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	State-of-the-Art of CO₂ Capture with Ionic Liquids. Industrial & Engineering Chemistry Research, 2012, 51, 8149-8177.	3.7	881
2	Quantum cutting by cooperative energy transfer inYbxY1â^'xPO4:Tb3+. Physical Review B, 2005, 71, .	3.2	537
3	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. Journal of Physical Chemistry B, 1999, 103, 1102-1118.	2.6	472
4	Adsorption-Driven Heat Pumps: The Potential of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 12205-12250.	47.7	410
5	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	2.6	314
6	Understanding the Role of Sodium during Adsorption:Â A Force Field for Alkanes in Sodium-Exchanged Faujasites. Journal of the American Chemical Society, 2004, 126, 11377-11386.	13.7	255
7	Improving the efficiency of the configurational-bias Monte Carlo algorithm. Molecular Physics, 1998, 94, 727-733.	1.7	212
8	Computing the Heat of Adsorption using Molecular Simulations: The Effect of Strong Coulombic Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1107-1118.	5.3	202
9	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. Journal of Physical Chemistry C, 2009, 113, 8814-8820.	3.1	199
10	Influence of Framework Flexibility on the Adsorption Properties of Hydrocarbons in the Zeolite Silicalite. Journal of Physical Chemistry B, 2002, 106, 12757-12763.	2.6	191
11	Downconversion for solar cells in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YF</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>Yb</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msup></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>Tm</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msup></mml:mrow></mml:math>. Physical Review B, 2010, 81, .	3.2	191
12	Force Network Ensemble: A New Approach to Static Granular Matter. Physical Review Letters, 2004, 92, 054302.	7.8	183
13	Understanding Water Adsorption in Cuâ^'BTC Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 15934-15939.	3.1	178
14	Molecular Simulations of Interacting Nanocrystals. Nano Letters, 2008, 8, 2930-2934.	9.1	165
15	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. Journal of the American Chemical Society, 1998, 120, 5599-5600.	13.7	163
16	Kirkwoodâ€“Buff Integrals for Finite Volumes. Journal of Physical Chemistry Letters, 2013, 4, 235-238.	4.6	163
17	Mechanical properties of clathrate hydrates: status and perspectives. Energy and Environmental Science, 2012, 5, 6779.	30.8	161
18	Force Field Parametrization through Fitting on Inflection Points in Isotherms. Physical Review Letters, 2004, 93, 088302.	7.8	144

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19	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. Journal of Chemical Physics, 2005, 122, 224712.	3.0	142
20	Adsorptive characterization of porous solids: Error analysis guides the way. Microporous and Mesoporous Materials, 2014, 200, 199-215.	4.4	134
21	The Shape Selectivity of Paraffin Hydroconversion on TON-, MTT-, and AEL-Type Sieves. Journal of Catalysis, 1999, 188, 403-412.	6.2	132
22	Adsorption and Binding of Ligands to CdSe Nanocrystals. Journal of Physical Chemistry C, 2009, 113, 12690-12698.	3.1	127
23	Metalâ€“Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. Langmuir, 2015, 31, 12783-12796.	3.5	123
24	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 2667-2677.	5.3	121
25	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. Journal of Physical Chemistry A, 1998, 102, 7727-7730.	2.5	118
26			

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37	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
38	Mechanical instability of monocrystalline and polycrystalline methane hydrates. Nature Communications, 2015, 6, 8743.	12.8	93
39	Molecular simulation of adsorption of short linear alkanes and their mixtures in silicalite. AICHE Journal, 1998, 44, 1756-1764.	3.6	90
40	Shape Selectivity in Hydrocarbon Conversion. Angewandte Chemie - International Edition, 2001, 40, 736-739.	13.8	88
41	Investigation of aerosol based emission of MEA due to sulphuric acid aerosol and soot in a Post Combustion CO2 Capture process. International Journal of Greenhouse Gas Control, 2013, 19, 138-144.	4.6	88
42	Polarizable Force Fields for CO₂ and CH₄ Adsorption in M-MOF-74. Journal of Physical Chemistry C, 2017, 121, 4659-4673.	3.1	87
43	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
44	Predictive Darken Equation for Maxwell-Stefan Diffusivities in Multicomponent Mixtures. Industrial & Engineering Chemistry Research, 2011, 50, 10350-10358.	3.7	84
45	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
46	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
47	Understanding interactions between capped nanocrystals: Three-body and chain packing effects. Journal of Chemical Physics, 2009, 131, 124705.	3.0	81
48	Morphological Transformations and Fusion of PbSe Nanocrystals Studied Using Atomistic Simulations. Nano Letters, 2010, 10, 3966-3971.	9.1	79
49	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2012, 51, 10247-10258.	3.7	79
50	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2013, 117, 7613-7622.	3.1	79
51	Simulation of Alkane Adsorption in the Aluminophosphate Molecular Sieve AlPO4â^'5. Journal of Physical Chemistry B, 1998, 102, 7183-7189.	2.6	77
52	Differences in Cross-Link Chemistry between Rigid and Flexible Dithiol Molecules Revealed by Optical Studies of CdTe Quantum Dots. Journal of Physical Chemistry C, 2007, 111, 11208-11215.	3.1	77
53	Entropy Maximization in the Force Network Ensemble for Granular Solids. Physical Review Letters, 2008, 100, 238001.	7.8	72
54	Thermodynamics of a small system in a Î¼T reservoir. Chemical Physics Letters, 2011, 504, 199-201.	2.6	71

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55	Conceptual Design of a Novel CO₂ Capture Process Based on Precipitating Amino Acid Solvents. Industrial & Engineering Chemistry Research, 2013, 52, 12223-12235.	3.7	71
56	Dual release of proteins from porous polymeric scaffolds. Journal of Controlled Release, 2006, 111, 95-106.	9.9	70
57	Fick Diffusion Coefficients of Liquid Mixtures Directly Obtained From Equilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 12921-12929.	2.6	70
58	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
59	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. Journal of Physical Chemistry C, 2009, 113, 14290-14301.	3.1	69
60	Influence of Nanoscale Intimacy and Zeolite Micropore Size on the Performance of Bifunctional Catalysts forn-Heptane Hydroisomerization. ACS Catalysis, 2020, 10, 14245-14257.	11.2	68
61	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metalâ"Organic Frameworks. Journal of Physical Chemistry C, 2009, 113, 20869-20874.	3.1	67
62	The force network ensemble for granular packings. Soft Matter, 2010, 6, 2908.	2.7	67
63	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
64	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
65	On the Mechanism Behind the Instability of Isoreticular Metalâ€"Organic Frameworks (IRMOFs) in Humid Environments. Chemistry - A European Journal, 2012, 18, 12260-12266.	3.3	66
66	Water adsorption in hydrophilic zeolites: experiment and simulation. Physical Chemistry Chemical Physics, 2013, 15, 17374.	2.8	66
67	Thermodynamics of small systems embedded in a reservoir: a detailed analysis of finite size effects. Molecular Physics, 2012, 110, 1069-1079.	1.7	62
68	Shape selectivity through entropy. Journal of Catalysis, 2003, 214, 88-99.	6.2	60
69	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	2.0	60
70	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
71	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. Journal of Physical Chemistry C, 2017, 121, 11273-11280.	3.1	60
72	Differences between MFI- and MEL-Type Zeolites in Paraffin Hydrocracking. Journal of Catalysis, 2001, 203, 281-291.	6.2	58

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73	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
74	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. Journal of Physical Chemistry C, 2008, 112, 9976-9979.	3.1	57
75	Tail of the contact force distribution in static granular materials. Physical Review E, 2007, 75, 060302.	2.1	55
76	Photon management with lanthanides. Optical Materials, 2006, 28, 575-581.	3.6	52
77	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	4.1	52
78	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
79	Diffusion of isobutane in silicalite studied by transition path sampling. Journal of Chemical Physics, 2000, 113, 8791-8799.	3.0	51
80	Solvent Effects in the Adsorption of Alkyl Thiols on Gold Structures:â€‰ A Molecular Simulation Study. Journal of Physical Chemistry C, 2007, 111, 10201-10212.	3.1	51
81	Optimisation of lean vapour compression (LVC) as an option for post-combustion CO2 capture: Net present value maximisation. International Journal of Greenhouse Gas Control, 2012, 11, S114-S121.	4.6	51
82	Computing solubility parameters of deep eutectic solvents from Molecular Dynamics simulations. Fluid Phase Equilibria, 2019, 497, 10-18.	2.5	51
83	Direct Water Injection in Catholyteâ€Free Zeroâ€Gap Carbon Dioxide Electrolyzers. ChemElectroChem, 2020, 7, 3839-3843.	3.4	51
84	Molecular Simulation of Propaneâ^'Propylene Binary Adsorption Equilibrium in Zeolite 13X. Industrial & Engineering Chemistry Research, 2007, 46, 7239-7245.	3.7	50
85	Multicomponent Maxwellâ^'Stefan Diffusivities at Infinite Dilution. Industrial & Engineering Chemistry Research, 2011, 50, 4776-4782.	3.7	50
86	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
87	How to apply the Kirkwoodâ€“Buff theory to individual species in salt solutions. Chemical Physics Letters, 2013, 582, 154-157.	2.6	49
88	Hydride Transfer versus Deprotonation Kinetics in the Isobutaneâ€“Propene Alkylation Reaction: A Computational Study. ACS Catalysis, 2017, 7, 8613-8627.	11.2	49
89	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
90	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

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91	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. Nature Communications, 2016, 7, 11503.	12.8	48
92	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
93	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. Journal of Chemical Theory and Computation, 2016, 12, 1481-1490.	5.3	47
94	Finite-size effects of Kirkwoodâ€“Buff integrals from molecular simulations. Molecular Simulation, 2018, 44, 599-612.	2.0	47
95	Ensemble theory for force networks in hyperstatic granular matter. Physical Review E, 2004, 70, 061306.	2.1	45
96	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
97	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
98	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
99	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
100	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. Journal of Chemical & Engineering Data, 2019, 64, 4103-4115.	1.9	43
101	Insight into the Effect of Dealumination on Mordenite Using Experimentally Validated Simulations. Journal of Physical Chemistry C, 2010, 114, 2056-2065.	3.1	41
102	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
103	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. Advanced Theory and Simulations, 2019, 2, 1900135.	2.8	41
104	High pressure solubility of CO2 in non-fluorinated phosphonium-based ionic liquids. Journal of Supercritical Fluids, 2013, 82, 41-49.	3.2	40
105	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
106	Size and shape dependence of finite-volume Kirkwood-Buff integrals. Physical Review E, 2018, 97, 051301.	2.1	40
107	Reversible Hydrogen Storage in Metal-Decorated Honeycomb Borophene Oxide. ACS Applied Materials & Interfaces, 2021, 13, 43233-43240.	8.0	40
108	Recoil growth algorithm for chain molecules with continuous interactions. Molecular Physics, 1999, 97, 1243-1254.	1.7	39

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109	Maxwellâ€“Stefan diffusivities in liquid mixtures: Using molecular dynamics for testing model predictions. Fluid Phase Equilibria, 2011, 301, 110-117.	2.5	39
110	Analysis of Process Configurations for CO₂ Capture by Precipitating Amino Acid Solvents. Industrial & Engineering Chemistry Research, 2014, 53, 2348-2361.	3.7	39
111	Absorption Refrigeration Cycles with Ammoniaâ€“Ionic Liquid Working Pairs Studied by Molecular Simulation. Industrial & Engineering Chemistry Research, 2018, 57, 5442-5452.	3.7	39
112	Recovery of Cerium from Glass Polishing Waste: A Critical Review. Metals, 2018, 8, 801.	2.3	39
113	Molecular Simulation of Propaneâ^'Propylene Binary Adsorption Equilibrium in Zeolite 4A. Industrial & Engineering Chemistry Research, 2007, 46, 321-328.	3.7	38
114	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
115	Recent advances in the continuous fractional component Monte Carlo methodology. Molecular Simulation, 2021, 47, 804-823.	2.0	38
116	Modeling the Loading Dependency of Diffusion in Zeolites: The Relevant Site Model. Journal of Physical Chemistry C, 2009, 113, 17840-17850.	3.1	37
117	Diffusion of propane, propylene and isobutane in 13X zeolite by molecular dynamics. Chemical Engineering Science, 2010, 65, 2656-2663.	3.8	37
118	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
119	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
120	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
121	Adsorption Selectivity of Benzene/Propene Mixtures for Various Zeolites. Journal of Physical Chemistry C, 2007, 111, 17241-17248.	3.1	36
122	Adsorption Equilibrium of Isobutane and 1-Butene in Zeolite 13X by Molecular Simulation. Industrial & Engineering Chemistry Research, 2008, 47, 6166-6174.	3.7	36
123	Prediction of adsorption isotherms from breakthrough curves. Microporous and Mesoporous Materials, 2019, 277, 237-244.	4.4	36
124	Maxwellâ€“Stefan Diffusivities in Binary Mixtures of Ionic Liquids with Dimethyl Sulfoxide (DMSO) and H₂O. Journal of Physical Chemistry B, 2011, 115, 8506-8517.	2.6	35
125	Solubility of CO₂ in the Ionic Liquids [TBMN][MeSO₄] and [TBMP][MeSO₄]. Journal of Chemical & Engineering Data, 2012, 57, 2275-2280.	1.9	35
126	Crystals for sustainability â€“ structuring Al-based MOFs for the allocation of heat and cold. CrystEngComm, 2015, 17, 281-285.	2.6	35

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127	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
128	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
129	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
130	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 22207-22213.	3.1	34
131	Stress fluctuations in granular force networks. Journal of Statistical Mechanics: Theory and Experiment, 2011, 2011, P04002.	2.3	34
132	Solubility of CO2/CH4 gas mixtures in ionic liquids. Fluid Phase Equilibria, 2014, 375, 134-142.	2.5	34
133	Determining Force Field Parameters Using a Physically Based Equation of State. Journal of Physical Chemistry B, 2011, 115, 7872-7880.	2.6	33
134	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. Langmuir, 2016, 32, 12664-12675.	3.5	33
135	Using molecular dynamics to obtain Maxwell-Stefan diffusion coefficients in liquid systems. Molecular Physics, 1998, 94, 495-503.	1.7	33
136	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
137	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
138	Modeling the release of proteins from degrading crosslinked dextran microspheres using kinetic Monte Carlo simulations. Journal of Controlled Release, 2006, 111, 117-127.	9.9	31
139	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
140	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
141	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
142	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
143	Sheared Force Networks: Anisotropies, Yielding, and Geometry. Physical Review Letters, 2006, 96, 098001.	7.8	30
144	Liquid permeation through PTMSP: One polymer for two different membrane applications. Journal of Membrane Science, 2013, 440, 98-107.	8.2	30

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145	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
146	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
147	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
148	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
149	Modeling the Loading Dependency of Diffusion in Zeolites: the Relevant Site Model Extended to Mixtures in DDR-Type Zeolite. Journal of Physical Chemistry C, 2009, 113, 21856-21865.	3.1	28
150	Validation of the CO₂/N₂O Analogy Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2014, 53, 18081-18090.	3.7	28
151	Computation of partial molar properties using continuous fractional component Monte Carlo. Molecular Physics, 2018, 116, 3331-3344.	1.7	28
152	Solving vapor-liquid flash problems using artificial neural networks. Fluid Phase Equilibria, 2019, 490, 39-47.	2.5	28
153	Selective adsorption of alkyl thiols on gold in different geometries. Computer Physics Communications, 2007, 177, 154-157.	7.5	26
154	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
155	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
156	A Coarse-Graining Approach for the Proton Complex in Protonated Aluminosilicates. Journal of Physical Chemistry B, 2006, 110, 5838-5841.	2.6	25
157	Investigating polarization effects of CO2 adsorption in MgMOF-74. Journal of Computational Science, 2016, 15, 86-94.	2.9	25
158	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	8.0	25
159	Zeolite microporosity studied by molecular simulation. Molecular Simulation, 2009, 35, 1105-1115.	2.0	24
160	Toward a Possibility To Exchange CO₂ and CH₄ in sI Clathrate Hydrates. Journal of Physical Chemistry B, 2012, 116, 3745-3753.	2.6	24
161	Selectivity and self-diffusion of CO2 and H2 in a mixture on a graphite surface. Frontiers in Chemistry, 2013, 1, 38.	3.6	24
162	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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163	Strategies to Simultaneously Enhance the Hydrostability and the Alcoholâ€“Water Separation Behavior of Cu-BTC. Journal of Physical Chemistry C, 2013, 117, 20706-20714.	3.1	23
164	Mechanical Response of Nanocrystalline Ice-Contained Methane Hydrates: Key Role of Water Ice. ACS Applied Materials & Interfaces, 2020, 12, 14016-14028.	8.0	23
165	On the validity of the Stokesâ€“Einstein relation for various water force fields. Molecular Physics, 2020, 118, e1702729.	1.7	22
166	Exploring new methods and materials for enantioselective separations and catalysis. Molecular Simulation, 2014, 40, 585-598.	2.0	21
167	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
168	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
169	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
170	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. Nanomaterials, 2020, 10, 771.	4.1	21
171	Adsorption of Volatile Organic Compounds. Experimental and Theoretical Study. Industrial & Engineering Chemistry Research, 2012, 51, 16697-16708.	3.7	20
172	Partial molar enthalpies and reaction enthalpies from equilibrium molecular dynamics simulation. Journal of Chemical Physics, 2014, 141, 144501.	3.0	20
173	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
174	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. Molecular Simulation, 2017, 43, 189-195.	2.0	20
175	Adsorption equilibrium of nitrogen dioxide in porous materials. Physical Chemistry Chemical Physics, 2018, 20, 4189-4199.	2.8	20
176	Theoretical study on cation codoped SrTiO₃ photocatalysts for water splitting. Journal of Materials Chemistry A, 2018, 6, 24342-24349.	10.3	20
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