Predicting Multicomponent Phase Equilibria and Free E Molecular Simulation

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Citation Report

#	Article	IF	Citations
2	Intermolecular potentials and vapor–liquid phase equilibria of perfluorinated alkanes. Fluid Phase Equilibria, 1998, 146, 51-61.	2.5	92
3	On the simulation of vapor–liquid equilibria for alkanes. Journal of Chemical Physics, 1998, 108, 9905-9911.	3.0	418
4	Thermodynamic Properties of the Williams, OPLS-AA, and MMFF94 All-Atom Force Fields for Normal Alkanes. Journal of Physical Chemistry B, 1998, 102, 2578-2586.	2.6	93
5	Determination of the Local Environment Surrounding Pyrene in Supercritical Alkanes: A First Step toward Solvation in Supercritical Aviation Fuels. Energy & Fuels, 1998, 12, 823-827.	5.1	5
6	Transferable Potentials for Phase Equilibria. 1. United-Atom Description of n-Alkanes. Journal of Physical Chemistry B, 1998, 102, 2569-2577.	2.6	2,480
7	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. Journal of Physical Chemistry A, 1998, 102, 7727-7730.	2.5	118
8	Vapor–Liquid Equilibria of Binary and Ternary Mixtures Containing Methane, Ethane, and Carbon Dioxide from Gibbs Ensemble Simulations. Journal of Physical Chemistry B, 1998, 102, 7627-7631.	2.6	28
9	Novel pseudoensembles for simulation of multicomponent phase equilibria. Journal of Chemical Physics, 1998, 108, 8761-8772.	3.0	69
10	Improving the efficiency of the configurational-bias Monte Carlo algorithm. Molecular Physics, 1998, 94, 727-733.	1.7	212
11	Vapour-liquid coexistence curves of the united-atom and anisotropic united-atom force fields for alkane mixtures. Molecular Physics, 1999, 96, 1517-1524.	1.7	34
12	Molecular simulations on volumetric properties of natural gas. Fluid Phase Equilibria, 1999, 161, 45-62.	2.5	18
13	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. Journal of Physical Chemistry B, 1999, 103, 1102-1118.	2.6	472
14	A New Intermolecular Potential Model for the n-Alkane Homologous Series. Journal of Physical Chemistry B, 1999, 103, 6314-6322.	2.6	171
15	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. Journal of Physical Chemistry B, 1999, 103, 5370-5379.	2.6	266
16	Molecular simulation of phase equilibria for mixtures of polar and non-polar components. Molecular Physics, 1999, 97, 1073-1083.	1.7	137
17	Origins of the Solvent Chain-Length Dependence of Gibbs Free Energies of Transfer. Journal of Physical Chemistry B, 1999, 103, 2977-2980.	2.6	13
18	Efficiency of Parallel CBMC Simulations. Molecular Simulation, 1999, 23, 63-78.	2.0	13
19	Exploring Multicomponent Phase Equilibria by Monte Carlo Simulations: Toward a Description of Gas-Liquid Chromatography. ACS Symposium Series, 1999, , 82-95.	0.5	4

#	Article	IF	Citations
20	Transferable Potentials for Phase Equilibria. 4. United-Atom Description of Linear and Branched Alkenes and Alkylbenzenes. Journal of Physical Chemistry B, 2000, 104, 8008-8016.	2.6	528
21	The Chemical Meaning of the Standard Free Energy of Transfer:Â Use of van der Waals' Equation of State To Unravel the Interplay between Free Volume, Volume Entropy, and the Role of Standard States. Journal of Physical Chemistry B, 2000, 104, 5343-5349.	2.6	30
22	Self-Adapting Fixed-End-Point Configurational-Bias Monte Carlo Method for the Regrowth of Interior Segments of Chain Molecules with Strong Intramolecular Interactions. Macromolecules, 2000, 33, 7207-7218.	4.8	116
23	Molecular Structure and Phase Diagram of the Binary Mixture ofn-Heptane and Supercritical Ethane:Â A Gibbs Ensemble Monte Carlo Study. Journal of Physical Chemistry B, 2000, 104, 2415-2423.	2.6	20
24	Inadequacy of the Lorentz-Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation. Molecular Physics, 2001, 99, 619-625.	1.7	332
25	Separation of Alkane Isomers by Exploiting Entropy Effects during Adsorption on Silicalite-1:â€‰A Configurational-Bias Monte Carlo Simulation Study. Langmuir, 2001, 17, 1558-1570.	3.5	104
26	Simulating Retention in Gasâ€"Liquid Chromatography: Benzene, Toluene, and Xylene Solutes. International Journal of Thermophysics, 2001, 22, 111-122.	2.1	9
27	Computing phase equilibria by parallel excluded volume tempering. Journal of Chemical Physics, 2001, 115, 8731-8741.	3.0	10
28	Molecular Dynamics Simulations of Model Perhydrogenated and Perfluorinated Alkyl Chains, Droplets, and Micelles. Langmuir, 2002, 18, 9067-9079.	3.5	3
29	Vaporˆ˘Liquid Interfacial Properties of Mutually Saturated Water/1-Butanol Solutions. Journal of the American Chemical Society, 2002, 124, 12232-12237.	13.7	76
30	Influence of Framework Flexibility on the Adsorption Properties of Hydrocarbons in the Zeolite Silicalite. Journal of Physical Chemistry B, 2002, 106, 12757-12763.	2.6	191
31	Simulating vaporâ€"liquid nucleation of n-alkanes. Journal of Chemical Physics, 2002, 116, 4317-4329.	3.0	65
32	Molecular dynamics simulations of the surface tension of n-hexane, n-decane and n-hexadecane. Molecular Physics, 2002, 100, 2471-2475.	1.7	52
33	Vaporâ€"liquid phase equilibria of triacontane isomers: Deviations from the principle of corresponding states. Fluid Phase Equilibria, 2002, 202, 307-324.	2.5	28
34	Temperature effects on the retention of n-alkanes and arenes in heliumâ€"squalane gasâ€"liquid chromatography. Journal of Chromatography A, 2002, 954, 181-190.	3.7	66
35	Adsorption and Separation of Ternary and Quaternary Mixtures of Short Linear Alkanes in Zeolites by Molecular Simulation. Langmuir, 2003, 19, 10617-10623.	3.5	32
36	Many-Body Optimization Using an Ab Initio Monte Carlo Method. Journal of Chemical Information and Computer Sciences, 2003, 43, 68-74.	2.8	8
37	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. Journal of Physical Chemistry B, 2003, 107, 12088-12096.	2.6	95

#	Article	IF	Citations
38	Effect of cyclic chain architecture on properties of dilute solutions of polyethylene from molecular dynamics simulations. Journal of Chemical Physics, 2003, 119, 1843-1854.	3.0	44
39	Efficiency of Various Lattices from Hard Ball to Soft Ball:Â Theoretical Study of Thermodynamic Properties of Dendrimer Liquid Crystal from Atomistic Simulation. Journal of the American Chemical Society, 2004, 126, 1872-1885.	13.7	98
40	Molecular modelling of adsorption in novel nanoporous metalâ€"organic materials. Molecular Physics, 2004, 102, 211-221.	1.7	126
41	Molecular Dynamics Study of a Surfactant-Mediated Decaneˆ̃Water Interface:â€‰ Effect of Molecular Architecture of Alkyl Benzene Sulfonate. Journal of Physical Chemistry B, 2004, 108, 12130-12140.	2.6	244
42	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	2.6	314
43	Toluene Model for Molecular Dynamics Simulations in the Ranges 298 < T (K) < 350 and 0.1 < P (MPa) < 10. Journal of Physical Chemistry B, 2004, 108, 11774-11781.	2.6	23
44	Simulation of 1-alkene and n-alkane binary vapourâ€"liquid equilibrium using different united-atom transferable force fields. Fluid Phase Equilibria, 2005, 232, 136-148.	2.5	4
45	Rapid shear viscosity calculation by momentum impulse relaxation molecular dynamics. Journal of Chemical Physics, 2005, 123, 224904.	3.0	17
46	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO2. Journal of the American Chemical Society, 2005, 127, 12338-12342.	13.7	28
47	Pressure Dependence of the Vaporˆ̃Liquidˆ̃Liquid Phase Behavior in Ternary Mixtures Consisting ofn-Alkanes,n-Perfluoroalkanes, and Carbon Dioxide. Journal of Physical Chemistry B, 2005, 109, 2911-2919.	2.6	81
48	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, 18974-18982.	2.6	212
49	Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2005, 109, 18988-18999.	2.6	193
50	Microscopic Structure and Solvation in Dry and Wet Octanolâ€. Journal of Physical Chemistry B, 2006, 110, 3555-3563.	2.6	130
51	Equilibrium Distributions of Dipalmitoyl Phosphatidylcholine and Dilauroyl Phosphatidylcholine in a Mixed Lipid Bilayer:Â Atomistic Semigrand Canonical Ensemble Simulations. Journal of Physical Chemistry B, 2006, 110, 25875-25882.	2.6	28
52	Direct calculation of Henryâ€™s law constants from Gibbs ensemble Monte Carlo simulations: nitrogen, oxygen, carbon dioxide and methane in ethanol. Theoretical Chemistry Accounts, 2006, 115, 391-397.	1.4	101
53	Combining reactive and configurational-bias Monte Carlo: Confinement influence on the propene metathesis reaction system in various zeolites. Journal of Chemical Physics, 2006, 125, 224709.	3.0	38
54	Solvent Effects in the Adsorption of Alkyl Thiols on Gold Structures:â€‰ A Molecular Simulation Study. Journal of Physical Chemistry C, 2007, 111, 10201-10212.	3.1	51
55	On the Atomistic Mechanisms of Alkane (Methaneˆ̃Pentane) Separation by Distillation:â€‰ A Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 12518-12523.	2.6	3

#	ARTICLE	IF	CITATIONS
56	Continuous Fractional Component Monte Carlo:â€‰ An Adaptive Biasing Method for Open System Atomistic Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1451-1463.	5.3	188
57	Selective adsorption of alkyl thiols on gold in different geometries. Computer Physics Communications, 2007, 177, 154-157.	7.5	26
58	Prediction of viscosities and vaporâ€"liquid equilibria for five polyhydric alcohols by molecular simulation. Fluid Phase Equilibria, 2007, 260, 218-231.	2.5	67
59	Molecular simulation of adsorption and separation of mixtures of short linear alkanes in pillared layered materials at ambient temperature. Journal of Colloid and Interface Science, 2007, 312, 179-185.	9.4	21
60	Wax Inhibition by Comb-like Polymers:â€‰ Support of the Incorporationâˆ'Perturbation Mechanism from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 13173-13179.	2.6	67
61	Influence of bonded-phase coverage in reversed-phase liquid chromatography via molecular simulation. Journal of Chromatography A, 2008, 1204, 11-19.	3.7	51
62	Influence of bonded-phase coverage in reversed-phase liquid chromatography via molecular simulation. Journal of Chromatography A, 2008, 1204, 20-27.	3.7	45
63	Molecular-Level Comparison of Alkylsilane and Polar-Embedded Reversed-Phase Liquid Chromatography Systems. Analytical Chemistry, 2008, 80, 6214-6221.	6.5	75
65	The effects of chain length, embedded polar groups, pressure, and pore shape on structure and retention in reversed-phase liquid chromatography: Molecular-level insights from Monte Carlo simulations. Journal of Chromatography A, 2009, 1216, 2320-2331.	3.7	61
66	Solvation of Nitrophenol Isomers: Consequences for Solute Electronic Structure and Alkane/Water Partitioning. Journal of Physical Chemistry B, 2009, 113, 759-766.	2.6	3
67	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metalâˆ'Organic Framework Materials. Industrial & Engineering Chemistry Research, 2009, 48, 2355-2371.	3.7	283
68	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metalâˆ'Organic Frameworks. Journal of Physical Chemistry C, 2009, 113, 20869-20874.	3.1	67
69	Investigation of the driving forces for retention in reversed-phase liquid chromatography: Monte Carlo simulations of solute partitioning between n-hexadecane and various aqueousâ€"organic mixtures. Fluid Phase Equilibria, 2010, 290, 25-35.	2.5	31
70	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. Journal of Physical Chemistry C, 2010, 114, 10527-10534.	3.1	82
71	Computational Investigation of the Influence of Surfactants on the Airâˆ'Water Interfacial Behavior of Polycylic Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2010, 114, 14520-14527.	3.1	25
72	Mitosis method for directly calculating the interfacial free energy of nuclei. Molecular Simulation, 2010, 36, 498-504.	2.0	9
73	Atomistic simulation of mixed-lipid bilayers: mixed methods for mixed membranes. Molecular Simulation, 2011, 37, 516-524.	2.0	11
74	Experimental and Theoretical Studies of Supercritical Methane Adsorption in the MIL-53(Al) Metal Organic Framework. Journal of Physical Chemistry C, 2011, 115, 20628-20638.	3.1	33

#	ARTICLE	IF	CITATIONS
75	Molecular Simulations of Retention in Chromatographic Systems: Use of Biased Monte Carlo Techniques to Access Multiple Time and Length Scales. Topics in Current Chemistry, 2011, 307, 181-200.	4.0	0
76	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. Journal of Physical Chemistry C, 2011, 115, 15355-15360.	3.1	18
77	Gibbs ensemble Monte Carlo simulations for the liquid–liquid phase equilibria of dipropylene glycol dimethyl ether and water: A preliminary report. Fluid Phase Equilibria, 2011, 310, 11-18.	2.5	17
78	Retention mechanism for polycyclic aromatic hydrocarbons in reversed-phase liquid chromatography with monomeric stationary phases. Journal of Chromatography A, 2011, 1218, 9183-9193.	3.7	32
79	Role of Surfactant Molecular Structure on Self-Assembly: Aqueous SDBS on Carbon Nanotubes. Journal of Physical Chemistry C, 2011, 115, 17286-17296.	3.1	73
80	The composition of liquid methane–nitrogen aerosols in Titan's lower atmosphere from Monte Carlo simulations. Icarus, 2011, 212, 779-789.	2.5	12
81	Mobile phase effects in reversed-phase liquid chromatography: A comparison of acetonitrile/water and methanol/water solvents as studied by molecular simulation. Journal of Chromatography A, 2011, 1218, 2203-2213.	3.7	84
82	Toward a Possibility To Exchange CO_2 and CH_4 in sI Clathrate Hydrates. Journal of Physical Chemistry B, 2012, 116, 3745-3753.	2.6	24
83	Calculation of Partition Functions and Free Energies of a Binary Mixture Using the Energy Partitioning Method: Application to Carbon Dioxide and Methane. Journal of Physical Chemistry B, 2012, 116, 4535-4542.	2.6	21
84	Multicomponent Adsorption of Alcohols onto Silicalite-1 from Aqueous Solution: Isotherms, Structural Analysis, and Assessment of Ideal Adsorbed Solution Theory. Langmuir, 2012, 28, 15566-15576.	3.5	71
85	Recent Advances in Molecular Dynamics Simulations of Gas Diffusion in Metal Organic Frameworks. , 0, , .		3
86	Computational screening of metal organic frameworks for mixed matrix membrane applications. Journal of Membrane Science, 2012, 407-408, 221-230.	8.2	43
87	Selective adsorption from dilute solutions: Gibbs ensemble Monte Carlo simulations. Fluid Phase Equilibria, 2013, 351, 1-6.	2.5	10
88	On the inner workings of Monte Carlo codes. Molecular Simulation, 2013, 39, 1253-1292.	2.0	325
89	Molecular insights for the optimization of solvent–based selective extraction of ethanol from fermentation broths. AICHE Journal, 2013, 59, 3065-3070.	3.6	16
90	Mechanism of adsorption of p-cresol uremic toxin into faujasite zeolites in presence of water and sodium cations – A Monte Carlo study. Microporous and Mesoporous Materials, 2013, 173, 70-77.	4.4	13
91	Adsorption of glucose into zeolite beta from aqueous solution. AICHE Journal, 2013, 59, 3523-3529.	3.6	52
92	Adapting SAFT-γ perturbation theory to site-based molecular dynamics simulation. I. Homogeneous fluids. Journal of Chemical Physics, 2013, 139, 234104.	3.0	30

#	Article	IF	Citations
93	Effect of molecular flexibility of Lennard-Jones chains on vapor-liquid interfacial properties. Journal of Chemical Physics, 2014, 140, 114705.	3.0	12
94	Concentration effects on the selective extraction of ethanol from aqueous solution using silicalite-1 and decanol isomers. Fluid Phase Equilibria, 2014, 362, 118-124.	2.5	7
95	Fully atomistic molecular–mechanical model of liquid alkane oils: Computational validation. Journal of Computational Chemistry, 2014, 35, 776-788.	3.3	6
96	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. III. Impact of combining rules on mixtures properties. Journal of Chemical Physics, 2014, 140, 104109.	3.0	35
97	Prediction of Vapor–Liquid Coexistence Properties and Critical Points of Polychlorinated Biphenyls from Monte Carlo Simulations with the TraPPE–EH Force Field. Journal of Chemical & Engineering Data, 2014, 59, 3301-3306.	1.9	7
98	A Comparison of Advanced Monte Carlo Methods for Open Systems: CFCMC vs CBMC. Journal of Chemical Theory and Computation, 2014, 10, 942-952.	5.3	60
99	Molecular simulation of self-assembly structure and interfacial interaction for SDBS adsorption on graphene. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 462, 82-89.	4.7	29
100	In Silico Determination of Gas Permeabilities by Non-Equilibrium Molecular Dynamics: CO_2 and He through PIM-1. Membranes, 2015, 5, 99-119.	3.0	44
101	Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling. Nature Communications, 2015, 6, 5912.	12.8	94
102	Equimolar mixtures of aqueous linear and branched SDBS surfactant simulated on single walled carbon nanotubes. RSC Advances, 2015, 5, 90049-90060.	3.6	6
103	Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibrium Calculations: n-Alkanes and n-Olefins. Journal of Physical Chemistry B, 2015, 119, 11695-11707.	2.6	46
104	Molecular Simulation of Olefin Oligomer Blend Phase Behavior. Macromolecules, 2016, 49, 3975-3985.	4.8	28
105	Hierarchical atom type definitions and extensible all–atom force fields. Journal of Computational Chemistry, 2016, 37, 653-664.	3.3	24
106	Computational assessment of MOF membranes for CH_4/H_2 separations. Journal of Membrane Science, 2016, 514, 313-321.	8.2	37
107	Adsorptive Separation of 1-Butanol from Aqueous Solutions Using MFI- and FER-Type Zeolite Frameworks: A Monte Carlo Study. Langmuir, 2016, 32, 2093-2101.	3.5	28
108	A Monte Carlo simulation study of the liquid–liquid equilibria for binary dodecane/ethanol and ternary dodecane/ethanol/water mixtures. Fluid Phase Equilibria, 2016, 407, 269-279.	2.5	25
109	Performance of various models in structural characterization of n -butanol: Molecular dynamics and X-ray scattering studies. Journal of Molecular Liquids, 2017, 229, 346-357.	4.9	21
110	Assessment and Optimization of Configurational-Bias Monte Carlo Particle Swap Strategies for Simulations of Water in the Gibbs Ensemble. Journal of Chemical Theory and Computation, 2017, 13, 431-440.	5.3	23

#	Article	IF	Citations
111	Different locations of adenine in AOT and CTAB reverse micelles. Journal of Molecular Liquids, 2017, 232, 236-242.	4.9	9
112	Phase Equilibria and Critical Point Predictions of Mixtures of Molecular Fluids Using Grand Canonical Transition Matrix Monte Carlo. Industrial & Engineering Chemistry Research, 2017, 56, 6520-6534.	3.7	6
113	Effect of Vinyl-Acetate Moiety Molar Fraction on the Performance of Poly(Octadecyl Acrylate-Vinyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Fuels, 2017, 31, 448-457.	5.1	34
114	Development of a low-pressure materials pre-treatment process for improved energy efficiency. Metals and Materials International, 2017, 23, 1029-1036.	3.4	0
115	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. Chemistry of Materials, 2017, 29, 6315-6328.	6.7	65
116	Characterization of the supramolecular assembly in 1,4-butanediol. Journal of Molecular Liquids, 2018, 259, 291-303.	4.9	6
117	Calix[4]arene-Based Porous Organic Nanosheets. ACS Applied Materials & Interfaces, 2018, 10, 17359-17365.	8.0	39
118	Modeling of Diffusion in MOFs. , 2018, , 63-97.		2
119	Solubility of CO2 in triglycerides using Monte Carlo simulations. Fluid Phase Equilibria, 2018, 476, 39-47.	2.5	10
120	A Monte Carlo simulation study of the interfacial tension for water/oil mixtures at elevated temperatures and pressures: Water/n-dodecane, water/toluene, and water/(n-dodecaneÂ+ toluene). Fluid Phase Equilibria, 2018, 476, 16-24.	2.5	19
121	Efficient separation of helium from methane using MOF membranes. Separation and Purification Technology, 2018, 191, 192-199.	7.9	49
122	Monte Carlo Simulations of Fluid Phase Equilibria and Interfacial Properties for Water/Alkane Mixtures: An Assessment of Nonpolarizable Water Models and of Departures from the Lorentzâ€"Berthelot Combining Rules. Journal of Chemical & Engineering Data, 2018, 63, 4256-4268.	1.9	26
123	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 5. Hetero-Group Coarse-Grained Models of Linear Alkanes and the Importance of Intramolecular Interactions. Journal of Physical Chemistry B, 2018, 122, 9161-9177.	2.6	37
124	Calculation of the Saturation Properties of a Model Octaneâ€"Water System Using Monte Carlo Simulation. Journal of Physical Chemistry B, 2018, 122, 6260-6271.	2.6	6
125	Understanding the unique sorption of alkane-α, ω-diols in silicalite-1. Journal of Chemical Physics, 2018, 149, 072331.	3.0	8
126	Understanding the Molecular Weight Dependence of Ï‡ and the Effect of Dispersity on Polymer Blend Phase Diagrams. Macromolecules, 2018, 51, 3774-3787.	4.8	20
127	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
128	Partial molar properties from molecular simulation using multiple linear regression. Molecular Physics, 2019, 117, 3589-3602.	1.7	13

#	Article	IF	Citations
129	Effect of fluorination on the partitioning of alcohols. Molecular Physics, 2019, 117, 3827-3839.	1.7	2
130	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
131	Toward realistic computer modeling of paraffin-based composite materials: critical assessment of atomic-scale models of paraffins. RSC Advances, 2019, 9, 38834-38847.	3.6	39
132	Derivation of micelle size-dependent free energies of aggregation for octyl phosphocholine from molecular dynamics simulation. Fluid Phase Equilibria, 2019, 485, 83-93.	2.5	8
133	Vaporâ€•and liquidâ€•phase adsorption of alcohol and water in silicaliteâ€‘1 synthesized in fluoride media. AICHE Journal, 2020, 66, e16868.	3.6	12
134	Bulk Self-Assembly of Giant, Unilamellar Vesicles. ACS Nano, 2020, 14, 14627-14634.	14.6	37
135	Approach to evaluate the gas/aerosol partition coefficient of organic volatile compounds using DFT methods associated with polarizable continuum models. Atmospheric Environment, 2020, 224, 117363.	4.1	7
136	Evaluation of thermal conductivity of organic phase-change materials from equilibrium and non-equilibrium computer simulations: Paraffin as a test case. International Journal of Heat and Mass Transfer, 2021, 165, 120639.	4.8	30
137	Effects of Electrolytes on Thermodynamics and Structure of Oligo(ethylene oxide)/Salt Solutions and Liquidâ€"Liquid Equilibria of a Squalane/Tetraethylene Glycol Dimethyl Ether Blend. Macromolecules, 2021, 54, 1120-1136.	4.8	2
138	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
139	Molecular Modeling of Subsurface Phenomena Related to Petroleum Engineering. Energy & Fuels, 2021, 35, 2851-2869.	5.1	12
140	Free energy of micellization of dodecyl phosphocholine (DPC) from molecular simulation: Hybrid PEACHâ€'BAR method. Journal of Computational Chemistry, 2021, 42, 2221-2232.	3.3	2
141	Monte Carlo Methods for Simulating Phase Equilibria of Complex Fluids. Advances in Chemical Physics, 0, , 443-460.	0.3	12
142	Improving the efficiency of the configurational-bias Monte Carlo algorithm. Molecular Physics, 1998, 94, 727-733.	1.7	13
143	Monte Carlo Simulation for Vapor-Liquid Equilibrium of Binary Mixtures CO_2/CH_3OH CO_2/C_2H_5OH, and CO_2/$CH_3CH_2CH_2OH$. Bulletin of the Korean Chemical Society, 2002, 23, 811-817.	1.9	5
144	Effect of Branching on Mutual Solubility of Alkaneâ€"CO_2 Systems by Molecular Simulations. Journal of Physical Chemistry B, 2022, 126, 8300-8308.	2.6	5
145	MoSDeF-GOMC: Python Software for the Creation of Scientific Workflows for the Monte Carlo Simulation Engine GOMC. Journal of Chemical Information and Modeling, 2023, 63, 1218-1228.	5.4	1
146	Continuous fractional component Gibbs ensemble Monte Carlo. American Journal of Physics, 2023, 91, 235-246.	0.7	3

#	Article	IF	Citations
147	Current Practices and Continuing Needs in Thermophysical Properties for the Chemical Industry. Industrial & Engineering Chemistry Research, 2023, 62, 3394-3427.	3.7	4
148	United atom and coarse grained models for crosslinked polydimethylsiloxane with applications to the rheology of silicone fluids. Physical Chemistry Chemical Physics, 2023, 25, 9669-9684.	2.8	3
149	A review of GEMC method and its improved algorithms. Acta Geochimica, 0, , .	1.7	0
150	Auto-calibration strategy for the equilibration phase of Gibbs ensemble Monte Carlo simulations. Molecular Simulation, 2023, 49, 1143-1156.	2.0	0
151	Diffusion and Gas Flow Dynamics in Partially Saturated Smectites. Journal of Physical Chemistry C, 2023, 127, 14425-14438.	3.1	0
152	Interactions of Essential Oil Components to Their Payloads in Supramolecular Particulate Carriers of Cyclodextrin Metal-Organic Frameworks. Journal of Oleo Science, 2023, 72, 957-968.	1.4	0