

Jeffrey J Potoff

List of Publications by Year in descending order

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54
papers

4,599
citations

218677

26
h-index

168389

53
g-index

55
all docs

55
docs citations

55
times ranked

3417
citing authors

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

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19	Extension of the Transferable Potentials for Phase Equilibria Force Field to Dimethylmethyl Phosphonate, Sarin, and Soman. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10292-10297.	2.6	37
20	Effect of quadrupole moment on the phase behavior of binary mixtures containing ethene. <i>Fluid Phase Equilibria</i> , 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. <i>SoftwareX</i> , 2019, 9, 20-27.	2.6	32
22	Development of the TraPPE-UA force field for ethylene oxide. <i>Fluid Phase Equilibria</i> , 2008, 274, 44-49.	2.5	30
23	Mie Potentials for Phase Equilibria: Application to Alkenes. <i>Journal of Chemical & Engineering Data</i> , 2014, 59, 3144-3150.	1.9	30
24	Ca ²⁺ Bridging of Apposed Phospholipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13249-13254.	2.6	29
25	Membrane-directed molecular assembly of the neuronal SNARE complex. <i>Journal of Cellular and Molecular Medicine</i> , 2011, 15, 31-37.	3.6	29
26	Computational prediction of ionic liquid 1-octanol/water partition coefficients. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4339.	2.8	28
27	GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. <i>Computer Physics Communications</i> , 2013, 184, 2662-2669.	7.5	27
28	Monte Carlo predictions for the phase behavior of H ₂ S+n-alkane, H ₂ S+CO ₂ , CO ₂ +CH ₄ and H ₂ S+CO ₂ +CH ₄ mixtures. <i>Fluid Phase Equilibria</i> , 2006, 246, 71-78.	2.5	24
29	Prediction of 1-octanol-water and air-water partition coefficients for nitro-aromatic compounds from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6467.	2.8	24
30	Optimized Mie Potentials for Phase Equilibria: Application to Branched Alkanes. <i>Journal of Chemical & Engineering Data</i> , 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. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 73-82.	3.7	22
32	Effect of partial charge parameterization on the phase equilibria of dimethyl ether. <i>Molecular Simulation</i> , 2007, 33, 769-776.	2.0	20
33	Vapor-Liquid Phase Equilibria for Linear and Branched Alkane Monolayers Physisorbed on Au(111). <i>Langmuir</i> , 2002, 18, 6088-6095.	3.5	17
34	Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. <i>AIChE Journal</i> , 2021, 67, e17206.	3.6	16
35	Effect of Branching on the Fluid Phase Behavior of Alkane Monolayers. <i>Physical Review Letters</i> , 2000, 85, 3460-3463.	7.8	15
36	Biomolecular Simulations with the Transferable Potentials for Phase Equilibria: Extension to Phospholipids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9910-9921.	2.6	14

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37	Optimised Mie potentials for phase equilibria: application to alkynes. <i>Molecular Physics</i> , 2017, 115, 1378-1388.	1.7	14
38	Accurate determination of solvation free energies of neutral organic compounds from first principles. <i>Nature Communications</i> , 2022, 13, 414.	12.8	14
39	Prediction of Radon-222 Phase Behavior by Monte Carlo Simulation. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 1625-1631.	1.9	13
40	Effect of torsional potential on the predicted phase behavior of n-alkanes. <i>Fluid Phase Equilibria</i> , 2009, 279, 100-104.	2.5	10
41	py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Chemical Physics</i> , 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. <i>Fluid Phase Equilibria</i> , 2019, 486, 106-118.	2.5	8
44	Improving performance of GPU code using novel features of the NVIDIA kepler architecture. <i>Concurrency Computation Practice and Experience</i> , 2016, 28, 3586-3605.	2.2	7
45	Molecular exchange Monte Carlo: A generalized method for identity exchanges in grand canonical Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2018, 149, 072318.	3.0	7
46	The effect of fluorination on the physical properties and the free energies of hydration of 1-alcohols. <i>Fluid Phase Equilibria</i> , 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. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 3701-3717.	1.9	5
48	Update 2.70 to GOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluids. <i>SoftwareX</i> , 2021, 13, 100627.	2.6	5
49	Parallel Monte Carlo simulation in the canonical ensemble on the graphics processing unit. <i>International Journal of Parallel, Emergent and Distributed Systems</i> , 2014, 29, 379-400.	1.0	4
50	Self-Assembly and Biogenesis of the Cellular Membrane are Dictated by Membrane Stretch and Composition. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6997-7005.	2.6	3
51	Vapor-Liquid Equilibria of Diethylamine + Methanol, Diethylamine + Acetone and Diethylamine + Acetonitrile: Predictions of Atomistic Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1451-1458.	3.1	2
52	Effect of fluorination on the partitioning of alcohols. <i>Molecular Physics</i> , 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. <i>FASEB Journal</i> , 2018, 32, 671.11.	0.5	0