Hans Hasse

List of Publications by Year in Descending Order

379 papers	9,620 citations	53 h-index	78 g-index
397 ext. papers	10,795 ext. citations	3.2 avg, IF	6.57 L-index

#	Paper	IF	Citations
379	Solid–liquid Equilibria and Kinetics of the Solid Formation in Binary and Ternary Mixtures Containing (Formaldehyde + Water + Methanol). *Industrial & Engineering Chemistry Research*, **2022**, 61, 1871-1884	3.9	0
378	Diffusion coefficients at infinite dilution of carbon dioxide and methane in water, ethanol, cyclohexane, toluene, methanol, and acetone: A PFG-NMR and MD simulation study. *Journal of Chemical Thermodynamics*, **2022**, 166, 106691	2.9	3
377	Investigation of Radial Shaft Seal Swelling Using a Special Tribometer and Magnetic Resonance Imaging.. *ACS Omega*, **2022**, 7, 11671-11677	3.9	
376	Mutual Diffusion Coefficients from NMR Imaging. *Chemical Engineering Science*, **2022**, 117655	4.4	0
375	13C-NMR Spectroscopic Study of the Kinetics of Formaldehyde Oligomerization Reactions in the System (Formaldehyde + Water + Isoprenol). *Industrial & Engineering Chemistry Research*, **2022**, 61, 224-235	3.9	0
374	Influence of pH value and salts on the adsorption of lysozyme in mixed-mode chromatography. *Engineering in Life Sciences*, **2021**, 21, 753-768	3.4	1
373	Conceptual design of a crystallization-based trioxane production process. *Chemical Engineering and Processing: Process Intensification*, **2021**, 171, 108710	3.7	0
372	Reproducibility of atomistic friction computer experiments: a molecular dynamics simulation study. *Molecular Simulation*, **2021**, 47, 1509-1521	2	1
371	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. *Computer Physics Communications*, **2021**, 262, 107860	4.2	10
370	High Flow-Rate Benchtop NMR Spectroscopy Enabled by Continuous Overhauser DNP. *Analytical Chemistry*, **2021**, 93, 8897-8905	7.8	1
369	Molecular Dynamics Study of Wetting and Adsorption of Binary Mixtures of the Lennard-Jones Truncated and Shifted Fluid on a Planar Wall. *Langmuir*, **2021**, 37, 7405-7419	4	5
368	Speciation in CO2-loaded aqueous solutions of sixteen triacetoneamine-derivates (EvAs) and elucidation of structure-property relationships. *Chemical Engineering Science*, **2021**, 229, 115999	4.4	2
367	Mass transfer through vapour–liquid interfaces: a molecular dynamics simulation study. *Molecular Physics*, **2021**, 119, e1810798	1.7	12
366	Influence of Salts on the Adsorption of Lysozyme on a Mixed-Mode Resin. *Adsorption Science and Technology*, **2021**, 2021, 1-11	3.6	1
365	Phase Field Simulations of Wetting Based on Molecular Simulations. *Proceedings in Applied Mathematics and Mechanics*, **2021**, 20, e202000035	0.2	
364	Experimental Study of the Influence of the Adsorbate Layer Composition on the Wetting of Different Substrates with Water. *Adsorption Science and Technology*, **2021**, 2021, 1-11	3.6	2
363	Sub-zero metalworking fluids for high performance cutting of difficult to cut materials. *Procedia CIRP*, **2021**, 101, 342-345	1.8	0

362	Thermophysical Properties of Mixtures of Titanium(IV) Isopropoxide (TTIP) and 2-Propanol (iPOH). *Journal of Chemical & Engineering Data*, **2021**, 66, 1296-1304	2.8	1
361	Vapor–liquid Equilibria and Chemical Equilibria in the System (Formaldehyde + Water + Isoprenol). *Industrial & Engineering Chemistry Research*, **2021**, 60, 4471-4483	3.9	5
360	Machine Learning of Thermophysical Properties. *Fluid Phase Equilibria*, **2021**, 549, 113206	2.5	2
359	Automated Methods for Identification and Quantification of Structural Groups from Nuclear Magnetic Resonance Spectra Using Support Vector Classification. *Journal of Chemical Information and Modeling*, **2021**, 61, 143-155	6.1	3
358	Vapor-liquid interfacial properties of the system cyclohexane + CO2: Experiments, molecular simulation and density gradient theory. *Fluid Phase Equilibria*, **2020**, 518, 112583	2.5	11
357	Thermophysical Properties of Solutions of Iron(III) Nitrate-Nonahydrate in Mixtures of Ethanol and Water. *Journal of Chemical & Engineering Data*, **2020**, 65, 3519-3527	2.8	8
356	Spectroscopic investigations of solutions of lithium bis(fluorosulfonyl) imide (LiFSI) in valeronitrile. *Polyhedron*, **2020**, 183, 114458	2.7	2
355	Multicriteria Optimization of Molecular Models of Water Using a Reduced Units Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 5127-5138	6.4	1
354	Adsorption and reaction layers when turning AISI 304 using various cooling strategies. *Procedia CIRP*, **2020**, 87, 125-130	1.8	1
353	Enrichment at vapour–liquid interfaces of mixtures: establishing a link between nanoscopic and macroscopic properties. *International Reviews in Physical Chemistry*, **2020**, 39, 319-349	7	26
352	Thermophysical Properties of Mixtures of Titanium(IV) Isopropoxide (TTIP) and p-Xylene. *Journal of Chemical & Engineering Data*, **2020**, 65, 869-876	2.8	7
351	Online process monitoring of a batch distillation by medium field NMR spectroscopy. *Chemical Engineering Science*, **2020**, 219, 115561	4.4	10
350	Molecular interactions at vapor-liquid interfaces: Binary mixtures of simple fluids. *Physical Review E*, **2020**, 101, 012802	2.4	18
349	Machine Learning in Thermodynamics: Prediction of Activity Coefficients by Matrix Completion. *Journal of Physical Chemistry Letters*, **2020**, 11, 981-985	6.4	17
348	Prediction of flow effects in quantitative NMR measurements. *Journal of Magnetic Resonance*, **2020** , 312, 106683	3	5
347	Molecular dynamics and phase field simulations of droplets on surfaces with wettability gradient. *Computer Methods in Applied Mechanics and Engineering*, **2020**, 361, 112773	5.7	7
346	Triacetoneamine-derivates (EvAs) for CO2-absorption from process gases. *International Journal of Greenhouse Gas Control*, **2020**, 95, 102932	4.2	3
345	Two Simple and Highly Efficient Variants of the Griffith-Ley Oxidation of Alcohols. *ChemCatChem*, **2020**, 12, 3919-3928	5.2	4

344	A novel approach for infeasible path optimization of distillation-based flowsheets. *Chemical Engineering Science: X*, **2020**, 7, 100063	1.1	
343	Processes for the production of OME fuels **2020**, 191-203	0.3	0
342	Generalized Chemical Equilibrium Constant of Formaldehyde Oligomerization. *Industrial & Engineering Chemistry Research*, **2020**, 59, 11431-11440	3.9	5
341	Interfacial properties of binary mixtures of simple fluids and their relation to the phase diagram. *Physical Chemistry Chemical Physics*, **2020**, 22, 12544-12564	3.6	16
340	Application of NEAT for the simulation of liquid□quid extraction processes with poorly specified feeds. *AICHE Journal*, **2020**, 66, e16826	3.6	4
339	PFG-NMR and MD Simulation Study of Self-Diffusion Coefficients of Binary and Ternary Mixtures Containing Cyclohexane, Ethanol, Acetone, and Toluene. *Journal of Chemical & Engineering Data*, **2020**, 65, 793-803	2.8	7
338	Short-cut method for assessing solvents for gas cleaning by reactive absorption. *Chemical Engineering Research and Design*, **2020**, 153, 757-767	5.5	3
337	Influence of dispersive long-range interactions on properties of vapour□quid equilibria and interfaces of binary Lennard-Jones mixtures. *Molecular Physics*, **2020**, 118, e1699185	1.7	15
336	Thermophysical Properties of Solutions of Iron(III) Nitrate Nonahydrate in Mixtures of 1-Propanol and Water. *Journal of Chemical & Engineering Data*, **2020**, 65, 5413-5420	2.8	2
335	Formulation of sub-zero metalworking fluids for cutting processes: Influence of additives. *CIRP Journal of Manufacturing Science and Technology*, **2020**, 31, 25-33	3.4	1
334	Die Entwicklung der Verfahrenstechnik an der TU Kaiserslautern. *Chemie-Ingenieur-Technik*, **2020**, 92, 1011-1022	0.8	
333	Multi-criteria optimization for parametrizing excess Gibbs energy models. *Fluid Phase Equilibria*, **2020**, 522, 112676	2.5	5
332	Review and comparison of equations of state for the Lennard-Jones fluid. *Fluid Phase Equilibria*, **2020**, 523, 112772	2.5	14
331	Prediction of the elution profiles of proteins in mixed salt systems in hydrophobic interaction chromatography. *Separation and Purification Technology*, **2020**, 233, 116006	8.3	5
330	Thermal, caloric and transport properties of the Lennard□ones truncated and shifted fluid in the adsorbed layers at dispersive solid walls. *Molecular Physics*, **2020**, 118, e1669838	1.7	1
329	Estimating activity coefficients of target components in poorly specified mixtures with NMR spectroscopy and COSMO-RS. *Fluid Phase Equilibria*, **2020**, 516, 112604	2.5	3
328	A Force Field for Poly(oxymethylene) Dimethyl Ethers (OME). *Journal of Chemical Theory and Computation*, **2020**, 16, 2517-2528	6.4	3
327	Molecular Dynamics Study of Adsorption of the Lennard-Jones Truncated and Shifted Fluid on Planar Walls. *Journal of Chemical & Engineering Data*, **2019**, 64, 386-394	2.8	3

326	Application of NEAT for determining the composition dependence of activity coefficients in poorly specified mixtures. *Chemical Engineering Science*, **2019**, 208, 115161	4.4	3
325	Reaction Monitoring by Benchtop NMR Spectroscopy Using a Novel Stationary Flow Reactor Setup. *Industrial & Engineering Chemistry Research*, **2019**, 58, 18125-18133	3.9	13
324	TweTriS: Twenty trillion-atom simulation. *International Journal of High Performance Computing Applications*, **2019**, 33, 838-854	1.8	25
323	Shear-rate dependence of thermodynamic properties of the Lennard-Jones truncated and shifted fluid by molecular dynamics simulations. *Physics of Fluids*, **2019**, 31, 063103	4.4	1
322	NMR spectroscopic method for studying homogenous liquid phase reaction kinetics in systems used in reactive gas absorption and application to monoethanolamine–water–carbon dioxide. *Chemical Engineering Journal*, **2019**, 374, 1127-1137	14.7	1
321	NEAT–NMR Spectroscopy for the Estimation of Activity Coefficients of Target Components in Poorly Specified Mixtures. *Industrial & Engineering Chemistry Research*, **2019**, 58, 9155-9165	3.9	9
320	Solid-liquid equilibrium in the system 2-keto-L-gulonic acid + sodium-2-keto-L-gulonate + hydrochloric acid + sodium chloride + water. *Fluid Phase Equilibria*, **2019**, 495, 21-27	2.5	
319	Physicochemical Properties of the System N,N-Dimethyl-dipropylene-diamino-triacetonediamine (EvA34), Water, and Carbon Dioxide for Reactive Absorption. *Journal of Chemical & Engineering Data*, **2019**, 64, 2368-2379	2.8	3
318	NMR Spectroscopic Study of Chemical Reactions in Mixtures Containing Oleic Acid, Formic Acid, and Formoxystearic Acid. *Industrial & Engineering Chemistry Research*, **2019**, 58, 5622-5630	3.9	2
317	Vapor-liquid equilibrium of mixtures containing formaldehyde, water, and butynediol. *Fluid Phase Equilibria*, **2019**, 490, 101-106	2.5	1
316	Studying equilibria of polymers in solution by direct molecular dynamics simulations: poly(N-isopropylacrylamide) in water as a test case. *European Physical Journal: Special Topics*, **2019**, 227, 1547-1558	2.3	11
315	Monoalkylcarbonate formation in the system monoethanolamine–water–carbon dioxide. *Fluid Phase Equilibria*, **2019**, 486, 98-105	2.5	11
314	Measurement and Modeling of Phase Equilibria in Systems Containing Water, Xylose, Furfural, and Acetic Acid. *Journal of Chemical & Engineering Data*, **2019**, 64, 2634-2640	2.8	2
313	MolMod – an open access database of force fields for molecular simulations of fluids. *Molecular Simulation*, **2019**, 45, 806-814	2	32
312	Digitalization in Thermodynamics. *Chemie-Ingenieur-Technik*, **2019**, 91, 201-214	0.8	8
311	Physico-Chemical Properties of LiFSI Solutions I. LiFSI with Valeronitrile, Dichloromethane, 1,2-Dichloroethane, and 1,2-Dichlorobenzene. *Journal of Chemical & Engineering Data*, **2019**, 64, 868-877	2.8	2
310	Simultaneous determination of thermal conductivity and shear viscosity using two-gradient non-equilibrium molecular dynamics simulations. *Molecular Physics*, **2019**, 117, 189-199	1.7	10
309	Interfacial properties of binary Lennard-Jones mixtures by molecular simulation and density gradient theory. *Journal of Chemical Physics*, **2019**, 150, 174704	3.9	28

308	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. *Journal of Chemical Information and Modeling*, **2019**, 59, 4248-4265	6.1	40
307	Self-Diffusion Coefficients in Solutions of Lithium Bis(fluorosulfonyl)imide with Dimethyl Carbonate and Ethylene Carbonate. *Chemie-Ingenieur-Technik*, **2019**, 91, 1633-1639	0.8	3
306	Turning of AISI 4140 (42CrMo4): A Novel Sub-zero Cooling Approach **2019**, 313-323		3
305	A Simple Way for Implementing Extraction Columns of Infinite Height in Flowsheet Simulators. *Chemie-Ingenieur-Technik*, **2019**, 91, 314-322	0.8	
304	Physicochemical Properties of LiFSI Solutions II: LiFSI with Water, MTBE, and Anisole. *Journal of Chemical & Engineering Data*, **2019**, 64, 878-883	2.8	
303	A Navier-Stokes-Korteweg Model for Dynamic Wetting based on the PeTS Equation of State. *Proceedings in Applied Mathematics and Mechanics*, **2019**, 19, e201900091	0.2	
302	The Influence of Lubrication and the Solid-Fluid Interaction on Thermodynamic Properties in a Nanoscopic Scratching Process. *Langmuir*, **2019**, 35, 16948-16960	4	14
301	Transport properties of the Lennard-Jones truncated and shifted fluid from non-equilibrium molecular dynamics simulations. *Fluid Phase Equilibria*, **2019**, 482, 38-47	2.5	13
300	Associating lattice cluster theory and application to modeling oleic acid + formic acid + formoxystearic acid. *AICHE Journal*, **2019**, 65, 783-791	3.6	1
299	Effects of Lubrication on Friction and Heat Transfer in Machining Processes on the Nanoscale: A Molecular Dynamics Approach. *Procedia CIRP*, **2018**, 67, 296-301	1.8	6
298	Study of homogeneous bubble nucleation in liquid carbon dioxide by a hybrid approach combining molecular dynamics simulation and density gradient theory. *Journal of Chemical Physics*, **2018**, 148, 124702	3.9	8
297	SkaSim Skalierbare HPC-Software f molekulare Simulationen in der chemischen Industrie. *Chemie-Ingenieur-Technik*, **2018**, 90, 295-306	0.8	6
296	Equation of state for the Lennard-Jones truncated and shifted fluid with a cut-off radius of 2.5 based on perturbation theory and its applications to interfacial thermodynamics. *Molecular Physics*, **2018**, 116, 2083-2094	1.7	39
295	Multi-criteria optimization for parameterization of SAFT-type equations of state for water. *AICHE Journal*, **2018**, 64, 226-237	3.6	24
294	Investigating the stability of the phase field solution of equilibrium droplet configurations by eigenvalues and eigenvectors. *Computational Materials Science*, **2018**, 141, 185-192	3.2	9
293	Electrical conductivity of solutions of lithium bis(fluorosulfonyl)imide in mixed organic solvents and multi-objective solvent optimization for lithium-ion batteries. *Journal of Power Sources*, **2018**, 398, 215-223	8.9	7
292	Hierarchical design of extraction-distillation processes using short-cut apparatus models with piece-wise linearized thermodynamics. *Chemical Engineering Science*, **2018**, 192, 422-433	4.4	2
291	Separation of water from mixtures containing formaldehyde, water, methanol, methylal, and poly(oxymethylene) dimethyl ethers by pervaporation. *Journal of Membrane Science*, **2018**, 564, 806-812	9.6	18

290	A molecular dynamics simulation scenario for studying solvent-mediated interactions of polymers and application to thermoresponse of poly(N-isopropylacrylamide) in water. *Journal of Molecular Liquids*, **2018**, 268, 294-302	6	10
289	Sub-zero cooling: A novel strategy for high performance cutting. *CIRP Annals - Manufacturing Technology*, **2018**, 67, 95-98	4.9	12
288	Three-dimensional phase field modeling of inhomogeneous gas-liquid systems using the PeTS equation of state. *Journal of Chemical Physics*, **2018**, 149, 064701	3.9	8
287	Partial molar volume of NaCl and CsCl in mixtures of water and methanol by experiment and molecular simulation. *Fluid Phase Equilibria*, **2018**, 458, 30-39	2.5	4
286	Thermal and caloric properties of fluids from non-equilibrium molecular dynamics simulations using the two-gradient method. *Journal of Chemical Physics*, **2018**, 149, 244106	3.9	3
285	Vapor–liquid Interface of the Lennard-Jones Truncated and Shifted Fluid: Comparison of Molecular Simulation, Density Gradient Theory, and Density Functional Theory. *Journal of Physical Chemistry C* , **2018**, 122, 24705-24715	3.8	32
284	Mathematical modeling of adsorption isotherms in mixed salt systems in hydrophobic interaction chromatography. *Biotechnology Progress*, **2018**, 34, 1251-1260	2.8	4
283	Solid-Liquid Equilibrium in the System 2-Keto--Gulonic Acid + -Ascorbic Acid + Water. *Chemical Engineering and Technology*, **2018**, 41, 2306-2311	2	2
282	Recovery of Furfural and Acetic Acid from Wood Hydrolysates in Biotechnological Downstream Processing. *Chemical Engineering and Technology*, **2018**, 41, 2331-2336	2	5
281	Design of a Production Process for Poly(oxymethylene) Dimethyl Ethers from Dimethyl Ether and Trioxane. *Chemie-Ingenieur-Technik*, **2018**, 90, 1489-1496	0.8	18
280	Influence of pH and Salts on Partial Molar Volume of Lysozyme and Bovine Serum Albumin in Aqueous Solutions. *Chemical Engineering and Technology*, **2018**, 41, 2337-2345	2	
279	Method for Estimating Activity Coefficients of Target Components in Poorly Specified Mixtures. *Industrial & Engineering Chemistry Research*, **2018**, 57, 7310-7313	3.9	16
278	Physico-chemical properties of solutions of lithium bis(fluorosulfonyl)imide (LiFSI) in dimethyl carbonate, ethylene carbonate, and propylene carbonate. *Journal of Power Sources*, **2018**, 394, 148-159	8.9	17
277	Adsorption of oleic acid dissolved in isopropanol–water mixtures on hydrotalcite. *Adsorption Science and Technology*, **2018**, 36, 919-926	3.6	
276	Solid-liquid equilibrium in the system 2-keto-L-gulonic acid + sodium-2-keto-L-gulonate + water. *Fluid Phase Equilibria*, **2018**, 473, 318-322	2.5	3
275	Vapor-liquid equilibrium in the ternary systems acetic acid + water + (xylose or glucose). *Fluid Phase Equilibria*, **2018**, 473, 323-329	2.5	4
274	Vapor–liquid equilibrium and distillation of mixtures containing formaldehdye and poly(oxymethylene) dimethyl ethers. *Chemical Engineering and Processing: Process Intensification*, **2018**, 131, 116-124	3.7	16
273	Stage-to-stage calculations of distillation columns by fixed-point iteration and application of the Banach fixed-point theorem. *Chemical Engineering Science*, **2017**, 164, 188-201	4.4	6

272	Comparison of predictions of the PC-SAFT equation of state and molecular simulations for the metastable region of binary mixtures. *Fluid Phase Equilibria*, **2017**, 444, 31-36	2.5	1
271	NMR spectroscopic study of chemical equilibria in solutions of formaldehyde, water, and butynediol. *AICHE Journal*, **2017**, 63, 4442-4450	3.6	7
270	Static and Dynamic Wetting Behavior of Drops on Impregnated Structured Walls by Molecular Dynamics Simulation. *Journal of Physical Chemistry C*, **2017**, 121, 12669-12683	3.8	9
269	In situ measurement of liquid-liquid equilibria by medium field nuclear magnetic resonance. *Fluid Phase Equilibria*, **2017**, 438, 44-52	2.5	7
268	Molecular simulation study of the CO2-N2O analogy. *Fluid Phase Equilibria*, **2017**, 442, 44-52	2.5	4
267	Development of an Integrated Reaction□Distillation Process for the Production of Methylal. *Industrial & Engineering Chemistry Research*, **2017**, 56, 575-582	3.9	29
266	Molecular simulation of the surface tension of 33 multi-site models for real fluids. *Journal of Molecular Liquids*, **2017**, 235, 126-134	6	10
265	Influence of mixed electrolytes and pH on adsorption of bovine serum albumin in hydrophobic interaction chromatography. *Journal of Chromatography A*, **2017**, 1521, 73-79	4.5	13
264	Efficient Approach for Calculating Pareto Boundaries under Uncertainties in Chemical Process Design. *Industrial & Engineering Chemistry Research*, **2017**, 56, 12672-12681	3.9	19
263	Activity coefficients from molecular simulations using the OPAS method. *Journal of Chemical Physics*, **2017**, 147, 144108	3.9	11
262	Solubility of Carbon Dioxide in Poly(oxymethylene) Dimethyl Ethers. *Journal of Chemical & Engineering Data*, **2017**, 62, 4027-4031	2.8	13
261	Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. *Journal of Chemical Theory and Computation*, **2017**, 13, 4270-4280	6.4	32
260	Conceptual Design of a Novel Process for the Production of Poly(oxymethylene) Dimethyl Ethers from Formaldehyde and Methanol. *Industrial & Engineering Chemistry Research*, **2017**, 56, 11519-11530	3.9	44
259	Studying Fast Reaction Kinetics with Online NMR Spectroscopy. *Chemie-Ingenieur-Technik*, **2017**, 89, 369-378	0.8	10
258	Influence of mixed electrolytes on the adsorption of lysozyme, PEG, and PEGylated lysozyme on a hydrophobic interaction chromatography resin. *Biotechnology Progress*, **2017**, 33, 1104-1115	2.8	9
257	ms2: A molecular simulation tool for thermodynamic properties, release 3.0. *Computer Physics Communications*, **2017**, 221, 343-351	4.2	53
256	Simultaneous description of bulk and interfacial properties of fluids by the Mie potential. *Molecular Physics*, **2017**, 115, 1017-1030	1.7	13
255	Reactive Distillation in a Dividing-Wall Column: Model Development, Simulation, and Error Analysis. *Chemie-Ingenieur-Technik*, **2017**, 89, 1315-1324	0.8	7

254	Surface Wetting with Droplets: A Phase Field Approach. *Proceedings in Applied Mathematics and Mechanics*, **2017**, 17, 501-502	0.2	4
253	Boon and Bane: On the Role of Adjustable Parameters in Simulation Models. *Boston Studies in the Philosophy and History of Science*, **2017**, 93-115	0.2	16
252	Monoalkylcarbonate Formation in Methyldiethanolamine–H2O–CO2. *Industrial & Engineering Chemistry Research*, **2017**, 56, 9006-9015	3.9	17
251	Density of ethanolic alkali halide salt solutions by experiment and molecular simulation. *Fluid Phase Equilibria*, **2016**, 408, 141-150	2.5	5
250	A new scheme for process simulation by optimization: distillation as an example. *Computer Aided Chemical Engineering*, **2016**, 205-210	0.6	2
249	Application of a new micro-reactor 1H NMR probe head for quantitative analysis of fast esterification reactions. *Chemical Engineering Journal*, **2016**, 306, 413-421	14.7	16
248	Simulation of Surface Wetting by Droplets Using a Phase Field Model. *Proceedings in Applied Mathematics and Mechanics*, **2016**, 16, 519-520	0.2	5
247	Thermodynamic Study of a Complex System for Carbon Capture: Butyltriacetonediamine + Water + Carbon Dioxide. *Journal of Chemical & Engineering Data*, **2016**, 61, 3814-3826	2.8	6
246	Liquid-liquid equilibrium in binary and ternary mixtures containing formaldehyde, water, methanol, methylal, and poly(oxymethylene) dimethyl ethers. *Fluid Phase Equilibria*, **2016**, 425, 127-135	2.5	26
245	Process Design in World 3.0 – Challenges and Strategies to Master the Raw Material Change. *Chemical Engineering and Technology*, **2016**, 39, 219-224	2	3
244	Modeling, simulation and analysis of a process for the production of crotonaldehyde. *Chemical Engineering and Processing: Process Intensification*, **2016**, 101, 101-111	3.7	5
243	Parametrization of two-center Lennard-Jones plus point-quadrupole force field models by multicriteria optimization. *Fluid Phase Equilibria*, **2016**, 411, 33-42	2.5	27
242	Oberfl□henerzeugungs-Morphologie-Eigenschafts-Beziehungen. *ZWF Zeitschrift Fuer Wirtschaftlichen Fabrikbetrieb*, **2016**, 111, 213-216	0.5	4
241	Kryogener K□lschmierstoff auf der Basis von Ethylenglykol. *ZWF Zeitschrift Fuer Wirtschaftlichen Fabrikbetrieb*, **2016**, 111, 444-448	0.5	4
240	Investigation of the reaction of 1,3-dimethylurea with formaldehyde by quantitative on-line NMR spectroscopy: a model for the urea-formaldehyde system. *Magnetic Resonance in Chemistry*, **2016**, 54, 457-76	2.1	11
239	Solvent cleaning and wettability of technical steel and titanium surfaces. *Adsorption Science and Technology*, **2016**, 34, 261-274	3.6	10
238	Solvent activity in electrolyte solutions from molecular simulation of the osmotic pressure. *Journal of Chemical Physics*, **2016**, 144, 084112	3.9	22
237	Surface tension of the two center Lennard-Jones plus point dipole fluid. *Journal of Chemical Physics* , **2016**, 144, 054702	3.9	12

236	Slope curve method for the analysis of separations in extraction columns of infinite height. *Chemical Engineering Science*, **2016**, 143, 105-113	4.4	8
235	Activities in Aqueous Solutions of the Alkali Halide Salts from Molecular Simulation. *Journal of Chemical & Engineering Data*, **2016**, 61, 4068-4076	2.8	18
234	From methanol to the oxygenated diesel fuel poly(oxymethylene) dimethyl ether: An assessment of the production costs. *Fuel*, **2016**, 185, 67-72	7.1	92
233	Interfacial and bulk properties of vapor-liquid equilibria in the system toluene + hydrogen chloride + carbon dioxide by molecular simulation and density gradient theory + PC-SAFT. *Fluid Phase Equilibria*, **2016**, 427, 219-230	2.5	28
232	Interfacial tension and adsorption in the binary system ethanol and carbon dioxide: Experiments, molecular simulation and density gradient theory. *Fluid Phase Equilibria*, **2016**, 427, 476-487	2.5	32
231	Chemical Equilibrium of the Synthesis of Poly(oxymethylene) Dimethyl Ethers from Formaldehyde and Methanol in Aqueous Solutions. *Industrial & Engineering Chemistry Research*, **2015**, 54, 6409-6417	3.9	82
230	Decision Support by Multicriteria Optimization in Process Development: An Integrated Approach for Robust Planning and Design of Plant Experiments. *Computer Aided Chemical Engineering*, **2015**, 37, 2063-2068	0.6	6
229	Surface tension of the two center Lennard-Jones plus quadrupole model fluid. *Fluid Phase Equilibria* , **2015**, 392, 12-18	2.5	12
228	Density of Methanolic Alkali Halide Salt Solutions by Experiment and Molecular Simulation. *Journal of Chemical & Engineering Data*, **2015**, 60, 1614-1628	2.8	9
227	Carbonate complexes of vanadate. *Polyhedron*, **2015**, 95, 81-85	2.7	3
226	Molecular modelling and simulation of the surface tension of real quadrupolar fluids. *Chemical Engineering Science*, **2015**, 121, 110-117	4.4	28
225	Long-range correction for dipolar fluids at planar interfaces. *Molecular Physics*, **2015**, 113, 3750-3756	1.7	8
224	Comment on "The gas-liquid surface tension of argon: A reconciliation between experiment and simulation" [J. Chem. Phys. 140, 244710 (2014)]. *Journal of Chemical Physics*, **2015**, 142, 107101	3.9	10
223	Molecular Modeling and Simulation in Fluid Process Engineering. *ChemBioEng Reviews*, **2015**, 2, 303-310	5.2	
222	INES An Interface Between Experiments and Simulation to Support the Development of Robust Process Designs. *Chemie-Ingenieur-Technik*, **2015**, 87, 1810-1825	0.8	26
221	On the simultaneous description of h-bonding and dipolar interactions with point charges in force field models. *AICHE Journal*, **2015**, 61, 2926-2932	3.6	7
220	Reaction Kinetics of the Formation of Poly(oxymethylene) Dimethyl Ethers from Formaldehyde and Methanol in Aqueous Solutions. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12553-12560	3.9	64
219	On the effort of approaching pure components and azeotropes in distillation. *Chemical Engineering Science*, **2015**, 127, 253-259	4.4	4

218	1H- and 13C-NMR spectroscopic study of chemical equilibria in the system acetaldehyde + water. *AICHE Journal*, **2015**, 61, 177-187	3.6	19
217	Characterization of alkylsilane self-assembled monolayers by molecular simulation. *Langmuir*, **2015**, 31, 2630-8	4	22
216	Molecular simulation of nano-dispersed fluid phases. *Chemical Engineering Science*, **2014**, 107, 235-244	4.4	9
215	Thermostatted micro-reactor NMR probe head for monitoring fast reactions. *Journal of Magnetic Resonance*, **2014**, 242, 155-61	3	25
214	Long-range correction for multi-site Lennard-Jones models and planar interfaces. *Molecular Physics*, **2014**, 112, 2227-2234	1.7	19
213	Online 1H NMR Spectroscopic Study of the Reaction Kinetics in Mixtures of Acetaldehyde and Water Using a New Microreactor Probe Head. *Industrial & Engineering Chemistry Research*, **2014** , 53, 17589-17596	3.9	15
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