J Ilja Siepmann

List of Publications by Year in Descending Order

174 papers	13,486 citations	56 h-index	114 g-index
195 ext. papers	15,050 ext. citations	5.4 avg, IF	6.72 L-index

#	Paper	IF	Citations
174	In silico design of microporous polymers for chemical separations and storage. *Current Opinion in Chemical Engineering*, **2022**, 36, 100795	5.4	1
173	Phase Equilibria of Difluoromethane (R32), 1,1,1,2-Tetrafluoroethane (R134a), and trans-1,3,3,3-Tetrafluoro-1-propene (R1234ze(E)) Probed by Experimental Measurements and Monte Carlo Simulations. *Industrial & Engineering Chemistry Research*, **2021**, 60, 739-752	3.9	4
172	First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 6090-6098	3.8	3
171	Development of a PointNet for Detecting Morphologies of Self-Assembled Block Oligomers in Atomistic Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 5275-5284	3.4	1
170	Machine learning using host/guest energy histograms to predict adsorption in metal-organic frameworks: Application to short alkanes and Xe/Kr mixtures. *Journal of Chemical Physics*, **2021**, 155, 014701	3.9	6
169	Effects of Electrolytes on Thermodynamics and Structure of Oligo(ethylene oxide)/Salt Solutions and Liquid–Liquid Equilibria of a Squalane/Tetraethylene Glycol Dimethyl Ether Blend. *Macromolecules*, **2021**, 54, 1120-1136	5.5	1
168	Adsorption of furan, hexanoic acid, and alkanes in a hierarchical zeolite at reaction conditions: Insights from molecular simulations. *Journal of Computational Science*, **2021**, 48, 101267	3.4	2
167	Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. *AICHE Journal*, **2021**, 67, e17206	3.6	6
166	Simulating Vapor–Liquid Equilibria of PH3, AsH3, and SbH3 from First Principles. *Journal of Physical Chemistry C*, **2021**, 125, 5380-5385	3.8	1
165	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. *Science Advances*, **2021**, 7,	14.3	8
164	The Statistical Mechanics of Solution-Phase Nucleation: CaCO(_3) Revisited. *Molecular Modeling and Simulation*, **2021**, 101-122		1
163	Modeling and simulation of gas separations with spiral-wound membranes. *AICHE Journal*, **2020**, 66, e16274	3.6	2
162	From Order to Disorder: Computational Design of Triblock Amphiphiles with 1 nm Domains. *Journal of the American Chemical Society*, **2020**, 142, 9352-9362	16.4	7
161	One-dimensional intergrowths in two-dimensional zeolite nanosheets and their effect on ultra-selective transport. *Nature Materials*, **2020**, 19, 443-449	27	43
160	Temperature effects on the spatial distribution of electrolyte mixtures at the aqueous liquid-vapor interface. *Physical Chemistry Chemical Physics*, **2020**, 22, 10792-10801	3.6	
159	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. *Fluid Phase Equilibria*, **2020**, 523, 112785	2.5	10
158	Assessing the Quality of Molecular Simulations for Vapor–Liquid Equilibria: An Analysis of the TraPPE Database. *Journal of Chemical & Engineering Data*, **2020**, 65, 1330-1344	2.8	16

157	Identification Schemes for Metal Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
156	Renewable lubricants with tailored molecular architecture. *Science Advances*, **2019**, 5, eaav5487	14.3	30
155	Synthesis, Simulation, and Self-Assembly of a Model Amphiphile To Push the Limits of Block Polymer Nanopatterning. *Nano Letters*, **2019**, 19, 4458-4462	11.5	14
154	Molecular Simulations Probing the Thermophysical Properties of Homogeneously Stretched and Bubbly Water Systems. *Journal of Chemical & Engineering Data*, **2019**, 64, 3755-3771	2.8	3
153	Metal Organic Frameworks with Metal Catecholates for O2/N2 Separation. *Journal of Physical Chemistry C*, **2019**,	3.8	12
152	Deep neural network learning of complex binary sorption equilibria from molecular simulation data. *Chemical Science*, **2019**, 10, 4377-4388	9.4	26
151	A new equation of state for homo-polymers in dissipative particle dynamics. *Journal of Chemical Physics*, **2019**, 150, 124104	3.9	4
150	Partial molar properties from molecular simulation using multiple linear regression. *Molecular Physics*, **2019**, 117, 3589-3602	1.7	9
149	Highlighting 10 Years of NIST Cooperation and Service to the Thermophysical Properties Data Community. *Journal of Chemical & Engineering Data*, **2019**, 64, 4191-4192	2.8	2
148	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*, **2019**, 64, 5985-5998	2.8	183
147	Vapor- and Liquid-Phase Adsorption of Alcohol and Water in Silicalite-1 Synthesized in Fluoride Media. *AICHE Journal*, **2019**, 66, e16868	3.6	4
146	Computational screening of metal organic frameworks for biogas purification. *Molecular Systems Design and Engineering*, **2019**, 4, 1125-1135	4.6	10
145	Column selection for comprehensive two-dimensional liquid chromatography using the hydrophobic subtraction model. *Journal of Chromatography A*, **2019**, 1589, 47-55	4.5	13
144	Computational Design of High- Block Oligomers for Accessing 1 nm Domains. *ACS Nano*, **2018**, 12, 4351-4361	13.7	18
143	C2 adsorption in zeolites: in silico screening and sensitivity to molecular models. *Molecular Systems Design and Engineering*, **2018**, 3, 619-626	4.6	7
142	Supersaturated calcium carbonate solutions are classical. *Science Advances*, **2018**, 4, eaao6283	14.3	75
141	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-dodecane + toluene). *Fluid Phase Equilibria*, **2018**, 476, 16-24	2.5	16
140	Understanding the unique sorption of alkane-, -diols in silicalite-1. *Journal of Chemical Physics*, **2018**, 149, 072331	3.9	5

139	Understanding the Molecular Weight Dependence of and the Effect of Dispersity on Polymer Blend Phase Diagrams. *Macromolecules*, **2018**, 51, 3774-3787	5.5	13
138	First principles Monte Carlo simulations of unary and binary adsorption: CO, N, and HO in Mg-MOF-74. *Chemical Communications*, **2018**, 54, 10816-10819	5.8	25
137	Using molecular simulations to probe pore structures and polymer partitioning in size exclusion chromatography. *Journal of Chromatography A*, **2018**, 1573, 78-86	4.5	7
136	Cooperative Catalysis by Surface Lewis Acid/Silanol for Selective Fructose Etherification on Sn-SPP Zeolite. *ACS Catalysis*, **2018**, 8, 9056-9065	13.1	9
135	Mercury Capture from Petroleum Using Deep Eutectic Solvents. *Industrial & Engineering Chemistry Research*, **2018**, 57, 9222-9230	3.9	15
134	Probing Additive Loading in the Lamellar Phase of a Nonionic Surfactant: Gibbs Ensemble Monte Carlo Simulations Using the SDK Force Field. *Langmuir*, **2018**, 34, 8245-8254	4	3
133	First-Principles Molecular Dynamics Study of a Deep Eutectic Solvent: Choline Chloride/Urea and Its Mixture with Water. *Journal of Physical Chemistry B*, **2018**, 122, 1245-1254	3.4	110
132	Understanding the Reactive Adsorption of H S and CO in Sodium-Exchanged Zeolites. *ChemPhysChem*, **2018**, 19, 512-518	3.2	8
131	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 LorentzBerthelot Combining Rules. *Journal of Chemical & Engineering Data*, **2018**, 63, 4256-4268	2.8	12
130	Monte Carlo simulations probing the liquid/vapour interface of water/hexane mixtures: adsorption thermodynamics, hydrophobic effect, and structural analysis. *Molecular Physics*, **2018**, 116, 3283-3291	1.7	2
129	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	6.4	18
128	Using the k-d Tree Data Structure to Accelerate Monte Carlo Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1556-1565	6.4	12
127	Transferable potentials for phase equilibria. Improved united-atom description of ethane and ethylene. *AICHE Journal*, **2017**, 63, 5098-5110	3.6	20
126	Ultra-selective high-flux membranes from directly synthesized zeolite nanosheets. *Nature*, **2017**, 543, 690-694	50.4	310
125	A Review of Biorefinery Separations for Bioproduct Production via Thermocatalytic Processing. *Annual Review of Chemical and Biomolecular Engineering*, **2017**, 8, 115-137	8.9	15
124	Deconstructing the Confinement Effect upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials: Lessons Learned from Zeolites. *Journal of Physical Chemistry C*, **2017**, 121, 22015-22024	3.8	21
123	Comparative Study of the Effect of Defects on Selective Adsorption of Butanol from Butanol/Water Binary Vapor Mixtures in Silicalite-1 Films. *Langmuir*, **2017**, 33, 8420-8427	4	19
122	Separation of Thiophene from Aliphatic Hydrocarbons Using Tetrahexylammonium-Based Deep Eutectic Solvents as Extracting Agents. *Journal of Chemical & Engineering Data*, **2017**, 62, 2911-2919	2.8	35

121	Bioethanol enrichment using zeolite membranes: Molecular modeling, conceptual process design and techno-economic analysis. *Journal of Membrane Science*, **2017**, 540, 464-476	9.6	11
120	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. *Chemistry of Materials*, **2017**, 29, 6315-6328	9.6	46
119	Hydrogen Sulfide Capture: From Absorption in Polar Liquids to Oxide, Zeolite, and Metal-Organic Framework Adsorbents and Membranes. *Chemical Reviews*, **2017**, 117, 9755-9803	68.1	288
118	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	22
117	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. *ACS Central Science*, **2016**, 2, 409-15	16.8	14
116	Adsorptive Separation of 1-Butanol from Aqueous Solutions Using MFI- and FER-Type Zeolite Frameworks: A Monte Carlo Study. *Langmuir*, **2016**, 32, 2093-101	4	24
115	Structure and Phase Behavior of Mixed Self-Assembled Alkanethiolate Monolayers on Gold Nanoparticles: A Monte Carlo Study. *Journal of Physical Chemistry B*, **2016**, 120, 1972-8	3.4	21
114	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. *Angewandte Chemie*, **2016**, 128, 6042-6046	3.6	8
113	A mathematical model for zeolite membrane module performance and its use for techno-economic evaluation of improved energy efficiency hybrid membrane-distillation processes for butane isomer separations. *Journal of Membrane Science*, **2016**, 520, 434-449	9.6	20
112	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. *Angewandte Chemie - International Edition*, **2016**, 55, 5938-42	16.4	32
111	Molecular Simulation of Olefin Oligomer Blend Phase Behavior. *Macromolecules*, **2016**, 49, 3975-3985	5.5	17
110	Accelerated Computational Analysis of Metal–Organic Frameworks for Oxidation Catalysis. *Journal of Physical Chemistry C*, **2016**, 120, 18707-18712	3.8	33
109	Understanding Diffusion in Hierarchical Zeolites with House-of-Cards Nanosheets. *ACS Nano*, **2016**, 10, 7612-8	16.7	41
108	Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling. *Nature Communications*, **2015**, 6, 5912	17.4	75
107	Development of the Transferable Potentials for Phase Equilibria Model for Hydrogen Sulfide. *Journal of Physical Chemistry B*, **2015**, 119, 7041-52	3.4	37
106	Ab Initio Derived Force Fields for Predicting CO2 Adsorption and Accessibility of Metal Sites in the Metal–Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). *Journal of Physical Chemistry C*, **2015**, 119, 16058-16071	3.8	67
105	Monte Carlo Simulations Probing the Adsorptive Separation of Hydrogen Sulfide/Methane Mixtures Using All-Silica Zeolites. *Langmuir*, **2015**, 31, 12268-78	4	27
104	Liquid-liquid equilibria for soft-repulsive particles: improved equation of state and methodology for representing molecules of different sizes and chemistry in dissipative particle dynamics. *Journal of Chemical Physics*, **2015**, 142, 044902	3.9	19

103	Accurate and precise determination of critical properties from Gibbs ensemble Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 143, 114113	3.9	38
102	Understanding the sensitivity of nucleation free energies: The role of supersaturation and temperature. *Journal of Chemical Physics*, **2015**, 143, 164516	3.9	5
101	Understanding the unusual adsorption behavior in hierarchical zeolite nanosheets. *ChemPhysChem*, **2014**, 15, 2225-9	3.2	18
100	An online parameter and property database for the TraPPE force field. *Molecular Simulation*, **2014**, 40, 101-105	2	66
99	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	2.8	7
98	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. *Fluid Phase Equilibria*, **2014**, 366, 146-151	2.5	13
97	Deconstructing Hydrogen-Bond Networks in Confined Nanoporous Materials: Implications for Alcohol□Water Separation. *Journal of Physical Chemistry C*, **2014**, 118, 19723-19732	3.8	40
96	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	Selective adsorption from dilute solutions: Gibbs ensemble Monte Carlo simulations. *Fluid Phase Equilibria*, **2013**, 351, 1-6	2.5	9
94	TraPPE-zeo: Transferable Potentials for Phase Equilibria Force Field for All-Silica Zeolites. *Journal of Physical Chemistry C*, **2013**, 117, 24375-24387	3.8	87
93	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. *Molecular Simulation*, **2013**, 39, 1135-1142	2	36
92	Molecular insights for the optimization of solvent-based selective extraction of ethanol from fermentation broths. *AICHE Journal*, **2013**, 59, 3065-3070	3.6	13
91	Adsorption of glucose into zeolite beta from aqueous solution. *AICHE Journal*, **2013**, 59, 3523-3529	3.6	46
90	Transferable potentials for phase equilibria. 10. Explicit-hydrogen description of substituted benzenes and polycyclic aromatic compounds. *Journal of Physical Chemistry B*, **2013**, 117, 273-88	3.4	77
89	Modeling helical proteins using residual dipolar couplings, sparse long-range distance constraints and a simple residue-based force field. *Theoretical Chemistry Accounts*, **2013**, 132, 1388	1.9	3
88	Transferable potentials for phase equilibria-united atom description of five- and six-membered cyclic alkanes and ethers. *Journal of Physical Chemistry B*, **2012**, 116, 11234-46	3.4	79
87	Understanding the solubility of triamino-trinitrobenzene in hydrous tetramethylammonium fluoride: a first principles molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2012**, 14, 4884-90	3.6	11
86	Multicomponent adsorption of alcohols onto silicalite-1 from aqueous solution: isotherms, structural analysis, and assessment of ideal adsorbed solution theory. *Langmuir*, **2012**, 28, 15566-76	4	61

85	Transferable potentials for phase equilibria-coarse-grain description for linear alkanes. *Journal of Physical Chemistry B*, **2011**, 115, 3452-65	3.4	64
84	Vapor-liquid coexistence curves for methanol and methane using dispersion-corrected density functional theory. *Journal of Physical Chemistry B*, **2011**, 115, 11688-92	3.4	35
83	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	16
82	Retention mechanism for polycyclic aromatic hydrocarbons in reversed-phase liquid chromatography with monomeric stationary phases. *Journal of Chromatography A*, **2011**, 1218, 9183-93	4.5	29
81	Assessing group-based cutoffs and the Ewald method for electrostatic interactions in clusters and in saturated, superheated, and supersaturated vapor phases of dipolar molecules. *Theoretical Chemistry Accounts*, **2011**, 130, 83-93	1.9	6
80	Liquid structures of water, methanol, and hydrogen fluoride at ambient conditions from first principles molecular dynamics simulations with a dispersion corrected density functional. *Physical Chemistry Chemical Physics*, **2011**, 13, 19943-50	3.6	59
79	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, 2203-13	4.5	70
78	Effects of an applied electric field on the vapor-liquid equilibria of water, methanol, and dimethyl ether. *Journal of Physical Chemistry B*, **2010**, 114, 4261-70	3.4	34
77	Thermodynamic, structural and transport properties of tetramethyl ammonium fluoride: first principles molecular dynamics simulations of an unusual ionic liquid. *Journal of Physical Chemistry B*, **2010**, 114, 12577-84	3.4	35
76	Development of the trappe force field for ammonia. *Collection of Czechoslovak Chemical Communications*, **2010**, 75, 577-591		27
75	Investigation of the driving forces for retention in reversed-phase liquid chromatography: Monte Carlo simulations of solute partitioning between n-hexadecane and various aqueous–organic mixtures. *Fluid Phase Equilibria*, **2010**, 290, 25-35	2.5	30
74	Prediction of Hildebrand solubility parameters of acrylate and methacrylate monomers and their mixtures by molecular simulation. *Journal of Applied Polymer Science*, **2010**, 116, 1-9	2.9	20
73	TraPPE-UA force field for acrylates and Monte Carlo simulations for their mixtures with alkanes and alcohols. *Journal of Physical Chemistry B*, **2009**, 113, 6415-25	3.4	69
72	Exploring the formation of multiple layer hydrates for a complex pharmaceutical compound. *Journal of Physical Chemistry B*, **2009**, 113, 5929-37	3.4	12
71	Bond angle distributions of carbon dioxide in the gas, supercritical, and solid phases. *Journal of Physical Chemistry A*, **2009**, 113, 2053-9	2.8	19
70	Application of the TraPPE Force Field for Predicting the Hildebrand Solubility Parameters of Organic Solvents and Monomer Units. *Journal of Chemical Theory and Computation*, **2008**, 4, 136-44	6.4	26
69	Structure of the Methanol Liquid–Vapor Interface: A Comprehensive Particle-Based Simulation Study. *Journal of Physical Chemistry C*, **2008**, 112, 15412-15418	3.8	21
68	Size Effects on the Solvation of Anions at the Aqueous Liquid–Vapor Interface. *Journal of Physical Chemistry C*, **2008**, 112, 210-218	3.8	63

67	Molecular-level comparison of alkylsilane and polar-embedded reversed-phase liquid chromatography systems. *Analytical Chemistry*, **2008**, 80, 6214-21	7.8	74
66	Influence of bonded-phase coverage in reversed-phase liquid chromatography via molecular simulation I. Effects on chain conformation and interfacial properties. *Journal of Chromatography A*, **2008**, 1204, 11-9	4.5	48
65	Development of the TraPPE-UA force field for ethylene oxide. *Fluid Phase Equilibria*, **2008**, 274, 44-49	2.5	27
64	Monte Carlo Simulations of an Isolated n-Octadecane Chain Solvated in Water-Acetonitrile Mixtures. *Journal of Chemical Theory and Computation*, **2007**, 3, 350-7	6.4	13
63	Pressure Dependence of the Hildebrand Solubility Parameter and the Internal Pressure: Monte Carlo Simulations for External Pressures up to 300 MPa *Journal of Physical Chemistry C*, **2007**, 111, 15634-15641	3.8	40
62	Prediction of viscosities and vapor–liquid equilibria for five polyhydric alcohols by molecular simulation. *Fluid Phase Equilibria*, **2007**, 260, 218-231	2.5	58
61	Retention mechanism in reversed-phase liquid chromatography: a molecular perspective. *Analytical Chemistry*, **2007**, 79, 6551-8	7.8	117
60	Application of the TraPPE Force Field to Predicting Isothermal Pressure–Volume Curves at High Pressures and High Temperatures. *International Journal of Thermophysics*, **2007**, 28, 796-804	2.1	5
59	An Introduction to the Monte Carlo Method for Particle Simulations. *Advances in Chemical Physics*, **2007**, 1-12		4
58	Transferable potentials for phase equilibria. 9. Explicit hydrogen description of benzene and five-membered and six-membered heterocyclic aromatic compounds. *Journal of Physical Chemistry B*, **2007**, 111, 10790-9	3.4	162
57	Direct calculation of Henry's law constants from Gibbs ensemble Monte Carlo simulations: nitrogen, oxygen, carbon dioxide and methane in ethanol. *Theoretical Chemistry Accounts*, **2006**, 115, 391-397	1.9	75
56	Time-Dependent Properties of Liquid Water: A Comparison of Car-Parrinello and Born-Oppenheimer Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2006**, 2, 1274-81	6.4	72
55	Microscopic structure and solvation in dry and wet octanol. *Journal of Physical Chemistry B*, **2006**, 110, 3555-63	3.4	124
54	Simulating fluid-phase equilibria of water from first principles. *Journal of Physical Chemistry A*, **2006**, 110, 640-6	2.8	125
53	Conformation and solvation structure for an isolated n-octadecane chain in water, methanol, and their mixtures. *Journal of Physical Chemistry B*, **2006**, 110, 10519-25	3.4	36
52	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
51	Microscopic origins for the favorable solvation of carbonate ether copolymers in CO2. *Journal of the American Chemical Society*, **2005**, 127, 12338-42	16.4	26
50	Pressure dependence of the vapor-liquid-liquid phase behavior in ternary mixtures consisting of n-alkanes, n-perfluoroalkanes, and carbon dioxide. *Journal of Physical Chemistry B*, **2005**, 109, 2911-9	3.4	72

49	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
48	Vapor-liquid and vapor-solid phase equilibria for united-atom benzene models near their triple points: the importance of quadrupolar interactions. *Journal of Physical Chemistry B*, **2005**, 109, 5368-74	3.4	29
47	Transferable potentials for phase equilibria. 8. United-atom description for thiols, sulfides, disulfides, and thiophene. *Journal of Physical Chemistry B*, **2005**, 109, 24100-7	3.4	96
46	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
45	Simulating the vapour–liquid equilibria of large cyclic alkanes. *Molecular Physics*, **2005**, 103, 99-104	1.7	31
44	Isobaric-isothermal monte carlo simulations from first principles: application to liquid water at ambient conditions. *ChemPhysChem*, **2005**, 6, 1894-901	3.2	93
43	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
42	Liquid Water from First Principles: Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309
41	Temperature Dependence of Transfer Properties: Importance of Heat Capacity Effects. *Journal of Physical Chemistry B*, **2003**, 107, 10623-10627	3.4	18
40	Vapor–liquid phase equilibria of triacontane isomers: Deviations from the principle of corresponding states. *Fluid Phase Equilibria*, **2002**, 202, 307-324	2.5	27
39	Vapor-liquid interfacial properties of mutually saturated water/1-butanol solutions. *Journal of the American Chemical Society*, **2002**, 124, 12232-7	16.4	70
38	Molecular simulation of concurrent gas-liquid interfacial adsorption and partitioning in gas-liquid chromatography. *Analytical Chemistry*, **2002**, 74, 3518-24	7.8	33
37	Simulating vapor–liquid nucleation of n-alkanes. *Journal of Chemical Physics*, **2002**, 116, 4317-4329	3.9	57
36	Vapor–liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. *AICHE Journal*, **2001**, 47, 1676-1682	3.6	1229
35	Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium. *Journal of Chemical Physics*, **2001**, 115, 10903-10913	3.9	107
34	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	3.4	632
33	Improving the Efficiency of the Aggregation−Volume−Bias Monte Carlo Algorithm. *Journal of Physical Chemistry B*, **2001**, 105, 11275-11282	3.4	109
32	Direct Gibbs Ensemble Monte Carlo Simulations for Solid−Vapor Phase Equilibria: Applications to Lennard−Jonesium and Carbon Dioxide. *Journal of Physical Chemistry B*, **2001**, 105, 9840-9848	3.4	87

31	Simulation Studies of Retention in Isotropic or Oriented Liquid n-Octadecane. *Journal of Physical Chemistry B*, **2001**, 105, 10961-10966	3.4	7
30	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	3.4	435
29	Adiabatic Nuclear and Electronic Sampling Monte Carlo Simulations in the Gibbs Ensemble: Application to Polarizable Force Fields for Water. *Journal of Physical Chemistry B*, **2000**, 104, 2378-2390	3.4	66
28	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	5.5	104
27	A Novel Monte Carlo Algorithm for Simulating Strongly Associating Fluids: Applications to Water, Hydrogen Fluoride, and Acetic Acid. *Journal of Physical Chemistry B*, **2000**, 104, 8725-8734	3.4	150
26	Partitioning of Alkane and Alcohol Solutes between Water and (Dry or Wet) 1-Octanol. *Journal of the American Chemical Society*, **2000**, 122, 6464-6467	16.4	53
25	Development of Polarizable Water Force Fields for Phase Equilibrium Calculations. *Journal of Physical Chemistry B*, **2000**, 104, 2391-2401	3.4	200
24	Molecular Structure and Phase Diagram of the Binary Mixture of n-Heptane and Supercritical Ethane: A Gibbs Ensemble Monte Carlo Study. *Journal of Physical Chemistry B*, **2000**, 104, 2415-2423	3.4	19
23	Monte Carlo algorithms for simulating systems with adiabatic separation of electronic and nuclear degrees of freedom. *Theoretical Chemistry Accounts*, **1999**, 103, 87-104	1.9	29
22	Novel Configurational-Bias Monte Carlo Method for Branched Molecules. Transferable Potentials for Phase Equilibria. 2. United-Atom Description of Branched Alkanes. *Journal of Physical Chemistry B*, **1999**, 103, 4508-4517	3.4	707
21	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. *Journal of Physical Chemistry B*, **1999**, 103, 5370-5379	3.4	233
20	Exploring Multicomponent Phase Equilibria by Monte Carlo Simulations: Toward a Description of Gas-Liquid Chromatography. *ACS Symposium Series*, **1999**, 82-95	0.4	4
19	Calculating Gibbs free energies of transfer from Gibbs ensemble Monte Carlo simulations. *Theoretical Chemistry Accounts*, **1998**, 99, 347-350	1.9	57
18	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	3.4	81
17	Transferable Potentials for Phase Equilibria. 1. United-Atom Description of n-Alkanes. *Journal of Physical Chemistry B*, **1998**, 102, 2569-2577	3.4	2075
16	A novel Monte Carlo algorithm for polarizable force fields: Application to a fluctuating charge model for water. *Journal of Chemical Physics*, **1998**, 108, 3383-3385	3.9	44
15	Predicting Multicomponent Phase Equilibria and Free Energies of Transfer for Alkanes by Molecular Simulation. *Journal of the American Chemical Society*, **1997**, 119, 8921-8924	16.4	143
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