.	1.2	44
27	Computational prediction of ionic liquid 1-octanol/water partition coefficients. Physical Chemistry Chemical Physics, 2012, 14, 4339.	1.3	28
28	Membraneâ€directed molecular assembly of the neuronal SNARE complex. Journal of Cellular and Molecular Medicine, 2011, 15, 31-37.	1.6	29
29	Development of an Optimized Intermolecular Potential for Sulfur Dioxide. Journal of Physical Chemistry B, 2011, 115, 4949-4954.	1.2	65
30	Ca²⁺ Bridging of Apposed Phospholipid Bilayers. Journal of Physical Chemistry B, 2010, 114, 13249-13254.	1.2	29
31	Effect of torsional potential on the predicted phase behavior of n-alkanes. Fluid Phase Equilibria, 2009, 279, 100-104.	1.4	10
32	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.	1.2	37
33	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.	1.2	42
34	Mie Potentials for Phase Equilibria Calculations: Application to Alkanes and Perfluoroalkanes. Journal of Physical Chemistry B, 2009, 113, 14725-14731.	1.2	110
35	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.	1.4	40
36	Development of the TraPPE-UA force field for ethylene oxide. Fluid Phase Equilibria, 2008, 274, 44-49.	1.4	30

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37	Effect of partial charge parameterization on the phase equilibria of dimethyl ether. Molecular Simulation, 2007, 33, 769-776.	0.9	20
38	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.	1.5	2
39	Application of TraPPE-UA force field for determination of vaporâ€"liquid equilibria of carboxylate esters. Fluid Phase Equilibria, 2006, 240, 46-55.	1.4	51
40	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.	1.4	24
41	Effect of quadrupole moment on the phase behavior of binary mixtures containing ethene. Fluid Phase Equilibria, 2005, 234, 144-150.	1.4	33
42	Molecular Modeling of Phase Behavior and Microstructure of Acetoneâ˜'Chloroformâ˜'Methanol Binary Mixtures. Journal of Physical Chemistry B, 2005, 109, 19463-19473.	1.2	67
43	Transferable Potentials for Phase Equilibria. 8. United-Atom Description for Thiols, Sulfides, Disulfides, and Thiophene. Journal of Physical Chemistry B, 2005, 109, 24100-24107.	1.2	112
44	Effect of partial charge parametrization on the fluid phase behavior of hydrogen sulfide. Journal of Chemical Physics, 2005, 123, 124505.	1.2	69
45	Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. Journal of Physical Chemistry B, 2004, 108, 17596-17605.	1.2	410
46	An Improved Force Field for the Prediction of the Vaporâ˜'Liquid Equilibria for Carboxylic Acids. Journal of Physical Chemistry B, 2004, 108, 14130-14136.	1.2	82
47	Vaporâ˜'Liquid Phase Equilibria for Linear and Branched Alkane Monolayers Physisorbed on Au(111). Langmuir, 2002, 18, 6088-6095.	1.6	17
48	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.	1.2	730
49	Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. Fluid Phase Equilibria, 2001, 183-184, 301-309.	1.4	44
50	Vaporâ€"liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. AICHE Journal, 2001, 47, 1676-1682.	1.8	1,560
51	Effect of Branching on the Fluid Phase Behavior of Alkane Monolayers. Physical Review Letters, 2000, 85, 3460-3463.	2.9	15
52	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.	1.2	68
53	Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. Journal of Chemical Physics, 2000, 112, 6411-6415.	1.2	144
54	Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. Journal of Chemical Physics, 1998, 109, 10914-10920.	1.2	347