J Ilja Siepmann

List of Publications by Citations

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	Transferable Potentials for Phase Equilibria. 1. United-Atom Description of n-Alkanes. *Journal of Physical Chemistry B*, **1998**, 102, 2569-2577	3.4	2075
173	Vapor–liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. *AICHE Journal*, **2001**, 47, 1676-1682	3.6	1229
172	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
171	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
170	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
169	Computer simulations of vapor–liquid phase equilibria of n-alkanes. *Journal of Chemical Physics*, **1995**, 102, 2126-2140	3.9	423
168	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
167	Ultra-selective high-flux membranes from directly synthesized zeolite nanosheets. *Nature*, **2017**, 543, 690-694	50.4	310
166	Liquid Water from First Principles: Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309
165	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
164	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. *Journal of Physical Chemistry B*, **1999**, 103, 5370-5379	3.4	233
163	Computer Simulations of the Energetics and Siting of n-Alkanes in Zeolites. *The Journal of Physical Chemistry*, **1994**, 98, 8442-8452		203
162	Development of Polarizable Water Force Fields for Phase Equilibrium Calculations. *Journal of Physical Chemistry B*, **2000**, 104, 2391-2401	3.4	200
161	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
160	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
159	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
158	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

157	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
156	Simulating fluid-phase equilibria of water from first principles. *Journal of Physical Chemistry A*, **2006**, 110, 640-6	2.8	125
155	Microscopic structure and solvation in dry and wet octanol. *Journal of Physical Chemistry B*, **2006**, 110, 3555-63	3.4	124
154	Retention mechanism in reversed-phase liquid chromatography: a molecular perspective. *Analytical Chemistry*, **2007**, 79, 6551-8	7.8	117
153	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
152	Improving the Efficiency of the Aggregation□Volume□Bias Monte Carlo Algorithm. *Journal of Physical Chemistry B*, **2001**, 105, 11275-11282	3.4	109
151	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
150	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
149	Monte Carlo simulations of mixed monolayers. *Molecular Physics*, **1992**, 75, 255-259	1.7	101
148	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
147	Isobaric-isothermal monte carlo simulations from first principles: application to liquid water at ambient conditions. *ChemPhysChem*, **2005**, 6, 1894-901	3.2	93
146	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
145	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
144	Calculation of the shear viscosity of decane using a reversible multiple time-step algorithm. *Journal of Chemical Physics*, **1995**, 102, 3376-3380	3.9	83
143	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
142	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
141	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
140	Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling. *Nature Communications*, **2015**, 6, 5912	17.4	75

139	Supersaturated calcium carbonate solutions are classical. *Science Advances*, **2018**, 4, eaao6283	14.3	75
138	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
137	Molecular-level comparison of alkylsilane and polar-embedded reversed-phase liquid chromatography systems. *Analytical Chemistry*, **2008**, 80, 6214-21	7.8	74
136	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
135	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
134	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
133	Vapor-liquid interfacial properties of mutually saturated water/1-butanol solutions. *Journal of the American Chemical Society*, **2002**, 124, 12232-7	16.4	70
132	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
131	Continuum-configurational-bias Monte Carlo simulations of long-chain alkanes. *Molecular Physics*, **1993**, 80, 55-63	1.7	68
130	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
129	An online parameter and property database for the TraPPE force field. *Molecular Simulation*, **2014**, 40, 101-105	2	66
128	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
127	Transferable potentials for phase equilibria-coarse-grain description for linear alkanes. *Journal of Physical Chemistry B*, **2011**, 115, 3452-65	3.4	64
126	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
125	Monte Carlo investigations of hexadecane films on a metal substrate. *Journal of Chemical Physics*, **1995**, 103, 3184-3195	3.9	63
124	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
123	Identification Schemes for Metal□Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
122	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

121	Prediction of viscosities and vapor–liquid equilibria for five polyhydric alcohols by molecular simulation. *Fluid Phase Equilibria*, **2007**, 260, 218-231	2.5	58
120	Calculating Gibbs free energies of transfer from Gibbs ensemble Monte Carlo simulations. *Theoretical Chemistry Accounts*, **1998**, 99, 347-350	1.9	57
119	Simulating vapor–liquid nucleation of n-alkanes. *Journal of Chemical Physics*, **2002**, 116, 4317-4329	3.9	57
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117	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
116	Equilibrium and non-equilibrium simulation studies of fluid alkanes in bulk and at interfaces. *Faraday Discussions*, **1996**, 104, 17	3.6	51
115	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
114	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. *Chemistry of Materials*, **2017**, 29, 6315-6328	9.6	46
113	Adsorption of glucose into zeolite beta from aqueous solution. *AICHE Journal*, **2013**, 59, 3523-3529	3.6	46
112	Decane under shear: A molecular dynamics study using reversible NVT-SLLOD and NPT-SLLOD algorithms. *Journal of Chemical Physics*, **1995**, 103, 10192-10200	3.9	46
111	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
110	One-dimensional intergrowths in two-dimensional zeolite nanosheets and their effect on ultra-selective transport. *Nature Materials*, **2020**, 19, 443-449	27	43
109	Understanding Diffusion in Hierarchical Zeolites with House-of-Cards Nanosheets. *ACS Nano*, **2016**, 10, 7612-8	16.7	41
108	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
107	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
106	Accurate and precise determination of critical properties from Gibbs ensemble Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 143, 114113	3.9	38
105	Development of the Transferable Potentials for Phase Equilibria Model for Hydrogen Sulfide. *Journal of Physical Chemistry B*, **2015**, 119, 7041-52	3.4	37
104	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. *Molecular Simulation*, **2013**, 39, 1135-1142	2	36

103	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
102	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
101	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
100	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
99	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
98	Molecular simulation of concurrent gas-liquid interfacial adsorption and partitioning in gas-liquid chromatography. *Analytical Chemistry*, **2002**, 74, 3518-24	7.8	33
97	Accelerated Computational Analysis of Metal□Organic Frameworks for Oxidation Catalysis. *Journal of Physical Chemistry C*, **2016**, 120, 18707-18712	3.8	33
96	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. *Angewandte Chemie - International Edition*, **2016**, 55, 5938-42	16.4	32
95	Simulating the vapour□liquid equilibria of large cyclic alkanes. *Molecular Physics*, **2005**, 103, 99-104	1.7	31
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91	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
90	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
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87	Simulation Studies of Ultrathin Films of Linear and Branched Alkanes on a Metal Substrate. *The Journal of Physical Chemistry*, **1996**, 100, 11960-11963		27
86	Development of the TraPPE-UA force field for ethylene oxide. *Fluid Phase Equilibria*, **2008**, 274, 44-49	2.5	27

85	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
84	Vapor–liquid phase equilibria of triacontane isomers: Deviations from the principle of corresponding states. *Fluid Phase Equilibria*, **2002**, 202, 307-324	2.5	27
83	Deep neural network learning of complex binary sorption equilibria from molecular simulation data. *Chemical Science*, **2019**, 10, 4377-4388	9.4	26
82	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
81	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
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76	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
75	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
74	Transferable potentials for phase equilibria. Improved united-atom description of ethane and ethylene. *AICHE Journal*, **2017**, 63, 5098-5110	3.6	20
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71	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
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69	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
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64	Temperature Dependence of Transfer Properties: Importance of Heat Capacity Effects. *Journal of Physical Chemistry B*, **2003**, 107, 10623-10627	3.4	18
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62	Molecular Simulation of Olefin Oligomer Blend Phase Behavior. *Macromolecules*, **2016**, 49, 3975-3985	5.5	17
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60	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
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58	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
57	Mercury Capture from Petroleum Using Deep Eutectic Solvents. *Industrial & Engineering Chemistry Research*, **2018**, 57, 9222-9230	3.9	15
56	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
55	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. *ACS Central Science*, **2016**, 2, 409-15	16.8	14
54	Understanding the Molecular Weight Dependence of and the Effect of Dispersity on Polymer Blend Phase Diagrams. *Macromolecules*, **2018**, 51, 3774-3787	5.5	13
53	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. *Fluid Phase Equilibria*, **2014**, 366, 146-151	2.5	13
52	Molecular insights for the optimization of solvent-based selective extraction of ethanol from fermentation broths. *AICHE Journal*, **2013**, 59, 3065-3070	3.6	13
51	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
50	Column selection for comprehensive two-dimensional liquid chromatography using the hydrophobic subtraction model. *Journal of Chromatography A*, **2019**, 1589, 47-55	4.5	13

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46	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 Lorentz□Berthelot Combining Rules. *Journal of Chemical & Engineering Data*, **2018**, 63, 4256-4268	2.8	12
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44	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
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42	Computational screening of metal□organic frameworks for biogas purification. *Molecular Systems Design and Engineering*, **2019**, 4, 1125-1135	4.6	10
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40	Partial molar properties from molecular simulation using multiple linear regression. *Molecular Physics*, **2019**, 117, 3589-3602	1.7	9
39	Selective adsorption from dilute solutions: Gibbs ensemble Monte Carlo simulations. *Fluid Phase Equilibria*, **2013**, 351, 1-6	2.5	9
38	Identifying Optimal Zeolitic Sorbents for Sweetening of Highly Sour Natural Gas. *Angewandte Chemie*, **2016**, 128, 6042-6046	3.6	8
37	Understanding the Reactive Adsorption of H S and CO in Sodium-Exchanged Zeolites. *ChemPhysChem*, **2018**, 19, 512-518	3.2	8
36	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. *Science Advances*, **2021**, 7,	14.3	8
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34	C2 adsorption in zeolites: in silico screening and sensitivity to molecular models. *Molecular Systems Design and Engineering*, **2018**, 3, 619-626	4.6	7
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32	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

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30	Simulation Studies of Retention in Isotropic or Oriented Liquid n-Octadecane. *Journal of Physical Chemistry B*, **2001**, 105, 10961-10966	3.4	7
29	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
28	Monte carlo calculations for the mechanical relaxation of a self-assembled monolayer and for the structures of alkane/metal interfaces. *Tribology Letters*, **1995**, 1, 191	2.8	6
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21	A new equation of state for homo-polymers in dissipative particle dynamics. *Journal of Chemical Physics*, **2019**, 150, 124104	3.9	4
20	An Introduction to the Monte Carlo Method for Particle Simulations. *Advances in Chemical Physics*, **2007**, 1-12		4
19	Exploring Multicomponent Phase Equilibria by Monte Carlo Simulations: Toward a Description of Gas-Liquid Chromatography. *ACS Symposium Series*, **1999**, 82-95	0.4	4
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