Thijs J H Vlugt

List of Publications by Year in Descending Order

288 papers	11,626 citations	56 h-index	95 g-index
296 ext. papers	13,149 ext. citations	4.8 avg, IF	6.65 L-index

#	Paper	IF	Citations
288	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics.. *Journal of Physical Chemistry C*, **2022**, 126, 8121-8133	3.8	0
287	Reactive Grand-Canonical Monte Carlo Simulations for Modeling Hydration of MgCl.. *ACS Omega*, **2021**, 6, 32475-32484	3.9	0
286	Electroreduction of CO/CO to C Products: Process Modeling, Downstream Separation, System Integration, and Economic Analysis.. *Industrial & Engineering Chemistry Research*, **2021**, 60, 17862-17880	3.8	3
285	Interfacial Properties of Hydrophobic Deep Eutectic Solvents with Water. *Journal of Physical Chemistry B*, **2021**, 125, 12303-12314	3.4	2
284	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	2.8	5
283	Liquid-Liquid Extraction of Formic Acid with 2-Methyltetrahydrofuran: Experiments, Process Modeling, and Economics. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5588-5599	3.9	5
282	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. *Journal of Chemical & Engineering Data*, **2021**, 66, 2071-2087	2.8	4
281	Thermodynamic, transport, and structural properties of hydrophobic deep eutectic solvents composed of tetraalkylammonium chloride and decanoic acid. *Journal of Chemical Physics*, **2021**, 154, 144502	3.9	6
280	How sensitive are physical properties of choline chloride-urea mixtures to composition changes: Molecular dynamics simulations and Kirkwood-Buff theory. *Journal of Chemical Physics*, **2021**, 154, 184502	3.9	5
279	Adsorption of n-alkanes in ZIF-8: Influence of crystal size and framework dynamics. *Microporous and Mesoporous Materials*, **2021**, 312, 110730	5.3	2
278	Diffusivity of -, -, -cyclodextrin and the inclusion complex of -cyclodextrin: Ibuprofen in aqueous solutions; A molecular dynamics simulation study. *Fluid Phase Equilibria*, **2021**, 528, 112842	2.5	11
277	Gibbs Ensemble Monte Carlo for Reactive Force Fields to Determine the Vapor-Liquid Equilibrium of CO and HO. *Journal of Chemical Theory and Computation*, **2021**, 17, 322-329	6.4	5
276	Recent advances in the continuous fractional component Monte Carlo methodology. *Molecular Simulation*, **2021**, 47, 804-823	2	14
275	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	27
274	A multiscale modelling approach to elucidate the mechanism of the oxygen evolution reaction at the hematite-water interface. *Faraday Discussions*, **2021**, 229, 89-107	3.6	8
273	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. *ACS Applied Materials & Interfaces*, **2021**, 13, 8383-8394	9.5	1
272	Competitive Adsorption of Xylenes at Chemical Equilibrium in Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 4155-4174	3.8	1

271	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	6.1	2
270	Reversible Hydrogen Storage in Metal-Decorated Honeycomb Borophene Oxide. *ACS Applied Materials & Interfaces*, **2021**, 13, 43233-43240	9.5	6
269	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	3.9	1
268	Recovery of rare earths from glass polishing waste for the production of aluminium-rare earth alloys. *Resources, Conservation and Recycling*, **2021**, 174, 105766	11.9	1
267	Mechanical Response of Nanocrystalline Ice-Contained Methane Hydrates: Key Role of Water Ice. *ACS Applied Materials & Interfaces*, **2020**, 12, 14016-14028	9.5	17
266	Gibbs Ensemble Monte Carlo Simulation of Fluids in Confinement: Relation between the Differential and Integral Pressures. *Nanomaterials*, **2020**, 10,	5.4	5
265	Inclusion Complexation of Organic Micropollutants with Cyclodextrin. *Journal of Physical Chemistry B*, **2020**, 124, 1218-1228	3.4	10
264	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	6.4	6
263	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	6.1	14
262	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. *Nanomaterials*, **2020**, 10,	5.4	12
261	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	6.4	18
260	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	14.7	22
259	On the validity of the StokesEinstein relation for various water force fields. *Molecular Physics*, **2020**, 118, e1702729	1.7	13
258	Effects of Framework Flexibility on the Adsorption and Diffusion of Aromatics in MFI-Type Zeolites. *Journal of Physical Chemistry C*, **2020**, 124, 24488-24499	3.8	10
257	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	6	14
256	Artificial intelligence and thermodynamics help solving arson cases. *Scientific Reports*, **2020**, 10, 20502	4.9	1
255	Influence of Nanoscale Intimacy and Zeolite Micropore Size on the Performance of Bifunctional Catalysts for -Heptane Hydroisomerization. *ACS Catalysis*, **2020**, 10, 14245-14257	13.1	14
254	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. *Fluid Phase Equilibria*, **2020**, 523, 112785	2.5	10

253	Isobaric Vapor–Liquid Equilibrium Data of Binary Systems Containing 2-Ethoxyethanol, 2-Ethoxyethyl Acetate, and Toluene. *Journal of Chemical & Engineering Data*, **2020**, 65, 4798-4804	2.8	3
252	Adsorption of Aromatics in MFI-Type Zeolites: Experiments and Framework Flexibility in Monte Carlo Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 21782-21797	3.8	5
251	Direct Water Injection in Catholyte-Free Zero-Gap Carbon Dioxide Electrolyzers. *ChemElectroChem*, **2020**, 7, 3839-3843	4.3	20
250	Two-Phase Equilibrium Conditions in Nanopores. *Nanomaterials*, **2020**, 10,	5.4	9
249	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. *Journal of Chemical & Engineering Data*, **2019**, 64, 4103-4115	2.8	16
248	The dynamic behavior of gas hydrate dissociation by heating in tight sandy reservoirs: A molecular dynamics simulation study. *Fuel*, **2019**, 258, 116106	7.1	12
247	Improving the accuracy of computing chemical potentials in CFCMC simulations. *Molecular Physics*, **2019**, 117, 3493-3508	1.7	10
246	Computing solubility parameters of deep eutectic solvents from Molecular Dynamics simulations. *Fluid Phase Equilibria*, **2019**, 497, 10-18	2.5	33
245	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	4.2	8
244	Enhancing the Water Capacity in Zr-Based Metal–Organic Framework for Heat Pump and Atmospheric Water Generator Applications. *ACS Applied Nano Materials*, **2019**, 2, 3050-3059	5.6	10
243	Characterization and Feasibility Studies on Complete Recovery of Rare Earths from Glass Polishing Waste. *Metals*, **2019**, 9, 278	2.3	2
242	Highlights of (bio-)chemical tools and visualization software for computational science. *Current Opinion in Chemical Engineering*, **2019**, 23, 1-13	5.4	3
241	Modeling the Electrochemical Conversion of Carbon Dioxide to Formic Acid or Formate at Elevated Pressures. *Journal of the Electrochemical Society*, **2019**, 166, E77-E86	3.9	15
240	Rayleigh-Brillouin light scattering spectra of CO2 from molecular dynamics. *Journal of Chemical Physics*, **2019**, 151, 064201	3.9	1
239	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. *Advanced Theory and Simulations*, **2019**, 2, 1900135	3.5	27
238	Solving vapor-liquid flash problems using artificial neural networks. *Fluid Phase Equilibria*, **2019**, 490, 39-47	2.5	14
237	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	6.1	32
236	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	3.9	36

235	Structural, Thermodynamic, and Transport Properties of Aqueous Reline and Ethaline Solutions from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2019**, 123, 11014-11025	3.4	41
234	Effect of truncating electrostatic interactions on predicting thermodynamic properties of water–ethanol systems. *Molecular Simulation*, **2019**, 45, 336-350	2	10
233	High Pressure Electrochemical Reduction of CO to Formic Acid/Formate: A Comparison between Bipolar Membranes and Cation Exchange Membranes. *Industrial & Engineering Chemistry Research*, **2019**, 58, 1834-1847	3.9	66
232	Prediction of adsorption isotherms from breakthrough curves. *Microporous and Mesoporous Materials*, **2019**, 277, 237-244	5.3	19
231	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. *AICHE Journal*, **2019**, 65, 792-803	3.6	10
230	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
229	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. *ACS Applied Materials & Interfaces*, **2018**, 10, 16911-16917	9.5	20
228	Kirkwood–Buff integrals of finite systems: shape effects. *Molecular Physics*, **2018**, 116, 1573-1580	1.7	17
227	iRASPA: GPU-accelerated visualization software for materials scientists. *Molecular Simulation*, **2018**, 44, 653-676	2	61
226	Molecular Simulation of Vapor-Liquid Equilibria Using the Wolf Method for Electrostatic Interactions. *Journal of Chemical & Engineering Data*, **2018**, 63, 1096-1102	2.8	15
225	Finite-size effects of Kirkwood–Buff integrals from molecular simulations. *Molecular Simulation*, **2018**, 44, 599-612	2	35
224	Adsorption equilibrium of nitrogen dioxide in porous materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 4189-4199	3.6	17
223	Development of efficient formulation for the removal of iron sulphide scale in sour production wells. *Canadian Journal of Chemical Engineering*, **2018**, 96, 2526-2533	2.3	24
222	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 2667-2677	6.4	68
221	Absorption Refrigeration Cycles with Ammonia-Ionic Liquid Working Pairs Studied by Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5442-5452	3.9	28
220	CO2 stripping from ionic liquid at elevated pressures in gas-liquid membrane contactor. *International Journal of Greenhouse Gas Control*, **2018**, 71, 293-302	4.2	17
219	In Silico Screening of Metal-Organic Frameworks for Adsorption-Driven Heat Pumps and Chillers. *ACS Applied Materials & Interfaces*, **2018**, 10, 27074-27087	9.5	25
218	Combined Steam Reforming of Methane and Formic Acid To Produce Syngas with an Adjustable H:CO Ratio. *Industrial & Engineering Chemistry Research*, **2018**, 57, 10663-10674	3.9	20

217	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
216	Gibbs ensemble Monte Carlo simulations of multicomponent natural gas mixtures. *Molecular Simulation*, **2018**, 44, 377-383	2	8
215	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	13
214	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. *Fluid Phase Equilibria*, **2018**, 458, 1-8	2.5	7
213	Recovery of Cerium from Glass Polishing Waste: A Critical Review. *Metals*, **2018**, 8, 801	2.3	22
212	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	3.6	11
211	Theoretical study on cation codoped SrTiO3 photocatalysts for water splitting. *Journal of Materials Chemistry A*, **2018**, 6, 24342-24349	13	13
210	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	6.4	10
209	Mechanical properties of bi- and poly-crystalline ice. *AIP Advances*, **2018**, 8, 125108	1.5	11
208	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	3.9	15
207	Polarizable Force Field for CO in M-MOF-74 Derived from Quantum Mechanics. *Journal of Physical Chemistry C*, **2018**, 122, 24488-24498	3.8	16
206	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	6.4	24
205	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	10.6	28
204	Size and shape dependence of finite-volume Kirkwood-Buff integrals. *Physical Review E*, **2018**, 97, 051301	2.4	33
203	Identifying Zeolite Topologies for Storage and Release of Hydrogen. *Journal of Physical Chemistry C* , **2018**, 122, 12485-12493	3.8	7
202	Polarizable Force Fields for CO and CH Adsorption in M-MOF-74. *Journal of Physical Chemistry C*, **2017**, 121, 4659-4673	3.8	62
201	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)-MOF-74. *ChemistrySelect*, **2017** , 2, 665-672	1.8	14
200	Behavior of the Enthalpy of Adsorption in Nanoporous Materials Close to Saturation Conditions. *Journal of Chemical Theory and Computation*, **2017**, 13, 3326-3339	6.4	25

199	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. *Journal of Physical Chemistry C*, **2017**, 121, 11273-11280	3.8	41
198	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. *Molecular Simulation*, **2017**, 43, 189-195	2	17
197	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	3.8	5
196	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	7.3	30
195	Efficient Application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble. *Journal of Chemical Theory and Computation*, **2017**, 13, 4452-4466	6.4	23
194	Thermodynamic and Transport Properties of Crown-Ethers: Force Field Development and Molecular Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 8367-8376	3.4	10
193	Hydride Transfer versus Deprotonation Kinetics in the Isobutane-Propene Alkylation Reaction: A Computational Study. *ACS Catalysis*, **2017**, 7, 8613-8627	13.1	30
192	Phase Diagram of Methane and Carbon Dioxide Hydrates Computed by Monte Carlo Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 7336-7350	3.4	27
191	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	26
190	Solubilities of CO2, CH4, C2H6, and SO2 in ionic liquids and Selexol from Monte Carlo simulations. *Journal of Computational Science*, **2016**, 15, 74-80	3.4	24
189	Electron microscopy investigations of cation exchange in colloidal PbSe/CdSe nanocrystals **2016**, 37-38		
188	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. *Langmuir*, **2016**, 32, 12664-12675	4	24
187	Computing equation of state parameters of gases from Monte Carlo simulations. *Fluid Phase Equilibria*, **2016**, 428, 174-181	2.5	7
186	Computation of the Heat and Entropy of Adsorption in Proximity of Inflection Points. *Journal of Physical Chemistry C*, **2016**, 120, 1727-1738	3.8	19
185	Liquid-crystal phase equilibria of Lennard-Jones chains. *Molecular Physics*, **2016**, 114, 895-908	1.7	7
184	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	4.2	16
183	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. *Journal of Chemical Theory and Computation*, **2016**, 12, 1481-90	6.4	35
182	Computing bubble-points of CO2/CH4 gas mixtures in ionic liquids from Monte Carlo simulations. *Fluid Phase Equilibria*, **2016**, 418, 100-107	2.5	8

181	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. *Nature Communications*, **2016**, 7, 11503	17.4	41
180	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	3.9	4
179	Investigating polarization effects of CO2 adsorption in MgMOF-74. *Journal of Computational Science*, **2016**, 15, 86-94	3.4	15
178	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	3.8	15
177	Phase Behavior of Binary Mixtures of a Liquid Crystal and Methane. *Journal of Chemical & Engineering Data*, **2015**, 60, 2167-2171	2.8	3
176	Diffusion of Heat and Mass in a Chemically Reacting Mixture away from Equilibrium. *Journal of Physical Chemistry C*, **2015**, 119, 12838-12847	3.8	5
175	Real-Time Process Monitoring of CO2 Capture by Aqueous AMP-PZ Using Chemometrics: Pilot Plant Demonstration. *Industrial & Engineering Chemistry Research*, **2015**, 54, 5769-5776	3.9	14
174	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	3.9	15
173	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	10.7	76
172	Adsorption-Driven Heat Pumps: The Potential of Metal-Organic Frameworks. *Chemical Reviews*, **2015**, 115, 12205-50	68.1	294
171	Isotropic-nematic phase equilibria of hard-sphere chain fluids-Pure components and binary mixtures. *Journal of Chemical Physics*, **2015**, 142, 064903	3.9	7
170	On the vapor-liquid equilibrium of attractive chain fluids with variable degree of molecular flexibility. *Journal of Chemical Physics*, **2015**, 142, 224504	3.9	4
169	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	2.8	22
168	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	3.9	11
167	Mechanical instability of monocrystalline and polycrystalline methane hydrates. *Nature Communications*, **2015**, 6, 8743	17.4	57
166	Metal-Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. *Langmuir*, **2015**, 31, 12783-96	4	97
165	Crystals for sustainability: structuring Al-based MOFs for the allocation of heat and cold. *CrystEngComm*, **2015**, 17, 281-285	3.3	30
164	Compressibility, thermal expansion coefficient and heat capacity of CH4 and CO2 hydrate mixtures using molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2015**, 17, 2869-83	3.6	56

163	Crystal structure, stability, and electronic properties of hydrated metal sulfates MSO4(H2O)n (M=Ni, Mg; n=6, 7) and their mixed phases: A first principles study. *Chemical Engineering Science*, **2015**, 121, 77-86	4.4	13
162	Evaluating adsorbed-phase activity coefficient models using a 2D-lattice model. *Molecular Simulation*, **2015**, 41, 1234-1244	2	2
161	Binary and ternary mixtures of liquid crystals with CO2. *AICHE Journal*, **2015**, 61, 2977-2984	3.6	6
160	Heat-induced transformation of CdSe-CdS-ZnS core-multishell quantum dots by Zn diffusion into inner layers. *Chemical Communications*, **2015**, 51, 3320-3	5.8	17
159	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, 2661-9	6.4	26
158	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	4.6	51
157	Manufacture of dense CAU-10-H coatings for application in adsorption driven heat pumps: optimization and characterization. *CrystEngComm*, **2015**, 17, 5911-5920	3.3	32
156	COSMO-3D: Incorporating Three-Dimensional Contact Information into the COSMO-SAC Model. *Industrial & Engineering Chemistry Research*, **2015**, 54, 2214-2226	3.9	5
155	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	2.3	6
154	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	4.2	40
153	Chapter 5:Diffusion in Liquids: Experiments, Molecular Dynamics, and Engineering Models **2015**, 78-104		5
152	CO2 Solubility in Biodegradable Hydroxylammonium-Based Ionic Liquids. *Journal of Chemical & Engineering Data*, **2014**, 59, 702-708	2.8	13
151	New Ab Initio Based Pair Potential for Accurate Simulation of Phase Transitions in ZnO. *Journal of Physical Chemistry C*, **2014**, 118, 11050-11061	3.8	29
150	Atomic resolution monitoring of cation exchange in CdSe-PbSe heteronanocrystals during epitaxial solid-solid-vapor growth. *Nano Letters*, **2014**, 14, 3661-7	11.5	43
149	Validation of the CO2/N2O Analogy Using Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2014**, 53, 18081-18090	3.9	22
148	Acid Wash Scrubbing as a Countermeasure for Ammonia Emissions from a Postcombustion CO2 Capture Plant. *Industrial & Engineering Chemistry Research*, **2014**, 53, 13195-13204	3.9	27
147	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	3.8	56
146	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	4.2	41

145	Phase Behavior of Liquid Crystal + CO2 Mixtures. *Journal of Chemical & Engineering Data*, **2014**, 59, 1667-1672	2.8	7
144	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. *Chemical Communications*, **2014**, 50, 10849-52	5.8	43
143	Analysis of Process Configurations for CO2 Capture by Precipitating Amino Acid Solvents. *Industrial & Engineering Chemistry Research*, **2014**, 53, 2348-2361	3.9	32
142	A Comparison of Advanced Monte Carlo Methods for Open Systems: CFCMC vs CBMC. *Journal of Chemical Theory and Computation*, **2014**, 10, 942-52	6.4	50
141	Solubility of CO2 and CH4 in Ionic Liquids: Ideal CO2/CH4 Selectivity. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15427-15435	3.9	79
140	Thermodynamic assessment of amine based CO2 capture technologies in power plants based on European Benchmarking Task Force methodology. *Fuel*, **2014**, 129, 318-329	7.1	90
139	Precipitating Amino Acid Solvents for CO2 Capture. Opportunities to Reduce Costs in Post Combustion Capture.. *Energy Procedia*, **2014**, 63, 727-738	2.3	18
138	Predicting Aerosol Based Emissions in a Post Combustion CO2 Capture Process Using an Aspen Plus Model. *Energy Procedia*, **2014**, 63, 911-925	2.3	15
137	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	11
136	Exploring new methods and materials for enantioselective separations and catalysis. *Molecular Simulation*, **2014**, 40, 585-598	2	15
135	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	3.9	17
134	Partial molar enthalpies and reaction enthalpies from equilibrium molecular dynamics simulation. *Journal of Chemical Physics*, **2014**, 141, 144501	3.9	20
133	Adsorptive characterization of porous solids: Error analysis guides the way. *Microporous and Mesoporous Materials*, **2014**, 200, 199-215	5.3	109
132	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	3.9	5
131	Probing lipid coating dynamics of quantum dot core micelles via F□ster resonance energy transfer. *Small*, **2014**, 10, 1163-70	11	10
130	Core-shell reconfiguration through thermal annealing in Fe(x)O/CoFe2O4 ordered 2D nanocrystal arrays. *Nanotechnology*, **2014**, 25, 055601	3.4	8
129	Bridging scales with thermodynamics: from nano to macro. *Advances in Natural Sciences: Nanoscience and Nanotechnology*, **2014**, 5, 023002	1.6	13
128	A transferable force field for CdS-CdSe-PbS-PbSe solid systems. *Journal of Chemical Physics*, **2014**, 141, 244503	3.9	14

127	Solubility of CO2/CH4 gas mixtures in ionic liquids. *Fluid Phase Equilibria*, **2014**, 375, 134-142	2.5	30
126	Calculating thermodynamic factors of ternary and multicomponent mixtures using the Permuted Widom test particle insertion method. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	5
125	The isotropic-nematic phase transition of tangent hard-sphere chain fluids--pure components. *Journal of Chemical Physics*, **2013**, 139, 034505	3.9	15
124	High pressure solubility of CO2 in non-fluorinated phosphonium-based ionic liquids. *Journal of Supercritical Fluids*, **2013**, 82, 41-49	4.2	32
123	Conceptual Design of a Novel CO2 Capture Process Based on Precipitating Amino Acid Solvents. *Industrial & Engineering Chemistry Research*, **2013**, 52, 12223-12235	3.9	58
122	Thermal Conductivity in Zeolites Studied by Non-equilibrium Molecular Dynamics Simulations. *International Journal of Thermophysics*, **2013**, 34, 1197-1213	2.1	8
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