Thijs J H Vlugt

List of Publications by Citations

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	State-of-the-Art of CO2 Capture with Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2012**, 51, 8149-8177	3.9	740
287	Quantum cutting by cooperative energy transfer in YbxY1PO4:Tb3+. *Physical Review B*, **2005**, 71,	3.3	505
286	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. *Journal of Physical Chemistry B*, **1999**, 103, 1102-1118	3.4	420
285	Adsorption-Driven Heat Pumps: The Potential of Metal-Organic Frameworks. *Chemical Reviews*, **2015**, 115, 12205-50	68.1	294
284	United Atom Force Field for Alkanes in Nanoporous Materials. *Journal of Physical Chemistry B*, **2004**, 108, 12301-12313	3.4	282
283	Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. *Journal of the American Chemical Society*, **2004**, 126, 11377-86	16.4	222
282	Improving the efficiency of the configurational-bias Monte Carlo algorithm. *Molecular Physics*, **1998**, 94, 727-733	1.7	192
281	Influence of Framework Flexibility on the Adsorption Properties of Hydrocarbons in the Zeolite Silicalite. *Journal of Physical Chemistry B*, **2002**, 106, 12757-12763	3.4	167
280	Downconversion for solar cells in YF3:Nd3+, Yb3+. *Physical Review B*, **2010**, 81,	3.3	164
279	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2009**, 113, 8814-8820	3.8	160
278	Understanding Water Adsorption in CuBTC MetalOrganic Frameworks. *Journal of Physical Chemistry C*, **2008**, 112, 15934-15939	3.8	159
277	Computing the Heat of Adsorption using Molecular Simulations: The Effect of Strong Coulombic Interactions. *Journal of Chemical Theory and Computation*, **2008**, 4, 1107-18	6.4	157
276	Force network ensemble: a new approach to static granular matter. *Physical Review Letters*, **2004**, 92, 054302	7.4	154
275	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. *Journal of the American Chemical Society*, **1998**, 120, 5599-5600	16.4	145
274	Molecular simulations of interacting nanocrystals. *Nano Letters*, **2008**, 8, 2930-4	11.5	140
273	Force field parametrization through fitting on inflection points in isotherms. *Physical Review Letters* , **2004**, 93, 088302	7.4	136
272	Kirkwood-Buff Integrals for Finite Volumes. *Journal of Physical Chemistry Letters*, **2013**, 4, 235-8	6.4	131

271	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. *Journal of Chemical Physics*, **2005**, 122, 224712	3.9	128
270	Mechanical properties of clathrate hydrates: status and perspectives. *Energy and Environmental Science*, **2012**, 5, 6779	35.4	124
269	Adsorption and Binding of Ligands to CdSe Nanocrystals. *Journal of Physical Chemistry C*, **2009**, 113, 12690-12698	4.8	123
268	Adsorptive characterization of porous solids: Error analysis guides the way. *Microporous and Mesoporous Materials*, **2014**, 200, 199-215	5.3	109
267	The Shape Selectivity of Paraffin Hydroconversion on TON-, MTT-, and AEL-Type Sieves. *Journal of Catalysis*, **1999**, 188, 403-412	7.3	107
266	Energy transfer mechanism for downconversion in the (Pr3+, Yb3+) couple. *Physical Review B*, **2010**, 81,	3.3	106
265	Time-dependent photoluminescence spectroscopy as a tool to measure the ligand exchange kinetics on a quantum dot surface. *ACS Nano*, **2008**, 2, 1703-14	16.7	103
264	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. *Journal of Physical Chemistry A*, **1998**, 102, 7727-7730	2.8	100
263	Metal-Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. *Langmuir*, **2015**, 31, 12783-96	4	97
262	Calculating thermodynamic properties from fluctuations at small scales. *Journal of Physical Chemistry B*, **2011**, 115, 10911-8	3.4	92
261	Separation of Alkane Isomers by Exploiting Entropy Effects during Adsorption on Silicalite-1: A Configurational-Bias Monte Carlo Simulation Study. *Langmuir*, **2001**, 17, 1558-1570	4	91
260	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
259	Influence of isotherm inflection on diffusion in silicalite. *Chemical Engineering Science*, **1999**, 54, 1751-1757	4.4	90
258	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. *Journal of Physical Chemistry B*, **2003**, 107, 12088-12096	3.4	86
257	Molecular simulation of adsorption of short linear alkanes and their mixtures in silicalite. *AICHE Journal*, **1998**, 44, 1756-1764	3.6	83
256	Solubility of CO2 and CH4 in Ionic Liquids: Ideal CO2/CH4 Selectivity. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15427-15435	3.9	79
255	Diffusion Coefficients from Molecular Dynamics Simulations in Binary and Ternary Mixtures. *International Journal of Thermophysics*, **2013**, 34, 1169-1196	2.1	79
254	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

253	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	4.2	76
252	Shape Selectivity in Hydrocarbon Conversion. *Angewandte Chemie - International Edition*, **2001**, 40, 736-739	13.4	74
251	Simulation of Alkane Adsorption in the Aluminophosphate Molecular Sieve AlPO4-5. *Journal of Physical Chemistry B*, **1998**, 102, 7183-7189	3.4	74
250	Morphological transformations and fusion of PbSe nanocrystals studied using atomistic simulations. *Nano Letters*, **2010**, 10, 3966-71	11.5	72
249	Entropy maximization in the force network ensemble for granular solids. *Physical Review Letters*, **2008**, 100, 238001	7.4	69
248	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	3.8	69
247	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 2667-2677	6.4	68
246	Understanding interactions between capped nanocrystals: three-body and chain packing effects. *Journal of Chemical Physics*, **2009**, 131, 124705	3.9	67
245	Dual release of proteins from porous polymeric scaffolds. *Journal of Controlled Release*, **2006**, 111, 95-106	11.7	66
244	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
243	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. *Industrial & Engineering Chemistry Research*, **2012**, 51, 10247-10258	3.9	63
242	Polarizable Force Fields for CO and CH Adsorption in M-MOF-74. *Journal of Physical Chemistry C*, **2017**, 121, 4659-4673	3.8	62
241	Thermodynamics of a small system in a T reservoir. *Chemical Physics Letters*, **2011**, 504, 199-201	2.5	62
240	iRASPA: GPU-accelerated visualization software for materials scientists. *Molecular Simulation*, **2018**, 44, 653-676	2	61
239	Predictive Darken Equation for Maxwell-Stefan Diffusivities in Multicomponent Mixtures. *Industrial & Engineering Chemistry Research*, **2011**, 50, 10350-10358	3.9	61
238	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. *Journal of Physical Chemistry C*, **2009**, 113, 14290-14301	3.8	61
237	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	3.8	60
236	Fick diffusion coefficients of liquid mixtures directly obtained from equilibrium molecular dynamics. *Journal of Physical Chemistry B*, **2011**, 115, 12921-9	3.4	59

235	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
234	Mechanical instability of monocrystalline and polycrystalline methane hydrates. *Nature Communications*, **2015**, 6, 8743	17.4	57
233	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metal Organic Frameworks. *Journal of Physical Chemistry C*, **2009**, 113, 20869-20874	3.8	57
232	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
231	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
230	On the mechanism behind the instability of isoreticular metal-organic frameworks (IRMOFs) in humid environments. *Chemistry - A European Journal*, **2012**, 18, 12260-6	4.8	55
229	The force network ensemble for granular packings. *Soft Matter*, **2010**, 6, 2908	3.6	55
228	Shape selectivity through entropy. *Journal of Catalysis*, **2003**, 214, 88-99	7.3	54
227	Thermodynamics of small systems embedded in a reservoir: a detailed analysis of finite size effects. *Molecular Physics*, **2012**, 110, 1069-1079	1.7	53
226	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. *Molecular Simulation*, **2009**, 35, 1067-1076	2	52
225	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
224	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
223	Differences between MFI- and MEL-Type Zeolites in Paraffin Hydrocracking. *Journal of Catalysis*, **2001**, 203, 281-291	7.3	50
222	Water adsorption in hydrophilic zeolites: experiment and simulation. *Physical Chemistry Chemical Physics*, **2013**, 15, 17374-82	3.6	49
221	Tail of the contact force distribution in static granular materials. *Physical Review E*, **2007**, 75, 060302	2.4	49
220	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. *Journal of Physical Chemistry C*, **2008**, 112, 9976-9979	3.8	47
219	Solvent Effects in the Adsorption of Alkyl Thiols on Gold Structures: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2007**, 111, 10201-10212	3.8	47
218	Photon management with lanthanides. *Optical Materials*, **2006**, 28, 575-581	3.3	47

217	Molecular Simulation of Propane–Propylene Binary Adsorption Equilibrium in Zeolite 13X. *Industrial & Engineering Chemistry Research*, **2007**, 46, 7239-7245	3.9	45
216	Diffusion of isobutane in silicalite studied by transition path sampling. *Journal of Chemical Physics*, **2000**, 113, 8791-8799	3.9	45
215	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
214	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. *Chemical Communications*, **2014**, 50, 10849-52	5.8	43
213	How to apply the Kirkwood–Buff theory to individual species in salt solutions. *Chemical Physics Letters*, **2013**, 582, 154-157	2.5	43
212	Ensemble theory for force networks in hyperstatic granular matter. *Physical Review E*, **2004**, 70, 061306	2.4	42
211	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. *Journal of Physical Chemistry C*, **2017**, 121, 11273-11280	3.8	41
210	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
209	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. *Nature Communications*, **2016**, 7, 11503	17.4	41
208	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
207	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
206	Multicomponent Maxwell–Stefan Diffusivities at Infinite Dilution. *Industrial & Engineering Chemistry Research*, **2011**, 50, 4776-4782	3.9	40
205	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	4.2	37
204	Insight into the Effect of Dealumination on Mordenite Using Experimentally Validated Simulations. *Journal of Physical Chemistry C*, **2010**, 114, 2056-2065	3.8	37
203	Molecular Simulation of Propane–Propylene Binary Adsorption Equilibrium in Zeolite 4A. *Industrial & Engineering Chemistry Research*, **2007**, 46, 321-328	3.9	36
202	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
201	Finite-size effects of Kirkwood–Buff integrals from molecular simulations. *Molecular Simulation*, **2018**, 44, 599-612	2	35
200	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. *Journal of Chemical Theory and Computation*, **2016**, 12, 1481-90	6.4	35

199	Modeling the Loading Dependency of Diffusion in Zeolites: The Relevant Site Model. *Journal of Physical Chemistry C*, **2009**, 113, 17840-17850	3.8	34
198	Computing solubility parameters of deep eutectic solvents from Molecular Dynamics simulations. *Fluid Phase Equilibria*, **2019**, 497, 10-18	2.5	33
197	Adsorption Equilibrium of Isobutane and 1-Butene in Zeolite 13X by Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2008**, 47, 6166-6174	3.9	33
196	Recoil growth algorithm for chain molecules with continuous interactions. *Molecular Physics*, **1999**, 97, 1243-1254	1.7	33
195	Size and shape dependence of finite-volume Kirkwood-Buff integrals. *Physical Review E*, **2018**, 97, 051301	2.4	33
194	Analysis of Process Configurations for CO2 Capture by Precipitating Amino Acid Solvents. *Industrial & Engineering Chemistry Research*, **2014**, 53, 2348-2361	3.9	32
193	High pressure solubility of CO2 in non-fluorinated phosphonium-based ionic liquids. *Journal of Supercritical Fluids*, **2013**, 82, 41-49	4.2	32
192	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
191	Stress fluctuations in granular force networks. *Journal of Statistical Mechanics: Theory and Experiment*, **2011**, 2011, P04002	1.9	32
190	Diffusion of propane, propylene and isobutane in 13X zeolite by molecular dynamics. *Chemical Engineering Science*, **2010**, 65, 2656-2663	4.4	32
189	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
188	Solubility of CO2 in the Ionic Liquids [TBMN][MeSO4] and [TBMP][MeSO4]. *Journal of Chemical & Engineering Data*, **2012**, 57, 2275-2280	2.8	31
187	Determining force field parameters using a physically based equation of state. *Journal of Physical Chemistry B*, **2011**, 115, 7872-80	3.4	31
186	Adsorption Selectivity of Benzene/Propene Mixtures for Various Zeolites. *Journal of Physical Chemistry C*, **2007**, 111, 17241-17248	3.8	31
185	Crystals for sustainability: structuring Al-based MOFs for the allocation of heat and cold. *CrystEngComm*, **2015**, 17, 281-285	3.3	30
184	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
183	Hydride Transfer versus Deprotonation Kinetics in the Isobutane-Propene Alkylation Reaction: A Computational Study. *ACS Catalysis*, **2017**, 7, 8613-8627	13.1	30
182	Solubility of CO2/CH4 gas mixtures in ionic liquids. *Fluid Phase Equilibria*, **2014**, 375, 134-142	2.5	30

181	Maxwell–Stefan diffusivities in liquid mixtures: Using molecular dynamics for testing model predictions. *Fluid Phase Equilibria*, **2011**, 301, 110-117	2.5	30
180	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
179	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. *Journal of Physical Chemistry C*, **2010**, 114, 22207-22213	3.8	29
178	Maxwell-Stefan diffusivities in binary mixtures of ionic liquids with dimethyl sulfoxide (DMSO) and H2O. *Journal of Physical Chemistry B*, **2011**, 115, 8506-17	3.4	29
177	Sheared force networks: anisotropies, yielding, and geometry. *Physical Review Letters*, **2006**, 96, 098001	7.4	29
176	Absorption Refrigeration Cycles with Ammonia-Ionic Liquid Working Pairs Studied by Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5442-5452	3.9	28
175	Liquid permeation through PTMSP: One polymer for two different membrane applications. *Journal of Membrane Science*, **2013**, 440, 98-107	9.6	28
174	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
173	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. *Advanced Theory and Simulations*, **2019**, 2, 1900135	3.5	27
172	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
171	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
170	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
169	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
168	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
167	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
166	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
165	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	3.8	25
164	Using molecular dynamics to obtain Maxwell-Stefan diffusion coefficients in liquid systems. *Molecular Physics*, **1998**, 94, 495-503	1.7	25

163	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
162	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
161	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. *Langmuir*, **2016**, 32, 12664-12675	4	24
160	Modeling the release of proteins from degrading crosslinked dextran microspheres using kinetic Monte Carlo simulations. *Journal of Controlled Release*, **2006**, 111, 117-27	11.7	24
159	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
158	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
157	Selective adsorption of alkyl thiols on gold in different geometries. *Computer Physics Communications*, **2007**, 177, 154-157	4.2	23
156	A coarse-graining approach for the proton complex in protonated aluminosilicates. *Journal of Physical Chemistry B*, **2006**, 110, 5838-41	3.4	23
155	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
154	Validation of the CO2/N2O Analogy Using Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2014**, 53, 18081-18090	3.9	22
153	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
152	Recovery of Cerium from Glass Polishing Waste: A Critical Review. *Metals*, **2018**, 8, 801	2.3	22
151	Strategies to Simultaneously Enhance the Hydrostability and the Alcohol/Water Separation Behavior of Cu-BTC. *Journal of Physical Chemistry C*, **2013**, 117, 20706-20714	3.8	21
150	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. *ACS Applied Materials & Interfaces*, **2018**, 10, 16911-16917	9.5	20
149	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
148	Partial molar enthalpies and reaction enthalpies from equilibrium molecular dynamics simulation. *Journal of Chemical Physics*, **2014**, 141, 144501	3.9	20
147	Direct Water Injection in Catholyte-Free Zero-Gap Carbon Dioxide Electrolyzers. *ChemElectroChem*, **2020**, 7, 3839-3843	4.3	20
146	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

145	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
144	Toward a possibility to exchange CO2 and CH4 in sI clathrate hydrates. *Journal of Physical Chemistry B*, **2012**, 116, 3745-53	3.4	19
143	Selectivity and self-diffusion of CO2 and H2 in a mixture on a graphite surface. *Frontiers in Chemistry*, **2013**, 1, 38	5	19
142	Prediction of adsorption isotherms from breakthrough curves. *Microporous and Mesoporous Materials*, **2019**, 277, 237-244	5.3	19
141	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
140	Precipitating Amino Acid Solvents for CO2 Capture. Opportunities to Reduce Costs in Post Combustion Capture.. *Energy Procedia*, **2014**, 63, 727-738	2.3	18
139	From sphere to multipod: thermally induced transitions of CdSe nanocrystals studied by molecular dynamics simulations. *Journal of the American Chemical Society*, **2013**, 135, 5869-76	16.4	18
138	Zeolite microporosity studied by molecular simulation. *Molecular Simulation*, **2009**, 35, 1105-1115	2	18
137	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. *Molecular Simulation*, **2017**, 43, 189-195	2	17
136	Mechanical Response of Nanocrystalline Ice-Contained Methane Hydrates: Key Role of Water Ice. *ACS Applied Materials & Interfaces*, **2020**, 12, 14016-14028	9.5	17
135	KirkwoodBuff integrals of finite systems: shape effects. *Molecular Physics*, **2018**, 116, 1573-1580	1.7	17
134	Adsorption equilibrium of nitrogen dioxide in porous materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 4189-4199	3.6	17
133	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
132	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
131	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
130	Adsorption of Volatile Organic Compounds. Experimental and Theoretical Study. *Industrial & Engineering Chemistry Research*, **2012**, 51, 16697-16708	3.9	17
129	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. *Journal of Chemical & Engineering Data*, **2019**, 64, 4103-4115	2.8	16
128	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

127	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
126	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
125	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
124	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
123	The isotropic-nematic phase transition of tangent hard-sphere chain fluids--pure components. *Journal of Chemical Physics*, **2013**, 139, 034505	3.9	15
122	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
121	Exploring new methods and materials for enantioselective separations and catalysis. *Molecular Simulation*, **2014**, 40, 585-598	2	15
120	Simulation study on the adsorption properties of linear alkanes on closed nanotube bundles. *Journal of Physical Chemistry B*, **2012**, 116, 9812-9	3.4	15
119	Phase behavior of liquid crystals with CO2. *Journal of Physical Chemistry B*, **2012**, 116, 9101-6	3.4	15
118	The phase behavior of linear and partially flexible hard-sphere chain fluids and the solubility of hard spheres in hard-sphere chain fluids. *Journal of Chemical Physics*, **2013**, 138, 204905	3.9	15
117	Dynamic pruned-enriched Rosenbluth method. *Molecular Physics*, **2003**, 101, 1675-1682	1.7	15
116	Molecular Dynamics Simulation of Self-Diffusion and Maxwell-Stefan Diffusion Coefficients in Liquid Mixtures of Methanol and Water. *Molecular Simulation*, **1999**, 23, 79-94	2	15
115	Investigating polarization effects of CO2 adsorption in MgMOF-74. *Journal of Computational Science*, **2016**, 15, 86-94	3.4	15
114	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
113	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
112	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)-MOF-74. *ChemistrySelect*, **2017**, 2, 665-672	1.8	14
111	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
110	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

109	A transferable force field for CdS-CdSe-PbS-PbSe solid systems. *Journal of Chemical Physics*, **2014**, 141, 244503	3.9	14
108	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
107	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
106	Solving vapor-liquid flash problems using artificial neural networks. *Fluid Phase Equilibria*, **2019**, 490, 39-47	2.5	14
105	Recent advances in the continuous fractional component Monte Carlo methodology. *Molecular Simulation*, **2021**, 47, 804-823	2	14
104	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
103	CO2 Solubility in Biodegradable Hydroxylammonium-Based Ionic Liquids. *Journal of Chemical & Engineering Data*, **2014**, 59, 702-708	2.8	13
102	Bridging scales with thermodynamics: from nano to macro. *Advances in Natural Sciences: Nanoscience and Nanotechnology*, **2014**, 5, 023002	1.6	13
101	A direct method for calculating thermodynamic factors for liquid mixtures using the Permuted Widom test particle insertion method. *Molecular Physics*, **2013**, 111, 287-296	1.7	13
100	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. *Journal of Physical Chemistry C*, **2011**, 115, 15355-15360	3.8	13
99	An analytical approximation for the orientation-dependent excluded volume of tangent hard sphere chains of arbitrary chain length and flexibility. *Journal of Chemical Physics*, **2012**, 137, 044906	3.9	13
98	Coarse-grained model for gold nanocrystals with an organic capping layer. *Molecular Physics*, **2007**, 105, 3177-3184	1.7	13
97	On the validity of the StokesEinstein relation for various water force fields. *Molecular Physics*, **2020**, 118, e1702729	1.7	13
96	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
95	Theoretical study on cation codoped SrTiO3 photocatalysts for water splitting. *Journal of Materials Chemistry A*, **2018**, 6, 24342-24349	13	13
94	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
93	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. *Nanomaterials*, **2020**, 10,	5.4	12
92	Force balance in canonical ensembles of static granular packings. *Journal of Statistical Mechanics: Theory and Experiment*, **2010**, 2010, P01015	1.9	12

91	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
90	Influence of force field parameters on computed diffusion coefficients of CO2 in LTA-type zeolite. *Microporous and Mesoporous Materials*, **2012**, 158, 64-76	5.3	11
89	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
88	Soft Hedgehogs on Coarse Carpets: A Molecular Simulation Study of Capped Nanocrystals Interacting with Self-Assembled Monolayers of Alkylthiols on a Gold (111) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 2531-2537	3.8	11
87	Molecular simulations of the adsorption of cycloalkanes in MFI-type silica. *Physical Chemistry Chemical Physics*, **2005**, 7, 2622-8	3.6	11
86	On the efficient sampling of pathways in the transition path ensemble. *PhysChemComm*, **2001**, 4, 11		11
85	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
84	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
83	Mechanical properties of bi- and poly-crystalline ice. *AIP Advances*, **2018**, 8, 125108	1.5	11
82	Improving the accuracy of computing chemical potentials in CFCMC simulations. *Molecular Physics*, **2019**, 117, 3493-3508	1.7	10
81	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
80	Inclusion Complexation of Organic Micropollutants with Cyclodextrin. *Journal of Physical Chemistry B*, **2020**, 124, 1218-1228	3.4	10
79	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
78	Probing lipid coating dynamics of quantum dot core micelles via Fster resonance energy transfer. *Small*, **2014**, 10, 1163-70	11	10
77	Diffusion in zeolites: Extension of the relevant site model to light gases and mixtures thereof in zeolites DDR, CHA, MFI and FAU. *Separation and Purification Technology*, **2010**, 73, 151-163	8.3	10
76	Universal anisotropy in force networks under shear. *Physical Review E*, **2007**, 75, 030301	2.4	10
75	Efficiency of Parallel CBMC Simulations. *Molecular Simulation*, **1999**, 23, 63-78	2	10
74	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

73	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. *Fluid Phase Equilibria*, **2020**, 523, 112785	2.5	10
72	Effect of truncating electrostatic interactions on predicting thermodynamic properties of water–ethanol systems. *Molecular Simulation*, **2019**, 45, 336-350	2	10
71	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. *AICHE Journal*, **2019**, 65, 792-803	3.6	10
70	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
69	Adsorption of Argon on MFI Nanosheets: Experiments and Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 24503-24510	3.8	9
68	Two-Phase Equilibrium Conditions in Nanopores. *Nanomaterials*, **2020**, 10,	5.4	9
67	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
66	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
65	Thermal Conductivity in Zeolites Studied by Non-equilibrium Molecular Dynamics Simulations. *International Journal of Thermophysics*, **2013**, 34, 1197-1213	2.1	8
64	Core-shell reconfiguration through thermal annealing in Fe(x)O/CoFe2O4 ordered 2D nanocrystal arrays. *Nanotechnology*, **2014**, 25, 055601	3.4	8
63	Computing phase equilibria by parallel excluded volume tempering. *Journal of Chemical Physics*, **2001**, 115, 8731-8741	3.9	8
62	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
61	Thermal conductivity of aqueous solutions of reline, ethaline, and glyceline deep eutectic solvents; a molecular dynamics simulation study. *Molecular Physics*,e1876263	1.7	8
60	Gibbs ensemble Monte Carlo simulations of multicomponent natural gas mixtures. *Molecular Simulation*, **2018**, 44, 377-383	2	8
59	Isotropic-nematic phase equilibria of hard-sphere chain fluids-Pure components and binary mixtures. *Journal of Chemical Physics*, **2015**, 142, 064903	3.9	7
58	Computing equation of state parameters of gases from Monte Carlo simulations. *Fluid Phase Equilibria*, **2016**, 428, 174-181	2.5	7
57	Liquid-crystal phase equilibria of Lennard-Jones chains. *Molecular Physics*, **2016**, 114, 895-908	1.7	7
56	Phase Behavior of Liquid Crystal + CO2 Mixtures. *Journal of Chemical & Engineering Data*, **2014**, 59, 1667-1672	2.8	7

55	Phase behaviour of the system 4?-pentyloxy-4-cyanobiphenyl+CO2. *Journal of Chemical Thermodynamics*, **2013**, 59, 20-27	2.9	7
54	Potential Desorbents for Propane/Propylene Separation by Gas Phase Simulated Moving Bed: A Molecular Simulation Study. *Industrial & Engineering Chemistry Research*, **2010**, 49, 5826-5833	3.9	7
53	Shape Selectivity in Hydrocarbon Conversion. *Angewandte Chemie*, **2001**, 113, 758-761	3.6	7
52	Measurement of chemical potentials of systems with strong excluded volume interactions by computing the density of states. *Molecular Physics*, **2002**, 100, 2763-2771	1.7	7
51	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. *Fluid Phase Equilibria*, **2018**, 458, 1-8	2.5	7
50	Identifying Zeolite Topologies for Storage and Release of Hydrogen. *Journal of Physical Chemistry C* , **2018**, 122, 12485-12493	3.8	7
49	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
48	Binary and ternary mixtures of liquid crystals with CO2. *AICHE Journal*, **2015**, 61, 2977-2984	3.6	6
47	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
46	Using an Analytic Equation of State to Obtain Quantitative Solubilities of CO2 by Molecular Simulation. *Journal of Physical Chemistry Letters*, **2011**, 2, 393-396	6.4	6
45	Study on hexane adsorption in zeolite ITQ-29 by molecular simulation. *Adsorption*, **2008**, 14, 763-770	2.6	6
44	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
43	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
42	Reversible Hydrogen Storage in Metal-Decorated Honeycomb Borophene Oxide. *ACS Applied Materials & Interfaces*, **2021**, 13, 43233-43240	9.5	6
41	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
40	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
39	Gibbs Ensemble Monte Carlo Simulation of Fluids in Confinement: Relation between the Differential and Integral Pressures. *Nanomaterials*, **2020**, 10,	5.4	5
38	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

37	COSMO-3D: Incorporating Three-Dimensional Contact Information into the COSMO-SAC Model. *Industrial & Engineering Chemistry Research*, **2015**, 54, 2214-2226	3.9	5
36	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
35	Adsorption and Diffusion of Alkanes in Na-MOR: Modeling the Effect of the Aluminum Distribution. *Journal of Chemical Theory and Computation*, **2009**, 5, 2858-65	6.4	5
34	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
33	Chapter 5:Diffusion in Liquids: Experiments, Molecular Dynamics, and Engineering Models **2015**, 78-104		5
32	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
31	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
30	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
29	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
28	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
27	Reconciling the Relevant Site Model and dynamically corrected Transition State Theory. *Chemical Physics Letters*, **2010**, 495, 77-79	2.5	4
26	Simulation of 1-alkene and n-alkane binary vapour–liquid equilibrium using different united-atom transferable force fields. *Fluid Phase Equilibria*, **2005**, 232, 136-148	2.5	4
25	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. *Journal of Chemical & Engineering Data*, **2021**, 66, 2071-2087	2.8	4
24	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
23	Highlights of (bio-)chemical tools and visualization software for computational science. *Current Opinion in Chemical Engineering*, **2019**, 23, 1-13	5.4	3
22	Phase Behavior of Binary Mixtures of a Liquid Crystal and Methane. *Journal of Chemical & Engineering Data*, **2015**, 60, 2167-2171	2.8	3
21	Stretching a heteropolymer. *Journal of Chemical Physics*, **2005**, 122, 114904	3.9	3
20	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

19	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
18	Characterization and Feasibility Studies on Complete Recovery of Rare Earths from Glass Polishing Waste. *Metals*, **2019**, 9, 278	2.3	2
17	Evaluating adsorbed-phase activity coefficient models using a 2D-lattice model. *Molecular Simulation*, **2015**, 41, 1234-1244	2	2
16	Interfacial Properties of Hydrophobic Deep Eutectic Solvents with Water. *Journal of Physical Chemistry B*, **2021**, 125, 12303-12314	3.4	2
15	Adsorption of n-alkanes in ZIF-8: Influence of crystal size and framework dynamics. *Microporous and Mesoporous Materials*, **2021**, 312, 110730	5.3	2
14	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
13	Rayleigh-Brillouin light scattering spectra of CO2 from molecular dynamics. *Journal of Chemical Physics*, **2019**, 151, 064201	3.9	1
12	Predictive Model for Optimizing Guest–Host Lennard–Jones Interactions in Zeolites. *Journal of Physical Chemistry C*, **2011**, 115, 10187-10195	3.8	1
11	Artificial intelligence and thermodynamics help solving arson cases. *Scientific Reports*, **2020**, 10, 20502	4.9	1
10	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. *ACS Applied Materials & Interfaces*, **2021**, 13, 8383-8394	9.5	1
9	Competitive Adsorption of Xylenes at Chemical Equilibrium in Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 4155-4174	3.8	1
8	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
7	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
6	Shape Selectivity in Hydrocarbon Conversion These investigations were supported in part by the Netherlands Research Council for Chemical Sciences (CW) with financial aid from the Netherlands Technology Foundation and by the Netherlands Organization for Scientific Research (NWO) through PIONIER. We would like to thank Christa Roemkens, Rob van Veen, Henk Schenk, Daan	16.4	1
5	Reactive Grand-Canonical Monte Carlo Simulations for Modeling Hydration of MgCl.. *ACS Omega*, **2021**, 6, 32475-32484 *International Edition*, **2001**, 40, 736-739	3.9	0
4	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
3	Electron microscopy investigations of cation exchange in colloidal PbSe/CdSe nanocrystals **2016**, 37-38		
2	Force network ensemble for the triangular lattice: a tale of tiles. *Chaos*, **2009**, 19, 041107	3.3	

1 Molecular Simulation Techniques Using Classical Force Fields121-149