Hans Hasse

List of Publications by Citations

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	Poly(oxymethylene) dimethyl ethers as components of tailored diesel fuel: Properties, synthesis and purification concepts. *Fuel*, **2010**, 89, 3315-3319	7.1	307
378	A Set of Molecular Models for Symmetric Quadrupolar Fluids. *Journal of Physical Chemistry B*, **2001**, 105, 12126-12133	3.4	294
377	Prediction of self-diffusion coefficient and shear viscosity of water and its binary mixtures with methanol and ethanol by molecular simulation. *Journal of Chemical Physics*, **2011**, 134, 074508	3.9	161
376	Online NMR spectroscopic study of species distribution in MEA–H2O–CO2 and DEA–H2O–CO2. *Fluid Phase Equilibria*, **2008**, 263, 131-143	2.5	161
375	Comprehensive study of the vapour–liquid coexistence of the truncated and shifted Lennard–Jones fluid including planar and spherical interface properties. *Molecular Physics*, **2006**, 104, 1509-1527	1.7	158
374	Post combustion CO2 capture by reactive absorption: Pilot plant description and results of systematic studies with MEA. *International Journal of Greenhouse Gas Control*, **2012**, 6, 84-112	4.2	143
373	Molecular dynamics and experimental study of conformation change of poly(N-isopropylacrylamide) hydrogels in mixtures of water and methanol. *Journal of Physical Chemistry B*, **2012**, 116, 5251-9	3.4	129
372	Chemical Equilibrium and Reaction Kinetics of the Heterogeneously Catalyzed Formation of Poly(oxymethylene) Dimethyl Ethers from Methylal and Trioxane. *Industrial & Engineering Chemistry Research*, **2012**, 51, 12751-12761	3.9	128
371	Quantitative high-resolution on-line NMR spectroscopy in reaction and process monitoring. *Journal of Magnetic Resonance*, **2004**, 166, 135-46	3	126
370	FT-IR spectroscopic investigations of hydrogen bonding in alcohol–hydrocarbon solutions. *Fluid Phase Equilibria*, **2001**, 186, 1-25	2.5	119
369	Grand Equilibrium: vapour-liquid equilibria by a new molecular simulation method. *Molecular Physics*, **2002**, 100, 3375-3383	1.7	113
368	Experimental Pressure–Temperature Data on Three- and Four-Phase Equilibria of Fluid, Hydrate, and Ice Phases in the System Carbon Dioxide–Water. *Journal of Chemical & Engineering Data*, **1999**, 44, 901-906	2.8	109
367	1H- and 13C-NMR-Spectroscopic Study of Chemical Equilibria in Solutions of Formaldehyde in Water, Deuterium Oxide, and Methanol. *Industrial & Engineering Chemistry Research*, **1994**, 33, 1022-1029	3.9	106
366	NMR Spectroscopic and Densimetric Study of Reaction Kinetics of Formaldehyde Polymer Formation in Water, Deuterium Oxide, and Methanol. *Industrial & Engineering Chemistry Research*, **1995**, 34, 440-450	3.9	104
365	Pilot plant experimental studies of post combustion CO2 capture by reactive absorption with MEA and new solvents. *Energy Procedia*, **2009**, 1, 963-970	2.3	100
364	Prediction of transport properties by molecular simulation: methanol and ethanol and their mixture. *Journal of Physical Chemistry B*, **2008**, 112, 16664-74	3.4	97
363	Hydrogen bonding of methanol in supercritical CO2: comparison between 1H NMR spectroscopic data and molecular simulation results. *Journal of Physical Chemistry B*, **2007**, 111, 9871-8	3.4	97

362	Production process for diesel fuel components poly(oxymethylene) dimethyl ethers from methane-based products by hierarchical optimization with varying model depth. *Chemical Engineering Research and Design*, **2013**, 91, 2648-2662	5.5	96
361	A molecular simulation study of shear and bulk viscosity and thermal conductivity of simple real fluids. *Fluid Phase Equilibria*, **2004**, 221, 157-163	2.5	92
360	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
359	ls1 mardyn: The Massively Parallel Molecular Dynamics Code for Large Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 4455-64	6.4	88
358	Octahedral molecular sieves of the type K-OMS-2 with different particle sizes and morphologies: Impact on the catalytic properties in the aerobic partial oxidation of benzyl alcohol. *Applied Catalysis A: General*, **2009**, 355, 42-49	5.1	88
357	Molecular dynamics and experimental study of conformation change of poly(N-isopropylacrylamide) hydrogels in water. *Fluid Phase Equilibria*, **2010**, 296, 164-172	2.5	87
356	Unlike Lennard□ones parameters for vapor□quid equilibria. *Journal of Molecular Liquids*, **2007**, 135, 170-178	6	87
355	Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets. *Computers and Chemical Engineering*, **2014**, 60, 354-363	4	86
354	ms2: A molecular simulation tool for thermodynamic properties. *Computer Physics Communications*, **2011**, 182, 2350-2367	4.2	85
353	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
352	High-pressure multiphase behaviour of ternary systems carbon dioxide□water□olar solvent: review and modeling with the Peng□Robinson equation of state. *Journal of Supercritical Fluids*, **1998**, 12, 185-221	4.2	81
351	Fluid dynamics in reactive distillation packing Katapak□ -S. *Chemical Engineering Science*, **1999**, 54, 1367-1374	4.1	81
350	A set of molecular models for carbon monoxide and halogenated hydrocarbons. *Journal of Chemical Physics*, **2003**, 119, 11396-11407	3.9	79
349	Henry□ law constants of methane, nitrogen, oxygen and carbon dioxide in ethanol from 273 to 498 K: Prediction from molecular simulation. *Fluid Phase Equilibria*, **2005**, 233, 134-143	2.5	79
348	CO2 Capture for Fossil Fuel-Fired Power Plants. *Chemical Engineering and Technology*, **2011**, 34, 163-172	2	76
347	Vapor□quid equilibria of mixtures containing nitrogen, oxygen, carbon dioxide, and ethane. *AICHE Journal*, **2003**, 49, 2187-2198	3.6	71
346	Quantitative NMR Spectroscopy of Complex Liquid Mixtures: Methods and Results for Chemical Equilibria in Formaldehyde□Water□Methanol at Temperatures up to 383 K. *Industrial & Engineering Chemistry Research*, **2003**, 42, 259-266	3.9	70
345	Modification of the classical nucleation theory based on molecular simulation data for surface tension, critical nucleus size, and nucleation rate. *Physical Review E*, **2008**, 78, 011603	2.4	69

344	Osmotic Virial Coefficients of Aqueous Poly(ethylene glycol) from Laser-Light Scattering and Isopiestic Measurements. *Macromolecules*, **1995**, 28, 3540-3552	5.5	69
343	Influence of ion-exchange resin catalysts on side reactions of the esterification of n-Butanol with acetic acid. *Chemical Engineering Science*, **2006**, 61, 753-765	4.4	67
342	Comprehensive study of the vapour–liquid equilibria of the pure two-centre Lennard–Jones plus pointquadrupole fluid. *Fluid Phase Equilibria*, **2001**, 179, 339-362	2.5	67
341	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
340	Integration of a chemical process model in a power plant modelling tool for the simulation of an amine based CO2 scrubber. *Fuel*, **2009**, 88, 2481-2488	7.1	63
339	Development of a new industrial process for trioxane production. *Chemical Engineering Science*, **2007**, 62, 5613-5620	4.4	62
338	Mutual diffusion in the ternary mixture of water + methanol + ethanol and its binary subsystems. *Physical Chemistry Chemical Physics*, **2013**, 15, 3985-4001	3.6	60
337	Selection and Pilot Plant Tests of New Absorbents for Post-Combustion Carbon Dioxide Capture. *Chemical Engineering Research and Design*, **2007**, 85, 510-515	5.5	59
336	The influence of the liquid slab thickness on the planar vapor–liquid interfacial tension. *Physica A: Statistical Mechanics and Its Applications*, **2013**, 392, 2359-2367	3.3	58
335	ms2: A molecular simulation tool for thermodynamic properties, new version release. *Computer Physics Communications*, **2014**, 185, 3302-3306	4.2	56
334	Multi-objective optimization using reduced models in conceptual design of a fuel additive production process. *Chemical Engineering Science*, **2013**, 99, 118-126	4.4	56
333	Phase Equilibrium in Formaldehyde Containing Multicomponent Mixtures: Experimental Results for Fluid Phase Equilibria of (Formaldehyde + (Water or Methanol) + Methylal)) and (Formaldehyde + Water + Methanol + Methylal) and Comparison with Predictions. *Industrial & Engineering Chemistry Research*, **2006**, 45, 5155-5164	3.9	55
332	Solubility of Carbon Dioxide in Aqueous Solutions of Monoethanolamine in the Low and High Gas Loading Regions. *Journal of Chemical & Engineering Data*, **2013**, 58, 883-895	2.8	54
331	Pilot plant experiments for post combustion carbon dioxide capture by reactive absorption with novel solvents. *Energy Procedia*, **2011**, 4, 1-8	2.3	54
330	ms2: A molecular simulation tool for thermodynamic properties, release 3.0. *Computer Physics Communications*, **2017**, 221, 343-351	4.2	53
329	Pilot plant study of four new solvents for post combustion carbon dioxide capture by reactive absorption and comparison to MEA. *International Journal of Greenhouse Gas Control*, **2012**, 8, 205-216	4.2	53
328	Molecular model for carbon dioxide optimized to vapor-liquid equilibria. *Journal of Chemical Physics* , **2010**, 132, 234512	3.9	53
327	A set of molecular models for alkali and halide ions in aqueous solution. *Journal of Chemical Physics*, **2012**, 136, 084501	3.9	53

326	Contact angle of sessile drops in Lennard-Jones systems. *Langmuir*, **2014**, 30, 13606-14	4	52
325	Online NMR Spectroscopic Study of Species Distribution in MDEA–H2O–CO2 and MDEA–PIPE–H2O–CO2. *Industrial & Engineering Chemistry Research*, **2008**, 47, 7917-7926	3.9	52
324	Methyl Acetate Hydrolysis in a Reactive Divided Wall Column. *Chemical Engineering Research and Design*, **2007**, 85, 149-154	5.5	52
323	On the application of force fields for predicting a wide variety of properties: Ethylene oxide as an example. *Fluid Phase Equilibria*, **2008**, 274, 16-26	2.5	51
322	Pilot plant study of post-combustion carbon dioxide capture by reactive absorption: Methodology, comparison of different structured packings, and comprehensive results for monoethanolamine. *Chemical Engineering Research and Design*, **2011**, 89, 1216-1228	5.5	48
321	Pilot plant study of two new solvents for post combustion carbon dioxide capture by reactive absorption and comparison to monoethanolamine. *Chemical Engineering Science*, **2011**, 66, 5512-5522	4.4	47
320	Set of molecular models based on quantum mechanical ab initio calculations and thermodynamic data. *Journal of Physical Chemistry B*, **2008**, 112, 12710-21	3.4	46
319	Self Diffusion and Binary Maxwell–Stefan Diffusion in Simple Fluids with the Green–Kubo Method. *International Journal of Thermophysics*, **2004**, 25, 175-186	2.1	46
318	Chemical potential of quadrupolar two-centre Lennard-Jones fluids by gradual insertion. *Chemical Physics Letters*, **2002**, 356, 431-436	2.5	46
317	Comprehensive study of the vapour–liquid equilibria of the pure two-centre Lennard–Jones plus pointdipole fluid. *Fluid Phase Equilibria*, **2003**, 209, 29-53	2.5	46
316	Vapor–liquid equilibrium of formaldehyde mixtures: New data and model revision. *AICHE Journal*, **1996**, 42, 1741-1752	3.6	46
315	Molecular models for 267 binary mixtures validated by vapor–liquid equilibria: A systematic approach. *Fluid Phase Equilibria*, **2009**, 279, 120-135	2.5	45
314	Vapor–liquid and Liquid–liquid Equilibria in Binary and Ternary Mixtures of Water, Methanol, and Methylal. *Journal of Chemical & Engineering Data*, **2001**, 46, 897-903	2.8	45
313	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	3.8	44
312	Quantitative NMR spectroscopy of complex technical mixtures using a virtual reference: chemical equilibria and reaction kinetics of formaldehyde-water-1,3,5-trioxane. *Analytical and Bioanalytical Chemistry*, **2006**, 385, 910-7	4.4	43
311	Experimental study and model of reaction kinetics of heterogeneously catalyzed methylal synthesis. *Chemical Engineering Research and Design*, **2012**, 90, 696-703	5.5	42
310	A short-cut method for assessing absorbents for post-combustion carbon dioxide capture. *International Journal of Greenhouse Gas Control*, **2011**, 5, 413-421	4.2	42
309	Molecular models of unlike interactions in fluid mixtures. *Molecular Simulation*, **2005**, 31, 215-221	2	42

308	Prediction of Joule–Thomson inversion curves for pure fluids and one mixture by molecular simulation. *Cryogenics*, **2005**, 45, 253-258	1.8	42
307	Multi-Objective Optimization and Decision Support in Process Engineering—Implementation and Application. *Chemie-Ingenieur-Technik*, **2014**, 86, 1065-1072	0.8	41
306	Excess equimolar radius of liquid drops. *Physical Review E*, **2012**, 85, 031605	2.4	41
305	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. *Journal of Chemical Information and Modeling*, **2019**, 59, 4248-4265	6.1	40
304	Phase Equlibria for Hexyl Acetate Reactive Distillation. *Journal of Chemical & Engineering Data*, **2005**, 50, 1677-1683	2.8	40
303	Kinetics of oligomerization reactions in formaldehyde solutions: NMR experiments up to 373 K and thermodynamically consistent model. *Chemical Engineering and Processing: Process Intensification*, **2005**, 44, 653-660	3.7	40
302	Revised vapor-liquid equilibrium model for multicomponent formaldehyde mixtures. *AICHE Journal*, **1990**, 36, 1807-1814	3.6	40
301	Equation of state for the Lennard-Jones truncated and shifted fluid with a cut-off radius of 2.5 σ based on perturbation theory and its applications to interfacial thermodynamics. *Molecular Physics*, **2018**, 116, 2083-2094	1.7	39
300	An optimised molecular model for ammonia. *Molecular Physics*, **2008**, 106, 1039-1046	1.7	39
299	Synthesis of n-hexyl acetate by reactive distillation. *Chemical Engineering and Processing: Process Intensification*, **2004**, 43, 397-409	3.7	39
298	Multicriteria optimization of molecular force fields by Pareto approach. *Fluid Phase Equilibria*, **2014**, 373, 100-108	2.5	36
297	Chemical Equilibrium and Reaction Kinetics of Heterogeneously Catalyzed n-Hexyl Acetate Esterification. *Industrial & Engineering Chemistry Research*, **2006**, 45, 4123-4132	3.9	36
296	Modeling and simulation of reactive absorption of CO2 with MEA: Results for four different packings on two different scales. *Chemical Engineering Science*, **2014**, 105, 179-190	4.4	35
295	Thermodynamics of Phase and Chemical Equilibrium in a Strongly Nonideal Esterification System. *Journal of Chemical & Engineering Data*, **2005**, 50, 92-101	2.8	35
294	Vapor–liquid equilibrium of formaldehyde-containing mixtures at temperatures below 320 K. *Fluid Phase Equilibria*, **1991**, 64, 185-199	2.5	35
293	Multiphase high-pressure equilibria of carbon dioxide-water-isopropanol. *Journal of Supercritical Fluids*, **1993**, 6, 211-222	4.2	35
292	Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants. *Energy Procedia*, **2009**, 1, 1249-1256	2.3	34
291	Quantitative and qualitative 1H, 13C, and 15N NMR spectroscopic investigation of the urea-formaldehyde resin synthesis. *Magnetic Resonance in Chemistry*, **2014**, 52, 138-62	2.1	33

290	Self-Diffusion and Binary Maxwell–Stefan Diffusion Coefficients of Quadrupolar Real Fluids from Molecular Simulation. *International Journal of Thermophysics*, **2005**, 26, 1389-1407	2.1	33
289	MolMod – an open access database of force fields for molecular simulations of fluids. *Molecular Simulation*, **2019**, 45, 806-814	2	32
288	591 TFLOPS Multi-trillion Particles Simulation on SuperMUC. *Lecture Notes in Computer Science*, **2013**, 1-12	0.9	32
287	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
286	Molecular dispersion energy parameters for alkali and halide ions in aqueous solution. *Journal of Chemical Physics*, **2014**, 140, 044504	3.9	32
285	Quantitative on-line high-resolution NMR spectroscopy in process engineering applications. *Analytical and Bioanalytical Chemistry*, **2003**, 375, 1111-5	4.4	32
284	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
283	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
282	Thermodynamic Properties of Aqueous Poly(vinylpyrrolidone) Solutions from Laser-Light-Scattering, Membrane Osmometry, and Isopiestic Measurements. *Journal of Chemical & Engineering Data*, **2003**, 48, 689-698	2.8	31
281	Analysis of homogeneous distillation processes. *Chemical Engineering Science*, **2012**, 84, 315-332	4.4	30
280	Microcalorimetric study of adsorption of human monoclonal antibodies on cation exchange chromatographic materials. *Journal of Chromatography A*, **2008**, 1205, 1-9	4.5	30
279	Kinetics of the poly(oxymethylene) glycol formation in aqueous formaldehyde solutions. *Industrial & Engineering Chemistry Research*, **1991**, 30, 2195-2200	3.9	30
278	Development of an Integrated Reaction–Distillation Process for the Production of Methylal. *Industrial & Engineering Chemistry Research*, **2017**, 56, 575-582	3.9	29
277	A calorimetric study of carbamate formation. *Journal of Chemical Thermodynamics*, **2011**, 43, 664-669	2.9	29
276	Thermal properties of the metastable supersaturated vapor of the Lennard-Jones fluid. *Journal of Chemical Physics*, **2005**, 122, 144506	3.9	29
275	Molecular modelling and simulation of the surface tension of real quadrupolar fluids. *Chemical Engineering Science*, **2015**, 121, 110-117	4.4	28
274	Interfacial properties of binary Lennard-Jones mixtures by molecular simulation and density gradient theory. *Journal of Chemical Physics*, **2019**, 150, 174704	3.9	28
273	Microcalorimetric study of the adsorption of PEGylated lysozyme on a strong cation exchange resin. *Journal of Chromatography A*, **2011**, 1218, 4720-6	4.5	28

272	Vapor–liquid equilibria of hydrogen chloride, phosgene, benzene, chlorobenzene, ortho-dichlorobenzene, and toluene by molecular simulation. *AICHE Journal*, **2011**, 57, 1043-1060	3.6	28
271	Joule–Thomson inversion curves of mixtures by molecular simulation in comparison to advanced equations of state: Natural gas as an example. *Fluid Phase Equilibria*, **2007**, 258, 34-40	2.5	28
270	Solubility of Formaldehyde and Trioxane in Aqueous Solutions. *Journal of Chemical & Engineering Data*, **2004**, 49, 642-646	2.8	28
269	Thermodynamic and IR spectroscopic studies of solutions with simultaneous association and solvation. *Fluid Phase Equilibria*, **2003**, 208, 23-51	2.5	28
268	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
267	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
266	On-line 1H NMR spectroscopic investigation of hydrogen bonding in supercritical and near critical CO2–methanol up to 35MPa and 403K. *Journal of Supercritical Fluids*, **2007**, 43, 267-275	4.2	27
265	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
264	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
263	On-Line NMR Spectroscopic Reaction Kinetic Study of Urea–Formaldehyde Resin Synthesis. *Industrial & Engineering Chemistry Research*, **2014**, 53, 12602-12613	3.9	26
262	Hydrogen bonding of ethanol in supercritical mixtures with CO2 by 1H NMR spectroscopy and molecular simulation. *Journal of Supercritical Fluids*, **2012**, 68, 94-103	4.2	26
261	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
260	A set of molecular models for alkaline-earth cations in aqueous solution. *Journal of Physical Chemistry B*, **2012**, 116, 5448-57	3.4	26
259	Homogeneous nucleation in supersaturated vapors of methane, ethane, and carbon dioxide predicted by brute force molecular dynamics. *Journal of Chemical Physics*, **2008**, 128, 164510	3.9	26
258	Multiphase high-pressure equilibria of carbon dioxide-water-acetone. *Journal of Supercritical Fluids*, **1994**, 7, 245-250	4.2	26
257	TweTriS: Twenty trillion-atom simulation. *International Journal of High Performance Computing Applications*, **2019**, 33, 838-854	1.8	25
256	Thermostatted micro-reactor NMR probe head for monitoring fast reactions. *Journal of Magnetic Resonance*, **2014**, 242, 155-61	3	25
255	New Experimental Results for the Vapor–Liquid Equilibrium of the Binary System (Trioxane + Water) and the Ternary System (Formaldehyde + Trioxane + Water). *Journal of Chemical & Engineering Data*, **2005**, 50, 1218-1223	2.8	25

254	Distillation of formaldehyde containing mixtures: laboratory experiments, equilibrium stage modeling and simulation. *Chemical Engineering and Processing: Process Intensification*, **2005**, 44, 687-694	3.7	25
253	Multi-criteria optimization for parameterization of SAFT-type equations of state for water. *AICHE Journal*, **2018**, 64, 226-237	3.6	24
252	Microcalorimetric study of the adsorption of PEGylated lysozyme and PEG on a mildly hydrophobic resin: influence of ammonium sulfate. *Langmuir*, **2012**, 28, 11376-83	4	24
251	Molecular Modeling and Simulation of Vapor□liquid Equilibria of Ethylene Oxide, Ethylene Glycol, and Water as Well as their Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2012**, 51, 7428-7440	3.9	24
250	Contact angle dependence on the fluid-wall dispersive energy. *Langmuir*, **2010**, 26, 10913-7	4	24
249	Removal of carbon dioxide from flue gases with aqueous MEA solution containing ethanol. *Chemical Engineering and Processing: Process Intensification*, **2014**, 75, 81-89	3.7	23
248	Limiting Activity Coefficients in Alcohol-Containing Organic Solutions from Headspace Gas Chromatography. *Journal of Chemical & Engineering Data*, **1998**, 43, 74-80	2.8	23
247	Molecular simulation study of hydrogen bonding mixtures and new molecular models for mono- and dimethylamine. *Fluid Phase Equilibria*, **2008**, 263, 144-159	2.5	23
246	Reaction Kinetics of the Homogeneously Catalyzed Esterification of 1-Butanol with Acetic Acid in a Wide Range of Initial Compositions. *Industrial & Engineering Chemistry Research*, **2006**, 45, 1869-1874	3.9	23
245	Characterization of alkylsilane self-assembled monolayers by molecular simulation. *Langmuir*, **2015**, 31, 2630-8	4	22
244	Engineering Molecular Models: Efficient Parameterization Procedure and Cyclohexanol as Case Study. *Soft Materials*, **2012**, 10, 3-25	1.7	22
243	Solvent activity in electrolyte solutions from molecular simulation of the osmotic pressure. *Journal of Chemical Physics*, **2016**, 144, 084112	3.9	22
242	Temperature Dependence of the Density of Aqueous Alkali Halide Salt Solutions by Experiment and Molecular Simulation. *Journal of Chemical & Engineering Data*, **2014**, 59, 3434-3448	2.8	21
241	Microcalorimetric study of the adsorption of native and mono-PEGylated bovine serum albumin on anion-exchangers. *Journal of Chromatography A*, **2013**, 1277, 58-68	4.5	21
240	Pilot plant experiments for two new amine solvents for post-combustion carbon dioxide capture. *International Journal of Greenhouse Gas Control*, **2013**, 18, 305-314	4.2	21
239	Thermodynamic properties for applications in chemical industry via classical force fields. *Topics in Current Chemistry*, **2012**, 307, 201-49		21
238	Application of IR-spectroscopy in thermodynamic investigations of associating solutions. *Fluid Phase Equilibria*, **2003**, 205, 195-214	2.5	21
237	Sensitivity study for the rate-based simulation of the reactive absorption of CO2. *Energy Procedia*, **2011**, 4, 533-540	2.3	20

236	Shear viscosity and thermal conductivity of quadrupolar real fluids from molecular simulation. *Molecular Simulation*, **2005**, 31, 787-793	2	20
235	Efficient Approach for Calculating Pareto Boundaries under Uncertainties in Chemical Process Design. *Industrial & Engineering Chemistry Research*, **2017**, 56, 12672-12681	3.9	19
234	Long-range correction for multi-site Lennard-Jones models and planar interfaces. *Molecular Physics*, **2014**, 112, 2227-2234	1.7	19
233	Experimental study and modeling of the influence of mixed electrolytes on adsorption of macromolecules on a hydrophobic resin. *Journal of Chromatography A*, **2013**, 1315, 135-44	4.5	19
232	A thermodynamic model for vanadate in aqueous solution--equilibria and reaction enthalpies. *Dalton Transactions*, **2013**, 42, 2622-8	4.3	19
231	1H- and 13C-NMR spectroscopic study of chemical equilibria in the system acetaldehyde + water. *AICHE Journal*, **2015**, 61, 177-187	3.6	19
230	Molecular model for formic acid adjusted to vapor□quid equilibria. *Chemical Physics Letters*, **2007**, 435, 268-272	2.5	19
229	Molecular interactions at vapor-liquid interfaces: Binary mixtures of simple fluids. *Physical Review E*, **2020**, 101, 012802	2.4	18
228	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
227	Prediction of Transport Properties of Liquid Ammonia and Its Binary Mixture with Methanol by Molecular Simulation. *International Journal of Thermophysics*, **2012**, 33, 449-468	2.1	18
226	Prediction of ternary vapor□quid equilibria for 33 systems by molecular simulation. *Fluid Phase Equilibria*, **2009**, 287, 62-69	2.5	18
225	Thermodynamic Properties of Aqueous Dextran Solutions from Laser-Light-Scattering, Membrane Osmometry, and Isopiestic Measurements. *Journal of Chemical & Engineering Data*, **1999**, 44, 230-242	2.8	18
224	Activities in Aqueous Solutions of the Alkali Halide Salts from Molecular Simulation. *Journal of Chemical & Engineering Data*, **2016**, 61, 4068-4076	2.8	18
223	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
222	Machine Learning in Thermodynamics: Prediction of Activity Coefficients by Matrix Completion. *Journal of Physical Chemistry Letters*, **2020**, 11, 981-985	6.4	17
221	Topological analysis of vapor□quid equilibrium diagrams for distillation process design. *Physical Chemistry Chemical Physics*, **2002**, 4, 896-908	3.6	17
220	Monoalkylcarbonate Formation in Methyldiethanolamine□H2O□CO2. *Industrial & Engineering Chemistry Research*, **2017**, 56, 9006-9015	3.9	17
219	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

218	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
217	Automated development of force fields for the calculation of thermodynamic properties: acetonitrile as a case study. *Molecular Simulation*, **2013**, 39, 109-118	2	16
216	Thermodynamic analysis of reaction-distillation processes based on piecewise linear models. *Chemical Engineering Science*, **2014**, 109, 284-295	4.4	16
215	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
214	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
213	Method for Estimating Activity Coefficients of Target Components in Poorly Specified Mixtures. *Industrial & Engineering Chemistry Research*, **2018**, 57, 7310-7313	3.9	16
212	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
211	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
210	Henry's Law Constant from Molecular Simulation: A Systematic Study of 95 Systems. *International Journal of Thermophysics*, **2009**, 30, 1791-1810	2.1	15
209	Prediction of the overall enthalpy of CO2 absorption in aqueous amine systems from experimentally determined reaction enthalpies. *Energy Procedia*, **2011**, 4, 1542-1549	2.3	15
208	Shear viscosity and thermal conductivity of dipolar real fluids from equilibrium molecular dynamics simulation. *Cryogenics*, **2006**, 46, 711-717	1.8	15
207	Multiphase high-pressure equilibria of carbon dioxide-water-propionic acid and carbon dioxide-water-i sop ropanol. *Journal of Supercritical Fluids*, **1996**, 9, 19-25	4.2	15
206	Influence of dispersive long-range interactions on properties of vapour–liquid equilibria and interfaces of binary Lennard-Jones mixtures. *Molecular Physics*, **2020**, 118, e1699185	1.7	15
205	Molecular simulation study on the solubility of carbon dioxide in mixtures of cyclohexane + cyclohexanone. *Fluid Phase Equilibria*, **2012**, 315, 77-83	2.5	14
204	Study of heterogeneously catalysed reactive distillation using the D+R tray—A novel type of laboratory equipment. *Chemical Engineering Research and Design*, **2011**, 89, 1271-1280	5.5	14
203	Thermodynamic models for vapor–liquid equilibria of nitrogen+oxygen+carbon dioxide at low temperatures. *Cryogenics*, **2009**, 49, 72-79	1.8	14
202	Comment on "An optimized potential for carbon dioxide" [J. Chem. Phys. 122, 214507 (2005)]. *Journal of Chemical Physics*, **2008**, 129, 087101; author reply 087102	3.9	14
201	Feasibility and multiplicity in reaction–distillation processes for systems with competing irreversible reactions. *Chemical Engineering Science*, **2000**, 55, 5421-5436	4.4	14

200	Review and comparison of equations of state for the Lennard-Jones fluid. *Fluid Phase Equilibria*, **2020**, 523, 112772	2.5	14
199	The Influence of Lubrication and the Solid-Fluid Interaction on Thermodynamic Properties in a Nanoscopic Scratching Process. *Langmuir*, **2019**, 35, 16948-16960	4	14
198	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
197	Solubility of Carbon Dioxide in Poly(oxymethylene) Dimethyl Ethers. *Journal of Chemical & Engineering Data*, **2017**, 62, 4027-4031	2.8	13
196	Reaction Monitoring by Benchtop NMR Spectroscopy Using a Novel Stationary Flow Reactor Setup. *Industrial & Engineering Chemistry Research*, **2019**, 58, 18125-18133	3.9	13
195	Swelling equilibrium of hydrogels of (N-isopropyl acrylamide+anionic and cationic comonomers) in aqueous solutions of sodium chloride: Experimental results and modeling. *Fluid Phase Equilibria*, **2013**, 337, 137-149	2.5	13
194	Simultaneous description of bulk and interfacial properties of fluids by the Mie potential. *Molecular Physics*, **2017**, 115, 1017-1030	1.7	13
193	Mastering the Reaction Is the Key to Successful Design of Heterogeneously Catalyzed Reactive Distillation: A Comprehensive Case Study of Hexyl Acetate Synthesis. *Industrial & Engineering Chemistry Research*, **2008**, 47, 6014-6024	3.9	13
192	High-Pressure Phase Equilibria of Carbon Dioxide + 1-Hexanol at 303.15 and 313.15 K. *Journal of Chemical & Engineering Data*, **2003**, 48, 1365-1367	2.8	13
191	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
190	Surface tension of the two center Lennard-Jones plus quadrupole model fluid. *Fluid Phase Equilibria* , **2015**, 392, 12-18	2.5	12
189	Sub-zero cooling: A novel strategy for high performance cutting. *CIRP Annals - Manufacturing Technology*, **2018**, 67, 95-98	4.9	12
188	Analysis of heterogeneous distillation processes. *Chemical Engineering Science*, **2013**, 104, 374-388	4.4	12
187	A novel type of equipment for reactive distillation: Model development, simulation, sensitivity and error analysis. *AICHE Journal*, **2013**, 59, 1533-1543	3.6	12
186	Flexible or rigid molecular models? A study on vapour–liquid equilibrium properties of ammonia. *Molecular Physics*, **2011**, 109, 619-624	1.7	12
185	n-Hexyl acetate pilot plant reactive distillation with modified internals. *Chemical Engineering and Processing: Process Intensification*, **2005**, 44, 677-685	3.7	12
184	Enthalpy change on vaporization of aqueous and methanolic formaldehyde solutions. *AICHE Journal*, **1992**, 38, 1693-1702	3.6	12
183	Effects of Lubrication on the Friction in Nanometric Machining Processes: A Molecular Dynamics Approach. *Applied Mechanics and Materials*,869, 85-93	0.3	12

182	Surface tension of the two center Lennard-Jones plus point dipole fluid. *Journal of Chemical Physics*, **2016**, 144, 054702	3.9	12
181	Mass transfer through vapour–liquid interfaces: a molecular dynamics simulation study. *Molecular Physics*, **2021**, 119, e1810798	1.7	12
180	Activity coefficients from molecular simulations using the OPAS method. *Journal of Chemical Physics*, **2017**, 147, 144108	3.9	11
179	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
178	Monoalkylcarbonate formation in the system monoethanolamine–water–carbon dioxide. *Fluid Phase Equilibria*, **2019**, 486, 98-105	2.5	11
177	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
176	On the prediction of transport properties of monomethylamine, dimethylamine, dimethylether and hydrogen chloride by molecular simulation. *Fluid Phase Equilibria*, **2012**, 316, 46-54	2.5	11
175	Convex envelope method for the determination of fluid phase diagrams. *Fluid Phase Equilibria*, **2012**, 324, 108-116	2.5	11
174	On the difference between a point multipole and an equivalent linear arrangement of point charges in force field models for vapour–liquid equilibria; partial charge based models for 59 real fluids. *Molecular Physics*, **2011**, 109, 1975-1982	1.7	11
173	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
172	Molecular simulation of the surface tension of 33 multi-site models for real fluids. *Journal of Molecular Liquids*, **2017**, 235, 126-134	6	10
171	Online process monitoring of a batch distillation by medium field NMR spectroscopy. *Chemical Engineering Science*, **2020**, 219, 115561	4.4	10
170	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
169	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
168	Swelling behavior of chemically cross-linked poly(N-IPAAm-allylglycine) hydrogels: Effects of NaCl and pH. *Fluid Phase Equilibria*, **2014**, 361, 257-265	2.5	10
167	Proof of ether-bridged condensation products in UF resins by 2D NMR spectroscopy. *Journal of Polymer Research*, **2013**, 20, 1	2.7	10
166	Studying Fast Reaction Kinetics with Online NMR Spectroscopy. *Chemie-Ingenieur-Technik*, **2017**, 89, 369-378	0.8	10
165	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

164	13C-NMR, 13C-13C gCOSY, and ESI-MS characterization of ether-bridged condensation products in N,N?-dimethylurea-formaldehyde systems. *Journal of Applied Polymer Science*, **2013**, 128, 3957-3963	2.9	10
163	Gas Solubility in Binary Liquid Mixtures: Carbon Dioxide in Cyclohexane + Cyclohexanone. *Journal of Chemical & Engineering Data*, **2011**, 56, 2477-2481	2.8	10
162	Molecular Dynamics Based Analysis of Nucleation and Surface Energy of Droplets in Supersaturated Vapors of Methane and Ethane. *Journal of Heat Transfer*, **2009**, 131,	1.8	10
161	Top-down model for dynamic simulation of cold-storage plants. *International Journal of Refrigeration*, **1996**, 19, 10-18	3.8	10
160	Heat of Dilution in Aqueous and Methanolic Formaldehyde Solutions. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1992**, 96, 83-96		10
159	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. *Computer Physics Communications*, **2021**, 262, 107860	4.2	10
158	Solvent cleaning and wettability of technical steel and titanium surfaces. *Adsorption Science and Technology*, **2016**, 34, 261-274	3.6	10
157	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
156	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
155	Density of Methanolic Alkali Halide Salt Solutions by Experiment and Molecular Simulation. *Journal of Chemical & Engineering Data*, **2015**, 60, 1614-1628	2.8	9
154	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
153	Molecular simulation of nano-dispersed fluid phases. *Chemical Engineering Science*, **2014**, 107, 235-244	4.4	9
152	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
151	Reaction Kinetics for Reactive Distillation Using Different Laboratory Reactors. *Industrial & Engineering Chemistry Research*, **2013**, 52, 624-637	3.9	9
150	New Equipment for Laboratory Studies of Heterogeneously Catalyzed Reactive Distillation. *Chemical Engineering and Technology*, **2009**, 32, 1313-1317	2	9
149	Reaktive Verdampfung formaldehydhaltiger Mischungen und Process Monitoring mit Online-NMR-Spektroskopie. *Chemie-Ingenieur-Technik*, **2003**, 75, 240-244	0.8	9
148	Pilot plant formaldehyde distillation: experiments and modelling. *Chemical Engineering and Processing: Process Intensification*, **2005**, 44, 671-676	3.7	9
147	Digitalization in Thermodynamics. *Chemie-Ingenieur-Technik*, **2019**, 91, 201-214	0.8	8

146	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
145	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
144	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
143	Temperature dependence of adsorption of PEGylated lysozyme and pure polyethylene glycol on a hydrophobic resin: comparison of isothermal titration calorimetry and van't Hoff data. *Journal of Chromatography A*, **2014**, 1356, 188-96	4.5	8
142	Morphological analysis for the development of reliable models for heterogeneously catalysed reactive distillation. *Chemical Engineering Science*, **2013**, 91, 134-145	4.4	8
141	Long-range correction for dipolar fluids at planar interfaces. *Molecular Physics*, **2015**, 113, 3750-3756	1.7	8
140	Rechnergest□tzter konzeptioneller Entwurf von Destillations-/ Reaktionsprozessen. *Chemie-Ingenieur-Technik*, **2008**, 80, 207-213	0.8	8
139	Quantitative hochaufl□sende Online-NMR-Spektroskopie im Reaktions- und Prozessmonitoring. *Chemie-Ingenieur-Technik*, **2004**, 76, 965-969	0.8	8
138	Slope curve method for the analysis of separations in extraction columns of infinite height. *Chemical Engineering Science*, **2016**, 143, 105-113	4.4	8
137	NMR spectroscopic study of chemical equilibria in solutions of formaldehyde, water, and butynediol. *AICHE Journal*, **2017**, 63, 4442-4450	3.6	7
136	In situ measurement of liquid-liquid equilibria by medium field nuclear magnetic resonance. *Fluid Phase Equilibria*, **2017**, 438, 44-52	2.5	7
135	Thermophysical Properties of Mixtures of Titanium(IV) Isopropoxide (TTIP) and p-Xylene. *Journal of Chemical & Engineering Data*, **2020**, 65, 869-876	2.8	7
134	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
133	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
132	Predicting supersaturation by rate-based simulations of reactive absorption. *Chemical Engineering Science*, **2014**, 118, 41-49	4.4	7
131	NMR Spectroscopic Study of the Aldoxane Formation in Aqueous Acetaldehyde Solutions. *Industrial & Engineering Chemistry Research*, **2014**, 53, 8395-8403	3.9	7
130	Gas solubility of carbon dioxide and of oxygen in cyclohexanol by experiment and molecular simulation. *Journal of Chemical Thermodynamics*, **2012**, 49, 114-118	2.9	7
129	Fluid-phase coexistence for the oxidation of CO2 expanded cyclohexane: Experiment, molecular simulation, and COSMO-SAC. *AICHE Journal*, **2013**, 59, 2236-2250	3.6	7

128	Reactive Distillation in a Dividing-Wall Column: Model Development, Simulation, and Error Analysis. *Chemie-Ingenieur-Technik*, **2017**, 89, 1315-1324	0.8	7
127	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
126	The air pressure effect on the homogeneous nucleation of carbon dioxide by molecular simulation. *Atmospheric Research*, **2011**, 101, 519-526	5.4	7
125	Heterogen katalysierte Reaktivdestillation: Design und Scale-up am Beispiel von Methylacetat. *Chemie-Ingenieur-Technik*, **2002**, 74, 1207-1218	0.8	7
124	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
123	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
122	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
121	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
120	SkaSim Skalierbare HPC-Software für molekulare Simulationen in der chemischen Industrie. *Chemie-Ingenieur-Technik*, **2018**, 90, 295-306	0.8	6
119	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
118	Equilibrium swelling of some poly(N-IPAAm-sulfobetaine) hydrogels in water and in aqueous solutions of a single salt. *Fluid Phase Equilibria*, **2014**, 367, 194-203	2.5	6
117	CO2-Abtrennung für fossil befeuerte Kraftwerke. *Chemie-Ingenieur-Technik*, **2010**, 82, 1639-1653	0.8	6
116	Continuous Three-Phase Distillation. *Chemical Engineering Research and Design*, **2007**, 85, 144-148	5.5	6
115	Pareto-Navigation in Chemical Engineering. *Computer Aided Chemical Engineering*, **2011**, 29, 422-426	0.6	6
114	Density of ethanolic alkali halide salt solutions by experiment and molecular simulation. *Fluid Phase Equilibria*, **2016**, 408, 141-150	2.5	5
113	Prediction of flow effects in quantitative NMR measurements. *Journal of Magnetic Resonance*, **2020**, 312, 106683	3	5
112	Simulation of Surface Wetting by Droplets Using a Phase Field Model. *Proceedings in Applied Mathematics and Mechanics*, **2016**, 16, 519-520	0.2	5
111	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

110	Solubility of Carbon Dioxide in Activated Potash Solutions in the Low and High Gas Loading Regions. *Industrial & Engineering Chemistry Research*, **2013**, 52, 13477-13489	3.9	5
109	Fully Automated Weighing of Liquid Substances with a Laboratory Robot. *Chemical Engineering and Technology*, **2014**, 37, 168-172	2	5
108	Separation efficiency of thin-film evaporators: Experiments with water–ethylene glycol and methanol–water and stage-based modeling. *Chemical Engineering and Processing: Process Intensification*, **2008**, 47, 209-214	3.7	5
107	Computational Molecular Engineering as an Emerging Technology in Process Engineering. *IT - Information Technology*, **2013**, 55, 97-101	0.4	5
106	Generalized Chemical Equilibrium Constant of Formaldehyde Oligomerization. *Industrial & Engineering Chemistry Research*, **2020**, 59, 11431-11440	3.9	5
105	Multi-criteria optimization for parametrizing excess Gibbs energy models. *Fluid Phase Equilibria*, **2020**, 522, 112676	2.5	5
104	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
103	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
102	Vapor–liquid Equilibria and Chemical Equilibria in the System (Formaldehyde + Water + Isoprenol). *Industrial & Engineering Chemistry Research*, **2021**, 60, 4471-4483	3.9	5
101	Recovery of Furfural and Acetic Acid from Wood Hydrolysates in Biotechnological Downstream Processing. *Chemical Engineering and Technology*, **2018**, 41, 2331-2336	2	5
100	Molecular simulation study of the CO2-N2O analogy. *Fluid Phase Equilibria*, **2017**, 442, 44-52	2.5	4
99	Two Simple and Highly Efficient Variants of the Griffith-Ley Oxidation of Alcohols. *ChemCatChem*, **2020**, 12, 3919-3928	5.2	4
98	Surface Wetting with Droplets: A Phase Field Approach. *Proceedings in Applied Mathematics and Mechanics*, **2017**, 17, 501-502	0.2	4
97	On the effort of approaching pure components and azeotropes in distillation. *Chemical Engineering Science*, **2015**, 127, 253-259	4.4	4
96	INES – Interface between Experiments and Simulation. *Computer Aided Chemical Engineering*, **2014**, 1159-1164	0.4	4
95	Transport properties of anisotropic polar fluids. *Fluid Phase Equilibria*, **2006**, 249, 120-130	2.5	4
94	Transport properties of anisotropic polar fluids. *Fluid Phase Equilibria*, **2006**, 249, 131-139	2.5	4
93	Oberflächenerzeugungs-Morphologie-Eigenschafts-Beziehungen. *ZWF Zeitschrift Fuer Wirtschaftlichen Fabrikbetrieb*, **2016**, 111, 213-216	0.5	4

92	Kryogener Kühlschmierstoff auf der Basis von Ethylenglykol. *ZWF Zeitschrift Fuer Wirtschaftlichen Fabrikbetrieb*, **2016**, 111, 444-448	0.5	4
91	Application of NEAT for the simulation of liquid–liquid extraction processes with poorly specified feeds. *AICHE Journal*, **2020**, 66, e16826	3.6	4
90	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
89	Mathematical modeling of adsorption isotherms in mixed salt systems in hydrophobic interaction chromatography. *Biotechnology Progress*, **2018**, 34, 1251-1260	2.8	4
88	Vapor-liquid equilibrium in the ternary systems acetic acid + water + (xylose or glucose). *Fluid Phase Equilibria*, **2018**, 473, 323-329	2.5	4
87	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
86	Application of NEAT for determining the composition dependence of activity coefficients in poorly specified mixtures. *Chemical Engineering Science*, **2019**, 208, 115161	4.4	3
85	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
84	Carbonate complexes of vanadate. *Polyhedron*, **2015**, 95, 81-85	2.7	3
83	Triacetoneamine-derivates (EvAs) for CO2-absorption from process gases. *International Journal of Greenhouse Gas Control*, **2020**, 95, 102932	4.2	3
82	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
81	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
80	Equilibrium swelling of (N-isopropyl acrylamide + hydrophobic comonomer) gels in aqueous solutions of ethanol. *Fluid Phase Equilibria*, **2014**, 382, 235-243	2.5	3
79	Thermophysical Properties of Dry and Humid Air by Molecular Simulation Including Dew Point Calculations with the Mollier Ensemble. *Industrial & Engineering Chemistry Research*, **2009**, 48, 10110-10119	3.9	3
78	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
77	Turning of AISI 4140 (42CrMo4): A Novel Sub-zero Cooling Approach **2019**, 313-323		3
76	Development of Models for Large Molecules and Electrolytes in Solution for Process Engineering **2010**, 165-176		3
75	Atomistic Simulations of Electrolyte Solutions and Hydrogels with Explicit Solvent Models **2012**, 185-199		3

74	Short-cut method for assessing solvents for gas cleaning by reactive absorption. *Chemical Engineering Research and Design*, **2020**, 153, 757-767	5.5	3
73	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
72	A Force Field for Poly(oxymethylene) Dimethyl Ethers (OME). *Journal of Chemical Theory and Computation*, **2020**, 16, 2517-2528	6.4	3
71	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
70	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
69	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
68	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
67	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
66	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
65	A new scheme for process simulation by optimization: distillation as an example. *Computer Aided Chemical Engineering*, **2016**, 205-210	0.6	2
64	Spectroscopic investigations of solutions of lithium bis(fluorosulfonyl) imide (LiFSI) in valeronitrile. *Polyhedron*, **2020**, 183, 114458	2.7	2
63	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
62	ms2: Ein Werkzeug zur Berechnung thermodynamischer Stoffeigenschaften mittels molekularer Simulation. *Chemie-Ingenieur-Technik*, **2012**, 84, 114-120	0.8	2
61	Molekulare Modellierung und Simulation in der Fluidverfahrenstechnik. *Chemie-Ingenieur-Technik*, **2014**, 86, 982-990	0.8	2
60	Second Osmotic Virial Coefficients and Aggregation of Monoclonal Antibodies by Static Laser Light Scattering. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227, 333-344	3.1	2
59	Simulation of Reactive Absorption: Model Validation for CO2-MEA system. *Computer Aided Chemical Engineering*, **2011**, 29, 61-65	0.6	2
58	Vorhersage thermophysikalischer Eigenschaften realer Fluide mit molekularen Modellen. *Chemie-Ingenieur-Technik*, **2004**, 76, 891-895	0.8	2
57	Erratum to Henry's law constants of methane, nitrogen, oxygen and carbon dioxide in ethanol from 273 to 498 K: Prediction from molecular simulation [Fluid Phase Equilib. 233 (2005) 134–143]. *Fluid Phase Equilibria*, **2005**, 236, 272	2.5	2

56	Molecular Modelling and Simulation of Electrolyte Solutions, Biomolecules, and Wetting of Component Surfaces **2013**, 647-661		2
55	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
54	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
53	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
52	Solid-Liquid Equilibrium in the System 2-Keto--Gulonic Acid + -Ascorbic Acid + Water. *Chemical Engineering and Technology*, **2018**, 41, 2306-2311	2	2
51	Machine Learning of Thermophysical Properties. *Fluid Phase Equilibria*, **2021**, 549, 113206	2.5	2
50	Prediction of Henry's Law Constants by Matrix Completion. *AICHE Journal*,	3.6	2
49	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
48	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
47	NMR spectroscopic method for studying homogenous liquid phase reaction kinetics in systems used in reactive gas absorption and application to monoethanolamine□water□arbon dioxide. *Chemical Engineering Journal*, **2019**, 374, 1127-1137	14.7	1
46	Vapor-liquid equilibrium of mixtures containing formaldehyde, water, and butynediol. *Fluid Phase Equilibria*, **2019**, 490, 101-106	2.5	1
45	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
44	Adsorption and reaction layers when turning AISI 304 using various cooling strategies. *Procedia CIRP*, **2020**, 87, 125-130	1.8	1
43	Influence of sodium chloride on hydrophobic adsorption of PEGylated lysozyme. *Engineering in Life Sciences*, **2014**, 14, 100-105	3.4	1
42	Vollautomatisierte Einwaage fl□siger Substanzen mittels Laborroboter. *Chemie-Ingenieur-Technik*, **2012**, 84, 530-534	0.8	1
41	CO2-Abtrennung aus Kraftwerksabgasen auf dem Weg von der Forschung und Entwicklung zur industriellen Anwendung. *Chemie-Ingenieur-Technik*, **2011**, 83, 1005-1015	0.8	1
40	Molecular Modeling of Hydrogen Bonding Fluids: Vapor-Liquid Coexistence and Interfacial Properties **2010**, 471-483		1
39	Online-NMR-Spektroskopie □Mischungen messen im Fluss. *Nachrichten Aus Der Chemie*, **2007**, 55, 745-749	0.1	1

38	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
37	Reproducibility of atomistic friction computer experiments: a molecular dynamics simulation study. *Molecular Simulation*, **2021**, 47, 1509-1521	2	1
36	Influence of Salt and pH on the Swelling Equilibrium of Ionizable N-IPAAm Based Hydrogels: Experimental Results and Modeling **2013**, 163-173		1
35	Molecular Modeling and Simulation of Thermophysical Properties: Application to Pure Substances and Mixtures **2009**, 119-133		1
34	Molecular Modeling of Hydrogen Bonding Fluids: New Cyclohexanol Model and Transport Properties of Short Monohydric Alcohols **2009**, 529-541		1
33	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
32	High Flow-Rate Benchtop NMR Spectroscopy Enabled by Continuous Overhauser DNP. *Analytical Chemistry*, **2021**, 93, 8897-8905	7.8	1
31	Associating lattice cluster theory and application to modeling oleic acid + formic acid + formoxystearic acid. *AICHE Journal*, **2019**, 65, 783-791	3.6	1
30	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
29	Influence of Salts on the Adsorption of Lysozyme on a Mixed-Mode Resin. *Adsorption Science and Technology*, **2021**, 2021, 1-11	3.6	1
28	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
27	Solid□iquid 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
26	Conceptual design of a crystallization-based trioxane production process. *Chemical Engineering and Processing: Process Intensification*, **2021**, 171, 108710	3.7	0
25	Processes for the production of OME fuels **2020**, 191-203	0.3	0
24	Sub-zero metalworking fluids for high performance cutting of difficult to cut materials. *Procedia CIRP*, **2021**, 101, 342-345	1.8	0
23	Mutual Diffusion Coefficients from NMR Imaging. *Chemical Engineering Science*, **2022**, 117655	4.4	0
22	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
21	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	

20	A novel approach for infeasible path optimization of distillation-based flowsheets. *Chemical Engineering Science: X*, **2020**, 7, 100063	1.1
19	Reprint of: Molecular simulation of nano-dispersed fluid phases. *Chemical Engineering Science*, **2014**, 115, 195-204	4.4
18	Molecular Modeling and Simulation in Fluid Process Engineering. *ChemBioEng Reviews*, **2015**, 2, 303-310	5.2
17	Bio- und Chemieingenieurwissenschaften an der TU Kaiserslautern. *Chemie in Unserer Zeit*, **2011**, 45, 162-162	0.2
16	Mehrphasengleichgewichte in ternären fluiden Systemen unter erhöhtem Druck. *Chemie-Ingenieur-Technik*, **2002**, 74, 1130-1135	0.8
15	Stability analysis of molality-based virial expansion GE-models. *Fluid Phase Equilibria*, **2005**, 227, 267-274	2.5
14	Thermodynamic Modeling of Phosphorus Recovery from Wastewater. *Waste and Biomass Valorization*,1	3.2
13	Molecular Modeling of Hydrogen Bonding Fluids **2006**, 319-328	
12	Molecular Modeling of Hydrogen Bonding Fluids: Monomethylamine, Dimethylamine, and Water Revised **2007**, 515-525	
11	Density of solutions of formaldehyde in water and alcohols. *AICHE Journal*,e17573	3.6
10	Molecular Modeling of Hydrogen Bonding Fluids: Transport Properties and Vapor-Liquid Coexistence **2011**, 543-551	
9	Molecular Modeling of Hydrogen Bonding Fluids: Phase Behavior of Industrial Fluids **2012**, 567-579	
8	Die Entwicklung der Verfahrenstechnik an der TU Kaiserslautern. *Chemie-Ingenieur-Technik*, **2020**, 92, 1011-1022	0.8
7	A Simple Way for Implementing Extraction Columns of Infinite Height in Flowsheet Simulators. *Chemie-Ingenieur-Technik*, **2019**, 91, 314-322	0.8
6	Physicochemical Properties of LiFSI Solutions II: LiFSI with Water, MTBE, and Anisole. *Journal of Chemical & Engineering Data*, **2019**, 64, 878-883	2.8
5	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
4	Phase Field Simulations of Wetting Based on Molecular Simulations. *Proceedings in Applied Mathematics and Mechanics*, **2021**, 20, e202000035	0.2
3	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

2	Adsorption of oleic acid dissolved in isopropanol–water mixtures on hydrotalcite. *Adsorption Science and Technology*, **2018**, 36, 919-926	3.6
1	Investigation of Radial Shaft Seal Swelling Using a Special Tribometer and Magnetic Resonance Imaging.. *ACS Omega*, **2022**, 7, 11671-11677	3.9