Thijs J H Vlugt

List of Publications by Year
in descending order

289	14,771	18482 62	28297 105
papers	citations	h-index	g-index

296	296	296	11463
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Influence of UiOâ€66 Metalâ€“Organic Framework Structural Defects on Adsorption and Separation of Hexane Isomers. Chemistry - A European Journal, 2022, , .	3.3	2
2	Solubilities and Transport Properties of CO₂, Oxalic Acid, and Formic Acid in Mixed Solvents Composed of Deep Eutectic Solvents, Methanol, and Propylene Carbonate. Journal of Physical Chemistry B, 2022, 126, 3572-3584.	2.6	13
3	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics. Journal of Physical Chemistry C, 2022, 126, 8121-8133.	3.1	8
4	Negative Effects of Inorganic Salt Invasion on the Dissociation Kinetics of Silica-Confined Gas Hydrate via Thermal Stimulation. Energy & Fuels, 2022, 36, 6216-6228.	5.1	8
5	Surface Coverage as an Important Parameter for Predicting Selectivity Trends in Electrochemical CO₂ Reduction. Journal of Physical Chemistry C, 2022, 126, 11927-11936.	3.1	9
6	Adsorption of n-alkanes in ZIF-8: Influence of crystal size and framework dynamics. Microporous and Mesoporous Materials, 2021, 312, 110730.	4.4	11
7	Diffusivity of Î±-, Î²-, Î³-cyclodextrin and the inclusion complex of Î²-cyclodextrin: Ibuprofen in aqueous solutions; A molecular dynamics simulation study. Fluid Phase Equilibria, 2021, 528, 112842.	2.5	30
8	Gibbs Ensemble Monte Carlo for Reactive Force Fields to Determine the Vaporâ€“Liquid Equilibrium of CO₂ and H₂O. Journal of Chemical Theory and Computation, 2021, 17, 322-329.	5.3	6
9	Recent advances in the continuous fractional component Monte Carlo methodology. Molecular Simulation, 2021, 47, 804-823.	2.0	38
10	Finite-size effects of diffusion coefficients computed from molecular dynamics: a review of what we have learned so far. Molecular Simulation, 2021, 47, 831-845.	2.0	87
11	A multiscale modelling approach to elucidate the mechanism of the oxygen evolution reaction at the hematiteâ€“water interface. Faraday Discussions, 2021, 229, 89-107.	3.2	11
12	Thermal conductivity of aqueous solutions of reline, ethaline, and glyceline deep eutectic solvents; a molecular dynamics simulation study. Molecular Physics, 2021, 119, .	1.7	13
13	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. ACS Applied Materials & Interfaces, 2021, 13, 8383-8394.	8.0	7
14	Competitive Adsorption of Xylenes at Chemical Equilibrium in Zeolites. Journal of Physical Chemistry C, 2021, 125, 4155-4174.	3.1	11
15	Liquidâ€“Liquid Extraction of Formic Acid with 2-Methyltetrahydrofuran: Experiments, Process Modeling, and Economics. Industrial & Engineering Chemistry Research, 2021, 60, 5588-5599.	3.7	14
16	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. Journal of Chemical & Engineering Data, 2021, 66, 2071-2087.	1.9	8
17	Thermodynamic, transport, and structural properties of hydrophobic deep eutectic solvents composed of tetraalkylammonium chloride and decanoic acid. Journal of Chemical Physics, 2021, 154, 144502.	3.0	16
18	How sensitive are physical properties of choline chlorideâ€“urea mixtures to composition changes: Molecular dynamics simulations and Kirkwoodâ€“Buff theory. Journal of Chemical Physics, 2021, 154, 184502.	3.0	24

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19	New Features of the Open Source Monte Carlo Software Brick-CFCMC: Thermodynamic Integration and Hybrid Trial Moves. Journal of Chemical Information and Modeling, 2021, 61, 3752-3757.	5.4	14
20	Reversible Hydrogen Storage in Metal-Decorated Honeycomb Borophene Oxide. ACS Applied Materials & Interfaces, 2021, 13, 43233-43240.	8.0	40
21	Vapor pressures and vapor phase compositions of choline chloride urea and choline chloride ethylene glycol deep eutectic solvents from molecular simulation. Journal of Chemical Physics, 2021, 155, 114504.	3.0	16
22	Recovery of rare earths from glass polishing waste for the production of aluminium-rare earth alloys. Resources, Conservation and Recycling, 2021, 174, 105766.	10.8	12
23	Solubility of Carbon Dioxide, Hydrogen Sulfide, Methane, and Nitrogen in Monoethylene Glycol; Experiments and Molecular Simulation. Journal of Chemical & Engineering Data, 2021, 66, 524-534.	1.9	7
24	Interfacial Properties of Hydrophobic Deep Eutectic Solvents with Water. Journal of Physical Chemistry B, 2021, 125, 12303-12314.	2.6	12
25	Reactive Grand-Canonical Monte Carlo Simulations for Modeling Hydration of MgCl2. ACS Omega, 2021, 6, 32475-32484.	3.5	1
26	Electroreduction of CO₂/CO to C₂ Products: Process Modeling, Downstream Separation, System Integration, and Economic Analysis. Industrial & Engineering Chemistry Research, 2021, 60, 17862-17880.	3.7	35
27	The adsorption mechanisms of organic micropollutants on high-silica zeolites causing S-shaped adsorption isotherms: An experimental and Monte Carlo simulation study. Chemical Engineering Journal, 2020, 389, 123968.	12.7	49
28	On the validity of the Stokesâ€“Einstein relation for various water force fields. Molecular Physics, 2020, 118, e1702729.	1.7	22
29	Effects of Framework Flexibility on the Adsorption and Diffusion of Aromatics in MFI-Type Zeolites. Journal of Physical Chemistry C, 2020, 124, 24488-24499.	3.1	16
30	Computation of gas solubilities in choline chloride urea and choline chloride ethylene glycol deep eutectic solvents using Monte Carlo simulations. Journal of Molecular Liquids, 2020, 316, 113729.	4.9	31
31	Artificial intelligence and thermodynamics help solving arson cases. Scientific Reports, 2020, 10, 20502.	3.3	3
32	Influence of Nanoscale Intimacy and Zeolite Micropore Size on the Performance of Bifunctional Catalysts for<i>n</i>-Heptane Hydroisomerization. ACS Catalysis, 2020, 10, 14245-14257.	11.2	68
33	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. Fluid Phase Equilibria, 2020, 523, 112785.	2.5	13
34	Isobaric Vaporâ€“Liquid Equilibrium Data of Binary Systems Containing 2-Ethoxyethanol, 2-Ethoxyethyl Acetate, and Toluene. Journal of Chemical & Engineering Data, 2020, 65, 4798-4804.	1.9	4
35	Adsorption of Aromatics in MFI-Type Zeolites: Experiments and Framework Flexibility in Monte Carlo Simulations. Journal of Physical Chemistry C, 2020, 124, 21782-21797.	3.1	9
36	Direct Water Injection in Catholyteâ€Free Zeroâ€Gap Carbon Dioxide Electrolyzers. ChemElectroChem, 2020, 7, 3839-3843.	3.4	51

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37	Mechanical Response of Nanocrystalline Ice-Contained Methane Hydrates: Key Role of Water Ice. ACS Applied Materials & Interfaces, 2020, 12, 14016-14028.	8.0	23
38	Gibbs Ensemble Monte Carlo Simulation of Fluids in Confinement: Relation between the Differential and Integral Pressures. Nanomaterials, 2020, 10, 293.	4.1	15
39	Inclusion Complexation of Organic Micropollutants with Î²-Cyclodextrin. Journal of Physical Chemistry B, 2020, 124, 1218-1228.	2.6	20
40	Multiple Free Energy Calculations from Single State Point Continuous Fractional Component Monte Carlo Simulation Using Umbrella Sampling. Journal of Chemical Theory and Computation, 2020, 16, 1757-1767.	5.3	9
41	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. Journal of Chemical Information and Modeling, 2020, 60, 2678-2682.	5.4	32
42	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. Nanomaterials, 2020, 10, 771.	4.1	21
43	Generalized Form for Finite-Size Corrections in Mutual Diffusion Coefficients of Multicomponent Mixtures Obtained from Equilibrium Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2020, 16, 3799-3806.	5.3	45
44	Two-Phase Equilibrium Conditions in Nanopores. Nanomaterials, 2020, 10, 608.	4.1	17
45	Rayleigh-Brillouin light scattering spectra of CO2 from molecular dynamics. Journal of Chemical Physics, 2019, 151, 064201.	3.0	3
46	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. Advanced Theory and Simulations, 2019, 2, 1900135.	2.8	41
47	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. Journal of Chemical & Engineering Data, 2019, 64, 4103-4115.	1.9	43
48	The dynamic behavior of gas hydrate dissociation by heating in tight sandy reservoirs: A molecular dynamics simulation study. Fuel, 2019, 258, 116106.	6.4	35
49	Improving the accuracy of computing chemical potentials in CFCMC simulations. Molecular Physics, 2019, 117, 3493-3508.	1.7	15
50	Computing solubility parameters of deep eutectic solvents from Molecular Dynamics simulations. Fluid Phase Equilibria, 2019, 497, 10-18.	2.5	51
51	In-situ experimental investigation on the growth of aerosols along the absorption column in post combustion carbon capture. International Journal of Greenhouse Gas Control, 2019, 85, 86-99.	4.6	13
52	Enhancing the Water Capacity in Zr-Based Metalâ€“Organic Framework for Heat Pump and Atmospheric Water Generator Applications. ACS Applied Nano Materials, 2019, 2, 3050-3059.	5.0	18
53	Characterization and Feasibility Studies on Complete Recovery of Rare Earths from Glass Polishing Waste. Metals, 2019, 9, 278.	2.3	5
54	Highlights of (bio-)chemical tools and visualization software for computational science. Current Opinion in Chemical Engineering, 2019, 23, 1-13.	7.8	7

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55	Modeling the Electrochemical Conversion of Carbon Dioxide to Formic Acid or Formate at Elevated Pressures. Journal of the Electrochemical Society, 2019, 166, E77-E86.	2.9	38
56	Solving vapor-liquid flash problems using artificial neural networks. Fluid Phase Equilibria, 2019, 490, 39-47.	2.5	28
57	OCTP: A Tool for On-the-Fly Calculation of Transport Properties of Fluids with the Order-n Algorithm in LAMMPS. Journal of Chemical Information and Modeling, 2019, 59, 1290-1294.	5.4	67
58	High-Pressure Electrochemical Reduction of CO₂ to Formic Acid/Formate: Effect of pH on the Downstream Separation Process and Economics. Industrial & Engineering Chemistry Research, 2019, 58, 22718-22740.	3.7	84
59	Structural, Thermodynamic, and Transport Properties of Aqueous Reline and Ethaline Solutions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2019, 123, 11014-11025.	2.6	70
60	Effect of truncating electrostatic interactions on predicting thermodynamic properties of waterâ€“methanol systems. Molecular Simulation, 2019, 45, 336-350.	2.0	17
61	High Pressure Electrochemical Reduction of CO₂ to Formic Acid/Formate: A Comparison between Bipolar Membranes and Cation Exchange Membranes. Industrial & Engineering Chemistry Research, 2019, 58, 1834-1847.	3.7	116
62	Prediction of adsorption isotherms from breakthrough curves. Microporous and Mesoporous Materials, 2019, 277, 237-244.	4.4	36
63	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. AICHE Journal, 2019, 65, 792-803.	3.6	11
64	Molecular simulation of the vapor-liquid equilibria of xylene mixtures: Force field performance, and Wolf vs. Ewald for electrostatic interactions. Fluid Phase Equilibria, 2019, 485, 239-247.	2.5	6
65	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	8.0	25
66	Kirkwoodâ€“Buff integrals of finite systems: shape effects. Molecular Physics, 2018, 116, 1573-1580.	1.7	19
67	iRASPA: GPU-accelerated visualization software for materials scientists. Molecular Simulation, 2018, 44, 653-676.	2.0	112
68	Molecular Simulation of Vaporâ€“Liquid Equilibria Using the Wolf Method for Electrostatic Interactions. Journal of Chemical & Engineering Data, 2018, 63, 1096-1102.	1.9	18
69	Finite-size effects of Kirkwoodâ€“Buff integrals from molecular simulations. Molecular Simulation, 2018, 44, 599-612.	2.0	47
70	Adsorption equilibrium of nitrogen dioxide in porous materials. Physical Chemistry Chemical Physics, 2018, 20, 4189-4199.	2.8	20
71	Development of efficient formulation for the removal of iron sulphide scale in sour production wells. Canadian Journal of Chemical Engineering, 2018, 96, 2526-2533.	1.7	31
72	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 2667-2677.	5.3	121

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73	Absorption Refrigeration Cycles with Ammoniaâ€“Ionic Liquid Working Pairs Studied by Molecular Simulation. Industrial & Engineering Chemistry Research, 2018, 57, 5442-5452.	3.7	39
74	CO2 stripping from ionic liquid at elevated pressures in gas-liquid membrane contactor. International Journal of Greenhouse Gas Control, 2018, 71, 293-302.	4.6	31
75	Gibbs ensemble Monte Carlo simulations of multicomponent natural gas mixtures. Molecular Simulation, 2018, 44, 377-383.	2.0	11
76	Chemical potentials of water, methanol, carbon dioxide and hydrogen sulphide at low temperatures using continuous fractional component Gibbs ensemble Monte Carlo. Molecular Simulation, 2018, 44, 405-414.	2.0	17
77	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. Fluid Phase Equilibria, 2018, 458, 1-8.	2.5	7
78	Recovery of Cerium from Glass Polishing Waste: A Critical Review. Metals, 2018, 8, 801.	2.3	39
79	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. Physical Chemistry Chemical Physics, 2018, 20, 28848-28859.	2.8	18
80	Theoretical study on cation codoped SrTiO₃ photocatalysts for water splitting. Journal of Materials Chemistry A, 2018, 6, 24342-24349.	10.3	20
81	Optimizing Nonbonded Interactions of the OPLS Force Field for Aqueous Solutions of Carbohydrates: How to Capture Both Thermodynamics and Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 6690-6700.	5.3	20
82	Mechanical properties of bi- and poly-crystalline ice. AIP Advances, 2018, 8, .	1.3	14
83	Prediction of Composition-Dependent Self-Diffusion Coefficients in Binary Liquid Mixtures: The Missing Link for Darken-Based Models. Industrial & Engineering Chemistry Research, 2018, 57, 14784-14794.	3.7	26
84	Polarizable Force Field for CO₂ in M-MOF-74 Derived from Quantum Mechanics. Journal of Physical Chemistry C, 2018, 122, 24488-24498.	3.1	29
85	Shear Viscosity Computed from the Finite-Size Effects of Self-Diffusivity in Equilibrium Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 5959-5968.	5.3	50
86	Ammonia/ionic liquid based double-effect vapor absorption refrigeration cycles driven by waste heat for cooling in fishing vessels. Energy Conversion and Management, 2018, 174, 824-843.	9.2	40
87	Size and shape dependence of finite-volume Kirkwood-Buff integrals. Physical Review E, 2018, 97, 051301.	2.1	40
88	Identifying Zeolite Topologies for Storage and Release of Hydrogen. Journal of Physical Chemistry C, 2018, 122, 12485-12493.	3.1	20
89	In Silico Screening of Metalâ€“Organic Frameworks for Adsorption-Driven Heat Pumps and Chillers. ACS Applied Materials & Interfaces, 2018, 10, 27074-27087.	8.0	32
90	Combined Steam Reforming of Methane and Formic Acid To Produce Syngas with an Adjustable H₂:CO Ratio. Industrial & Engineering Chemistry Research, 2018, 57, 10663-10674.	3.7	37

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91	Computation of partial molar properties using continuous fractional component Monte Carlo. Molecular Physics, 2018, 116, 3331-3344.	1.7	28
92	Polarizable Force Fields for CO₂ and CH₄ Adsorption in M-MOF-74. Journal of Physical Chemistry C, 2017, 121, 4659-4673.	3.1	87
93	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)â€MOFâ€74. ChemistrySelect, 2017, 2, 665-672.	1.5	16
94	Behavior of the Enthalpy of Adsorption in Nanoporous Materials Close to Saturation Conditions. Journal of Chemical Theory and Computation, 2017, 13, 3326-3339.	5.3	41
95	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. Journal of Physical Chemistry C, 2017, 121, 11273-11280.	3.1	60
96	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. Molecular Simulation, 2017, 43, 189-195.	2.0	20
97	Modeling Thermodynamic Properties of Propane or Tetrahydrofuran Mixed with Carbon Dioxide or Methane in Structure-II Clathrate Hydrates. Journal of Physical Chemistry C, 2017, 121, 23911-23925.	3.1	15
98	Product shape selectivity of MFI-type, MEL-type, and BEA-type zeolites in the catalytic hydroconversion of heptane. Journal of Catalysis, 2017, 353, 54-62.	6.2	44
99	Efficient Application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble. Journal of Chemical Theory and Computation, 2017, 13, 4452-4466.	5.3	37
100	Thermodynamic and Transport Properties of Crown-Ethers: Force Field Development and Molecular Simulations. Journal of Physical Chemistry B, 2017, 121, 8367-8376.	2.6	15
101	Hydride Transfer versus Deprotonation Kinetics in the Isobutaneâ€“Propene Alkylation Reaction: A Computational Study. ACS Catalysis, 2017, 7, 8613-8627.	11.2	49
102	Phase Diagram of Methane and Carbon Dioxide Hydrates Computed by Monte Carlo Simulations. Journal of Physical Chemistry B, 2017, 121, 7336-7350.	2.6	35
103	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. Fluid Phase Equilibria, 2017, 433, 50-55.	2.5	29
104	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. Nature Communications, 2016, 7, 11503.	12.8	48
105	In-Line Monitoring of the CO₂, MDEA, and PZ Concentrations in the Liquid Phase during High Pressure CO₂ Absorption. Industrial & Engineering Chemistry Research, 2016, 55, 3804-3812.	3.7	4
106	Investigating polarization effects of CO2 adsorption in MgMOF-74. Journal of Computational Science, 2016, 15, 86-94.	2.9	25
107	Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC. Journal of Physical Chemistry C, 2016, 120, 9148-9159.	3.1	18
108	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. Langmuir, 2016, 32, 12664-12675.	3.5	33

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109	Computing equation of state parameters of gases from Monte Carlo simulations. Fluid Phase Equilibria, 2016, 428, 174-181.	2.5	9
110	Computation of the Heat and Entropy of Adsorption in Proximity of Inflection Points. Journal of Physical Chemistry C, 2016, 120, 1727-1738.	3.1	21
111	Liquid-crystal phase equilibria of Lennard-Jones chains. Molecular Physics, 2016, 114, 895-908.	1.7	8
112	Comparison of Raman, NIR, and ATR FTIR spectroscopy as analytical tools for in-line monitoring of CO 2 concentration in an amine gas treating process. International Journal of Greenhouse Gas Control, 2016, 47, 17-24.	4.6	19
113	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. Journal of Chemical Theory and Computation, 2016, 12, 1481-1490.	5.3	47
114	Computing bubble-points of CO2/CH4 gas mixtures in ionic liquids from Monte Carlo simulations. Fluid Phase Equilibria, 2016, 418, 100-107.	2.5	9
115	Solubilities of CO2, CH4, C2H6, and SO2 in ionic liquids and Selexol from Monte Carlo simulations. Journal of Computational Science, 2016, 15, 74-80.	2.9	31
116	Binary and ternary mixtures of liquid crystals with CO₂. AICHE Journal, 2015, 61, 2977-2984.	3.6	7
117	Heat-induced transformation of CdSeâ€“CdSâ€“ZnS coreâ€“multishell quantum dots by Zn diffusion into inner layers. Chemical Communications, 2015, 51, 3320-3323.	4.1	20
118	Simulating the Reactions of CO2 in Aqueous Monoethanolamine Solution by Reaction Ensemble Monte Carlo Using the Continuous Fractional Component Method. Journal of Chemical Theory and Computation, 2015, 11, 2661-2669.	5.3	30
119	Study of glassy polymers fractional accessible volume (FAV) by extended method of hydrostatic weighing: Effect of porous structure on liquid transport. Reactive and Functional Polymers, 2015, 86, 269-281.	4.1	58
120	Manufacture of dense CAU-10-H coatings for application in adsorption driven heat pumps: optimization and characterization. CrystEngComm, 2015, 17, 5911-5920.	2.6	44
121	COSMO-3D: Incorporating Three-Dimensional Contact Information into the COSMO-SAC Model. Industrial & Engineering Chemistry Research, 2015, 54, 2214-2226.	3.7	5
122	Simulation of Pore Width and Pore Charge Effects on Selectivities of CO2 vs. H2 from a Syngas-like Mixture in Carbon Mesopores. Energy Procedia, 2015, 64, 150-159.	1.8	9
123	Understanding aerosol based emissions in a Post Combustion CO2 Capture process: Parameter testing and mechanisms. International Journal of Greenhouse Gas Control, 2015, 34, 63-74.	4.6	52
124	Phase Behavior of Binary Mixtures of a Liquid Crystal and Methane. Journal of Chemical & Engineering Data, 2015, 60, 2167-2171.	1.9	4
125	Diffusion of Heat and Mass in a Chemically Reacting Mixture away from Equilibrium. Journal of Physical Chemistry C, 2015, 119, 12838-12847.	3.1	6
126	Real-Time Process Monitoring of CO₂ Capture by Aqueous AMP-PZ Using Chemometrics: Pilot Plant Demonstration. Industrial & Engineering Chemistry Research, 2015, 54, 5769-5776.	3.7	21

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127	Online Corrosion Monitoring in a Postcombustion CO₂ Capture Pilot Plant and its Relation to Solvent Degradation and Ammonia Emissions. Industrial & Engineering Chemistry Research, 2015, 54, 5336-5344.	3.7	15
128	Economic assessment of novel amine based CO2 capture technologies integrated in power plants based on European Benchmarking Task Force methodology. Applied Energy, 2015, 138, 546-558.	10.1	94
129	Adsorption-Driven Heat Pumps: The Potential of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 12205-12250.	47.7	410
130	Isotropic-nematic phase equilibria of hard-sphere chain fluidsâ€”Pure components and binary mixtures. Journal of Chemical Physics, 2015, 142, 064903.	3.0	8
131	On the vapor-liquid equilibrium of attractive chain fluids with variable degree of molecular flexibility. Journal of Chemical Physics, 2015, 142, 224504.	3.0	5
132	Solubility of Natural Gas Species in Ionic Liquids and Commercial Solvents: Experiments and Monte Carlo Simulations. Journal of Chemical & Engineering Data, 2015, 60, 3039-3045.	1.9	26
133	An analytical equation of state for describing isotropic-nematic phase equilibria of Lennard-Jones chain fluids with variable degree of molecular flexibility. Journal of Chemical Physics, 2015, 142, 244903.	3.0	11
134	Mechanical instability of monocrystalline and polycrystalline methane hydrates. Nature Communications, 2015, 6, 8743.	12.8	93
135	Metalâ€“Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. Langmuir, 2015, 31, 12783-12796.	3.5	123
136	Crystals for sustainability â€“ structuring Al-based MOFs for the allocation of heat and cold. CrystEngComm, 2015, 17, 281-285.	2.6	35
137	Compressibility, thermal expansion coefficient and heat capacity of CH₄ and CO₂ hydrate mixtures using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2015, 17, 2869-2883.	2.8	82
138	Crystal structure, stability, and electronic properties of hydrated metal sulfates MSO4(H2O)n (M=Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 77-86.	3.8	13
139	Evaluating adsorbed-phase activity coefficient models using a 2D-lattice model. Molecular Simulation, 2015, 41, 1234-1244.	2.0	2
140	Chapter 5. Diffusion in Liquids: Experiments, Molecular Dynamics, and Engineering Models. , 2015, , 78-104.		7
141	Predicting Aerosol Based Emissions in a Post Combustion CO2 Capture Process Using an Aspen Plus Model. Energy Procedia, 2014, 63, 911-925.	1.8	19
142	An equation of state for the isotropic phase of linear, partially flexible and fully flexible tangent hard-sphere chain fluids. Molecular Physics, 2014, 112, 919-928.	1.7	12
143	Exploring new methods and materials for enantioselective separations and catalysis. Molecular Simulation, 2014, 40, 585-598.	2.0	21
144	Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics: A systematic study of several common force fields. Journal of Chemical Physics, 2014, 141, 134504.	3.0	21

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145	Partial molar enthalpies and reaction enthalpies from equilibrium molecular dynamics simulation. Journal of Chemical Physics, 2014, 141, 144501.	3.0	20
146	Adsorptive characterization of porous solids: Error analysis guides the way. Microporous and Mesoporous Materials, 2014, 200, 199-215.	4.4	134
147	The isotropic-nematic and nematic-nematic phase transition of binary mixtures of tangent hard-sphere chain fluids: An analytical equation of state. Journal of Chemical Physics, 2014, 140, 034504.	3.0	5
148	Probing Lipid Coating Dynamics of Quantum Dot Core Micelles via FÃ¶rster Resonance Energy Transfer. Small, 2014, 10, 1163-1170.	10.0	10
149	Coreâ€“shell reconfiguration through thermal annealing in Fe_xO/CoFe₂O₄ordered 2D nanocrystal arrays. Nanotechnology, 2014, 25, 055601.	2.6	9
150	Bridging scales with thermodynamics: from nano to macro. Advances in Natural Sciences: Nanoscience and Nanotechnology, 2014, 5, 023002.	1.5	15
151	A transferable force field for CdS-CdSe-PbS-PbSe solid systems. Journal of Chemical Physics, 2014, 141, 244503.	3.0	19
152	Solubility of CO2/CH4 gas mixtures in ionic liquids. Fluid Phase Equilibria, 2014, 375, 134-142.	2.5	34
153	CO₂ Solubility in Biodegradable Hydroxylammonium-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 702-708.	1.9	15
154	New Ab Initio Based Pair Potential for Accurate Simulation of Phase Transitions in ZnO. Journal of Physical Chemistry C, 2014, 118, 11050-11061.	3.1	45
155	Atomic Resolution Monitoring of Cation Exchange in CdSe-PbSe Heteronanocrystals during Epitaxial Solidâ€“Solidâ€“Vapor Growth. Nano Letters, 2014, 14, 3661-3667.	9.1	48
156	Validation of the CO₂/N₂O Analogy Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2014, 53, 18081-18090.	3.7	28
157	Acid Wash Scrubbing as a Countermeasure for Ammonia Emissions from a Postcombustion CO₂ Capture Plant. Industrial & Engineering Chemistry Research, 2014, 53, 13195-13204.	3.7	37
158	Solubility of the Precombustion Gases CO₂, CH₄, CO, H₂, N₂, and H₂S in the Ionic Liquid [bmim][Tf₂N] from Monte Carlo Simulations. Journal of Physical Chemistry C, 2014, 118, 23599-23604.	3.1	67
159	Field study of a Brownian Demister Unit to reduce aerosol based emission from a Post Combustion CO 2 Capture plant. International Journal of Greenhouse Gas Control, 2014, 28, 57-64.	4.6	47
160	Phase Behavior of Liquid Crystal + CO₂ Mixtures. Journal of Chemical & Engineering Data, 2014, 59, 1667-1672.	1.9	8
161	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	4.1	52
162	Analysis of Process Configurations for CO₂ Capture by Precipitating Amino Acid Solvents. Industrial & Engineering Chemistry Research, 2014, 53, 2348-2361.	3.7	39

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163	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
164	Solubility of CO₂ and CH₄ in Ionic Liquids: Ideal CO₂/CH₄ Selectivity. Industrial & Engineering Chemistry Research, 2014, 53, 15427-15435.	3.7	109
165	Thermodynamic assessment of amine based CO2 capture technologies in power plants based on European Benchmarking Task Force methodology. Fuel, 2014, 129, 318-329.	6.4	111
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