J Ilja Siepmann

List of Publications by Year
in descending order

190 papers	16,467 citations	23500 58 h-index	16127 124 g-index
195 all docs	195 docs citations	195 times ranked	9499 citing authors

#	Article	IF	Citations
1	Transferable Potentials for Phase Equilibria. 1. United-Atom Description ofn-Alkanes. Journal of Physical Chemistry B, 1998, 102, 2569-2577.	1.2	2,480
2	Vaporâ€“liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. AICHE Journal, 2001, 47, 1676-1682.	1.8	1,560
3	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.	1.2	795
4	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
5	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.	1.2	528
6	Computer simulations of vaporâ€“liquid phase equilibria ofnâ€alkanes. Journal of Chemical Physics, 1995, 102, 2126-2140.	1.2	467
7	Ultra-selective high-flux membranes from directly synthesized zeolite nanosheets. Nature, 2017, 543, 690-694.	13.7	446
8	Hydrogen Sulfide Capture: From Absorption in Polar Liquids to Oxide, Zeolite, and Metalâ€“Organic Framework Adsorbents and Membranes. Chemical Reviews, 2017, 117, 9755-9803.	23.0	434
9	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
10	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metalâ€“Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data, 2019, 64, 5985-5998.	1.0	372
11	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
12	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. Journal of Physical Chemistry B, 1999, 103, 5370-5379.	1.2	266
13	Computer Simulations of the Energetics and Siting of n-Alkanes in Zeolites. The Journal of Physical Chemistry, 1994, 98, 8442-8452.	2.9	223
14	Development of Polarizable Water Force Fields for Phase Equilibrium Calculations. Journal of Physical Chemistry B, 2000, 104, 2391-2401.	1.2	216
15	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.	1.2	212
16	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, 10790-10799.	1.2	185
17	A Novel Monte Carlo Algorithm for Simulating Strongly Associating Fluids:Â Applications to Water, Hydrogen Fluoride, and Acetic Acid. Journal of Physical Chemistry B, 2000, 104, 8725-8734.	1.2	165
18	Predicting Multicomponent Phase Equilibria and Free Energies of Transfer for Alkanes by Molecular Simulation. Journal of the American Chemical Society, 1997, 119, 8921-8924.	6.6	152

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19	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.	1.2	136
20	Microscopic Structure and Solvation in Dry and Wet Octanolâ€. Journal of Physical Chemistry B, 2006, 110, 3555-3563.	1.2	130
21	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	1.1	128
22	Retention Mechanism in Reversed-Phase Liquid Chromatography:â€‰ A Molecular Perspective. Analytical Chemistry, 2007, 79, 6551-6558.	3.2	125
23	TraPPE-zeo: Transferable Potentials for Phase Equilibria Force Field for All-Silica Zeolites. Journal of Physical Chemistry C, 2013, 117, 24375-24387.	1.5	124
24	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	1.4	123
25	Improving the Efficiency of the Aggregationâ^'Volumeâ^'Bias Monte Carlo Algorithm. Journal of Physical Chemistry B, 2001, 105, 11275-11282.	1.2	119
26	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.	2.2	116
27	Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium. Journal of Chemical Physics, 2001, 115, 10903-10913.	1.2	116
28	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
29	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
30	An online parameter and property database for the TraPPE force field. Molecular Simulation, 2014, 40, 101-105.	0.9	111
31	Transferable Potentials for Phase Equilibriaâ€“United Atom Description of Five- and Six-Membered Cyclic Alkanes and Ethers. Journal of Physical Chemistry B, 2012, 116, 11234-11246.	1.2	106
32	Monte Carlo simulations of mixed monolayers. Molecular Physics, 1992, 75, 255-259.	0.8	105
33	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.	0.5	101
34	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	1.0	99
35	Direct Gibbs Ensemble Monte Carlo Simulations for Solidâ^'Vapor Phase Equilibria:â€‰ Applications to Lennardâ^'Jonesium and Carbon Dioxide. Journal of Physical Chemistry B, 2001, 105, 9840-9848.	1.2	97
36	Transferable Potentials for Phase Equilibria. 10. Explicit-Hydrogen Description of Substituted Benzenes and Polycyclic Aromatic Compounds. Journal of Physical Chemistry B, 2013, 117, 273-288.	1.2	95

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37	Calculation of the shear viscosity of decane using a reversible multiple timeâ€step algorithm. Journal of Chemical Physics, 1995, 102, 3376-3380.	1.2	94
38	TraPPE-UA Force Field for Acrylates and Monte Carlo Simulations for Their Mixtures with Alkanes and Alcohols. Journal of Physical Chemistry B, 2009, 113, 6415-6425.	1.2	94
39	Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling. Nature Communications, 2015, 6, 5912.	5.8	94
40	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.	1.2	93
41	One-dimensional intergrowths in two-dimensional zeolite nanosheets and their effect on ultra-selective transport. Nature Materials, 2020, 19, 443-449.	13.3	91
42	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.	1.8	84
43	Ab Initio Derived Force Fields for Predicting CO₂ Adsorption and Accessibility of Metal Sites in the Metalâ€“Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). Journal of Physical Chemistry C, 2015, 119, 16058-16071.	1.5	84
44	Pressure Dependence of the Vaporâˆ’Liquidâˆ’Liquid Phase Behavior in Ternary Mixtures Consisting ofn-Alkanes,n-Perfluoroalkanes, and Carbon Dioxide. Journal of Physical Chemistry B, 2005, 109, 2911-2919.	1.2	81
45	Continuum-configurational-bias Monte Carlo simulations of long-chain alkanes. Molecular Physics, 1993, 80, 55-63.	0.8	78
46	Time-Dependent Properties of Liquid Water:â€‰ A Comparison of Carâˆ’Parrinello and Bornâˆ’Oppenheimer Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1274-1281.	2.3	77
47	Vaporâˆ’Liquid Interfacial Properties of Mutually Saturated Water/1-Butanol Solutions. Journal of the American Chemical Society, 2002, 124, 12232-12237.	6.6	76
48	Molecular-Level Comparison of Alkylsilane and Polar-Embedded Reversed-Phase Liquid Chromatography Systems. Analytical Chemistry, 2008, 80, 6214-6221.	3.2	75
49	Transferable Potentials for Phase Equilibriaâˆ’Coarse-Grain Description for Linear Alkanes. Journal of Physical Chemistry B, 2011, 115, 3452-3465.	1.2	73
50	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.	1.6	71
51	Monte Carlo investigations of hexadecane films on a metal substrate. Journal of Chemical Physics, 1995, 103, 3184-3195.	1.2	69
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	Size Effects on the Solvation of Anions at the Aqueous Liquidâˆ’Vapor Interface. Journal of Physical Chemistry C, 2008, 112, 210-218.	1.5	68
54	Prediction of viscosities and vaporâ€“liquid equilibria for five polyhydric alcohols by molecular simulation. Fluid Phase Equilibria, 2007, 260, 218-231.	1.4	67

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55	Simulating vaporâ€“liquid nucleation of n-alkanes. Journal of Chemical Physics, 2002, 116, 4317-4329.	1.2	65
56	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. Chemistry of Materials, 2017, 29, 6315-6328.	3.2	65
57	Calculating Gibbs free energies of transfer from Gibbs ensemble Monte Carlo simulations. Theoretical Chemistry Accounts, 1998, 99, 347-350.	0.5	63
58	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.	1.3	63
59	Development of the Transferable Potentials for Phase Equilibria Model for Hydrogen Sulfide. Journal of Physical Chemistry B, 2015, 119, 7041-7052.	1.2	59
60	Partitioning of Alkane and Alcohol Solutes between Water and (Dry or Wet) 1-Octanol. Journal of the American Chemical Society, 2000, 122, 6464-6467.	6.6	58
61	Decane under shear: A molecular dynamics study using reversible NVTâ€SLLOD and NPTâ€SLLOD algorithms. Journal of Chemical Physics, 1995, 103, 10192-10200.	1.2	57
62	Equilibrium and non-equilibrium simulation studies of fluid alkanes in bulk and at interfaces. Faraday Discussions, 1996, 104, 17.	1.6	57
63	Understanding Diffusion in Hierarchical Zeolites with House-of-Cards Nanosheets. ACS Nano, 2016, 10, 7612-7618.	7.3	56
64	Elucidating the Vibrational Spectra of Hydrogen-Bonded Aggregates in Solution:Â Electronic Structure Calculations with Implicit Solvent and First-Principles Molecular Dynamics Simulations with Explicit Solvent for 1-Hexanol inn-Hexane. Journal of the American Chemical Society, 2005, 127, 4722-4729.	6.6	54
65	Adsorption of glucose into zeolite beta from aqueous solution. AICHE Journal, 2013, 59, 3523-3529.	1.8	52
66	Influence of bonded-phase coverage in reversed-phase liquid chromatography via molecular simulation. Journal of Chromatography A, 2008, 1204, 11-19.	1.8	51
67	Deconstructing Hydrogen-Bond Networks in Confined Nanoporous Materials: Implications for Alcoholâ€“Water Separation. Journal of Physical Chemistry C, 2014, 118, 19723-19732.	1.5	50
68	Accurate and precise determination of critical properties from Gibbs ensemble Monte Carlo simulations. Journal of Chemical Physics, 2015, 143, 114113.	1.2	50
69	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.	1.2	49
70	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. Science Advances, 2021, 7, .	4.7	47
71	Pressure Dependence of the Hildebrand Solubility Parameter and the Internal Pressure:â€‰ Monte Carlo Simulations for External Pressures up to 300 MPa. Journal of Physical Chemistry C, 2007, 111, 15634-15641.	1.5	44
72	Accelerated Computational Analysis of Metalâ€“Organic Frameworks for Oxidation Catalysis. Journal of Physical Chemistry C, 2016, 120, 18707-18712.	1.5	44

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73	Renewable lubricants with tailored molecular architecture. Science Advances, 2019, 5, eaav5487.	4.7	44
74	Separation of Thiophene from Aliphatic Hydrocarbons Using Tetrahexylammonium-Based Deep Eutectic Solvents as Extracting Agents. Journal of Chemical & Engineering Data, 2017, 62, 2911-2919.	1.0	43
75	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. Angewandte Chemie - International Edition, 2016, 55, 5938-5942.	7.2	41
76	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. Molecular Simulation, 2013, 39, 1135-1142.	0.9	40
77	Effects of an Applied Electric Field on the Vaporâ^'Liquid Equilibria of Water, Methanol, and Dimethyl Ether. Journal of Physical Chemistry B, 2010, 114, 4261-4270.	1.2	38
78	Vaporâ€“Liquid Coexistence Curves for Methanol and Methane Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2011, 115, 11688-11692.	1.2	38
79	Deep neural network learning of complex binary sorption equilibria from molecular simulation data. Chemical Science, 2019, 10, 4377-4388.	3.7	38
80	Simulating the vapourâ€“liquid equilibria of large cyclic alkanes. Molecular Physics, 2005, 103, 99-104.	0.8	37
81	Conformation and Solvation Structure for an Isolatedn-Octadecane Chain in Water, Methanol, and Their Mixtures. Journal of Physical Chemistry B, 2006, 110, 10519-10525.	1.2	37
82	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, 12577-12584.	1.2	37
83	Monte Carlo Simulations Probing the Adsorptive Separation of Hydrogen Sulfide/Methane Mixtures Using All-Silica Zeolites. Langmuir, 2015, 31, 12268-12278.	1.6	37
84	Molecular Simulation of Concurrent Gasâ^'Liquid Interfacial Adsorption and Partitioning in Gasâ^'Liquid Chromatography. Analytical Chemistry, 2002, 74, 3518-3524.	3.2	34
85	Metalâ€“Organic Frameworks with Metalâ€“Catecholates for O₂/N₂ Separation. Journal of Physical Chemistry C, 2019, 123, 12935-12946.	1.5	33
86	Simulation Studies of Ultrathin Films of Linear and Branched Alkanes on a Metal Substrate. The Journal of Physical Chemistry, 1996, 100, 11960-11963.	2.9	32
87	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, 136-144.	2.3	32
88	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.	1.3	32
89	Retention mechanism for polycyclic aromatic hydrocarbons in reversed-phase liquid chromatography with monomeric stationary phases. Journal of Chromatography A, 2011, 1218, 9183-9193.	1.8	32
90	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.	1.4	31

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91	First principles Monte Carlo simulations of unary and binary adsorption: CO₂, N₂, and H₂O in Mg-MOF-74. Chemical Communications, 2018, 54, 10816-10819.	2.2	31
92	Assessing the Quality of Molecular Simulations for Vaporâ€“Liquid Equilibria: An Analysis of the TraPPE Database. Journal of Chemical & Engineering Data, 2020, 65, 1330-1344.	1.0	31
93	Vaporâ^'Liquid and Vaporâ^'Solid Phase Equilibria for United-Atom Benzene Models near Their Triple Points:â€‰ The Importance of Quadrupolar Interactions. Journal of Physical Chemistry B, 2005, 109, 5368-5374.	1.2	30
94	Development of the TraPPE-UA force field for ethylene oxide. Fluid Phase Equilibria, 2008, 274, 44-49.	1.4	30
95	Development of the trappe force field for ammonia. Collection of Czechoslovak Chemical Communications, 2010, 75, 577-591.	1.0	30
96	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.	4.1	30
97	Monte Carlo algorithms for simulating systems with adiabatic separation of electronic and nuclear degrees of freedom. Theoretical Chemistry Accounts, 1999, 103, 87-104.	0.5	29
98	Vaporâ€“liquid phase equilibria of triacontane isomers: Deviations from the principle of corresponding states. Fluid Phase Equilibria, 2002, 202, 307-324.	1.4	28
99	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO2. Journal of the American Chemical Society, 2005, 127, 12338-12342.	6.6	28
100	Partial Molar Volume and Solvation Structure of Naphthalene in Supercritical Carbon Dioxide:Â A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2005, 109, 19885-19892.	1.2	28
101	Molecular Simulation of Olefin Oligomer Blend Phase Behavior. Macromolecules, 2016, 49, 3975-3985.	2.2	28
102	Adsorptive Separation of 1-Butanol from Aqueous Solutions Using MFI- and FER-Type Zeolite Frameworks: A Monte Carlo Study. Langmuir, 2016, 32, 2093-2101.	1.6	28
103	Transferable potentials for phase equilibria. Improved unitedâ€atom description of ethane and ethylene. AICHE Journal, 2017, 63, 5098-5110.	1.8	28
104	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.	1.5	27
105	Bond Angle Distributions of Carbon Dioxide in the Gas, Supercritical, and Solid Phases. Journal of Physical Chemistry A, 2009, 113, 2053-2059.	1.1	26
106	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.	1.0	26
107	A Monte Carlo simulation study of the liquidâ€“liquid equilibria for binary dodecane/ethanol and ternary dodecane/ethanol/water mixtures. Fluid Phase Equilibria, 2016, 407, 269-279.	1.4	25
108	Computational Design of High-Ï‡ Block Oligomers for Accessing 1 nm Domains. ACS Nano, 2018, 12, 4351-4361.	7.3	25

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109	Structure and Phase Behavior of Mixed Self-Assembled Alkanethiolate Monolayers on Gold Nanoparticles: A Monte Carlo Study. Journal of Physical Chemistry B, 2016, 120, 1972-1978.	1.2	24
110	A Review of Biorefinery Separations for Bioproduct Production via Thermocatalytic Processing. Annual Review of Chemical and Biomolecular Engineering, 2017, 8, 115-137.	3.3	24
111	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.	1.6	24
112	Machine learning using host/guest energy histograms to predict adsorption in metalâ€“organic frameworks: Application to short alkanes and Xe/Kr mixtures. Journal of Chemical Physics, 2021, 155, 014701.	1.2	24
113	Structure of the Methanol Liquidâ^'Vapor Interface: A Comprehensive Particle-Based Simulation Study. Journal of Physical Chemistry C, 2008, 112, 15412-15418.	1.5	23
114	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.	2.3	23
115	Understanding the Unusual Adsorption Behavior in Hierarchical Zeolite Nanosheets. ChemPhysChem, 2014, 15, 2225-2229.	1.0	22
116	Mercury Capture from Petroleum Using Deep Eutectic Solvents. Industrial & Engineering Chemistry Research, 2018, 57, 9222-9230.	1.8	22
117	Liquidâ€“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.	1.2	21
118	Synthesis, Simulation, and Self-Assembly of a Model Amphiphile To Push the Limits of Block Polymer Nanopatterning. Nano Letters, 2019, 19, 4458-4462.	4.5	21
119	Determination of the Pressureâ^'Viscosity Coefficient of Decane by Molecular Simulation. The Journal of Physical Chemistry, 1996, 100, 16779-16781.	2.9	20
120	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.	1.2	20
121	Temperature Dependence of Transfer Properties:Â Importance of Heat Capacity Effects. Journal of Physical Chemistry B, 2003, 107, 10623-10627.	1.2	20
122	Understanding the Molecular Weight Dependence of Ï‡ and the Effect of Dispersity on Polymer Blend Phase Diagrams. Macromolecules, 2018, 51, 3774-3787.	2.2	20
123	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.	1.4	19
124	Bioethanol enrichment using zeolite membranes: Molecular modeling, conceptual process design and techno-economic analysis. Journal of Membrane Science, 2017, 540, 464-476.	4.1	18
125	Gibbs ensemble Monte Carlo simulations for the liquidâ€“liquid phase equilibria of dipropylene glycol dimethyl ether and water: A preliminary report. Fluid Phase Equilibria, 2011, 310, 11-18.	1.4	17
126	Using the k-d Tree Data Structure to Accelerate Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1556-1565.	2.3	17

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127	Cooperative Catalysis by Surface Lewis Acid/Silanol for Selective Fructose Etherification on Sn-SPP Zeolite. ACS Catalysis, 2018, 8, 9056-9065.	5.5	17
128	Molecular insights for the optimization of solventâ€based selective extraction of ethanol from fermentation broths. AICHE Journal, 2013, 59, 3065-3070.	1.8	16
129	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. ACS Central Science, 2016, 2, 409-415.	5.3	16
130	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
131	Computational screening of metalâ€“organic frameworks for biogas purification. Molecular Systems Design and Engineering, 2019, 4, 1125-1135.	1.7	15
132	Column selection for comprehensive two-dimensional liquid chromatography using the hydrophobic subtraction model. Journal of Chromatography A, 2019, 1589, 47-55.	1.8	15
133	Monte Carlo Simulations of an Isolated n-Octadecane Chain Solvated in Waterâ^'Acetonitrile Mixtures. Journal of Chemical Theory and Computation, 2007, 3, 350-357.	2.3	14
134	Understanding the solubility of triamino-trinitrobenzene in hydrous tetramethylammonium fluoride: a first principles molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2012, 14, 4884.	1.3	14
135	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. Fluid Phase Equilibria, 2014, 366, 146-151.	1.4	14
136	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.	1.8	14
137	Exploring the Formation of Multiple Layer Hydrates for a Complex Pharmaceutical Compound. Journal of Physical Chemistry B, 2009, 113, 5929-5937.	1.2	13
138	Partial molar properties from molecular simulation using multiple linear regression. Molecular Physics, 2019, 117, 3589-3602.	0.8	13
139	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. Fluid Phase Equilibria, 2020, 523, 112785.	1.4	13
140	Understanding the Reactive Adsorption of H₂S and CO₂ in Sodiumâ€Exchanged Zeolites. ChemPhysChem, 2018, 19, 512-518.	1.0	12
141	Vaporâ€and liquidâ€phase adsorption of alcohol and water in silicaliteâ€1 synthesized in fluoride media. AICHE Journal, 2020, 66, e16868.	1.8	12
142	Monte Carlo Methods for Simulating Phase Equilibria of Complex Fluids. Advances in Chemical Physics, 0, , 443-460.	0.3	12
143	C2 adsorption in zeolites: in silico screening and sensitivity to molecular models. Molecular Systems Design and Engineering, 2018, 3, 619-626.	1.7	11
144	First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites. Journal of Physical Chemistry C, 2021, 125, 6090-6098.	1.5	11

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145	Selective adsorption from dilute solutions: Gibbs ensemble Monte Carlo simulations. Fluid Phase Equilibria, 2013, 351, 1-6.	1.4	10
146	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. Angewandte Chemie, 2016, 128, 6042-6046.	1.6	9
147	ACS Virtual Issue on Multicomponent Systems: Absorption, Adsorption, and Diffusion. Journal of Chemical & Engineering Data, 2018, 63, 3651-3651.	1.0	9
148	From Order to Disorder: Computational Design of Triblock Amphiphiles with 1 nm Domains. Journal of the American Chemical Society, 2020, 142, 9352-9362.	6.6	9
149	Understanding the unique sorption of alkane-Î±, Ï‰-diols in silicalite-1. Journal of Chemical Physics, 2018, 149, 072331.	1.2	8
150	Using molecular simulations to probe pore structures and polymer partitioning in size exclusion chromatography. Journal of Chromatography A, 2018, 1573, 78-86.	1.8	8
151	Molecular Simulations Probing the Thermophysical Properties of Homogeneously Stretched and Bubbly Water Systems. Journal of Chemical & Engineering Data, 2019, 64, 3755-3771.	1.0	8
152	Simulation Studies of Retention in Isotropic or Oriented Liquidn-Octadecane. Journal of Physical Chemistry B, 2001, 105, 10961-10966.	1.2	7
153	An Introduction to the Monte Carlo Method for Particle Simulations. Advances in Chemical Physics, 2007, , 1-12.	0.3	7
154	Concentration effects on the selective extraction of ethanol from aqueous solution using silicalite-1 and decanol isomers. Fluid Phase Equilibria, 2014, 362, 118-124.	1.4	7
155	Prediction of Vaporâ€“Liquid Coexistence Properties and Critical Points of Polychlorinated Biphenyls from Monte Carlo Simulations with the TraPPEâ€“EH Force Field. Journal of Chemical & Engineering Data, 2014, 59, 3301-3306.	1.0	7
156	Editorial: Molecular Modeling and Simulation in JCED. Journal of Chemical & Engineering Data, 2016, 61, 1-2.	1.0	7
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