Hans Hasse

List of Publications by Year
in descending order

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384	12,057	23567 58	49909 87
papers	citations	h-index	g-index

397	397	397	6547
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Poly(oxymethylene) dimethyl ethers as components of tailored diesel fuel: Properties, synthesis and purification concepts. Fuel, 2010, 89, 3315-3319.	6.4	372
2	A Set of Molecular Models for Symmetric Quadrupolar Fluids. Journal of Physical Chemistry B, 2001, 105, 12126-12133.	2.6	346
3	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.	4.6	191
4	Comprehensive study of the vapourâ€“liquid coexistence of the truncated and shifted Lennardâ€“Jones fluid including planar and spherical interface properties. Molecular Physics, 2006, 104, 1509-1527.	1.7	189
5	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.	3.0	182
6	Online NMR spectroscopic study of species distribution in MEAâ€“H2Oâ€“CO2 and DEAâ€“H2Oâ€“CO2. Fluid Phase Equilibria, 2008, 263, 131-143.	2.5	178
7	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, 5251-5259.	2.6	145
8	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.	3.7	144
9	FT-IR spectroscopic investigations of hydrogen bonding in alcoholâ€“hydrocarbon solutions. Fluid Phase Equilibria, 2001, 186, 1-25.	2.5	139
10	Experimental Pressureâ^'Temperature Data on Three- and Four-Phase Equilibria of Fluid, Hydrate, and Ice Phases in the System Carbon Dioxideâ^'Water. Journal of Chemical & Engineering Data, 1999, 44, 901-906.	1.9	135
11	Quantitative high-resolution on-line NMR spectroscopy in reaction and process monitoring. Journal of Magnetic Resonance, 2004, 166, 135-146.	2.1	135
12	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.	3.7	126
13	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.	3.7	124
14	Grand Equilibrium: vapour-liquid equilibria by a new molecular simulation method. Molecular Physics, 2002, 100, 3375-3383.	1.7	124
15	Pilot plant experimental studies of post combustion CO2 capture by reactive absorption with MEA and new solvents. Energy Procedia, 2009, 1, 963-970.	1.8	120
16	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.	5.6	111
17	From methanol to the oxygenated diesel fuel poly(oxymethylene) dimethyl ether: An assessment of the production costs. Fuel, 2016, 185, 67-72.	6.4	110
18	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	108

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19	ls1 mardyn: The Massively Parallel Molecular Dynamics Code for Large Systems. Journal of Chemical Theory and Computation, 2014, 10, 4455-4464.	5.3	108
20	Prediction of Transport Properties by Molecular Simulation: Methanol and Ethanol and Their Mixture. Journal of Physical Chemistry B, 2008, 112, 16664-16674.	2.6	106
21	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.	3.7	106
22	ms2: A molecular simulation tool for thermodynamic properties. Computer Physics Communications, 2011, 182, 2350-2367.	7.5	102
23	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. Journal of Chemical Information and Modeling, 2019, 59, 4248-4265.	5.4	101
24	Hydrogen Bonding of Methanol in Supercritical CO₂:â€‰ Comparison between ¹H NMR Spectroscopic Data and Molecular Simulation Results. Journal of Physical Chemistry B, 2007, 111, 9871-9878.	2.6	100
25	Unlike Lennardâ€“Jones parameters for vaporâ€“liquid equilibria. Journal of Molecular Liquids, 2007, 135, 170-178.	4.9	100
26	Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets. Computers and Chemical Engineering, 2014, 60, 354-363.	3.8	100
27	Molecular dynamics and experimental study of conformation change of poly(N-isopropylacrylamide) hydrogels in water. Fluid Phase Equilibria, 2010, 296, 164-172.	2.5	98
28	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.	4.3	97
29	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.	3.7	93
30	Fluid dynamics in reactive distillation packing KatapakÂ®-S. Chemical Engineering Science, 1999, 54, 1367-1374.	3.8	92
31	Henryâ€™s law constants of methane, nitrogen, oxygen and carbon dioxide in ethanol from 273 to 498â€‰K: Prediction from molecular simulation. Fluid Phase Equilibria, 2005, 233, 134-143.	2.5	91
32	Vaporâ€“liquid equilibria of mixtures containing nitrogen, oxygen, carbon dioxide, and ethane. AICHE Journal, 2003, 49, 2187-2198.	3.6	88
33	A set of molecular models for carbon monoxide and halogenated hydrocarbons. Journal of Chemical Physics, 2003, 119, 11396-11407.	3.0	88
34	High-pressure multiphase behaviour of ternary systems carbon dioxideâ€“waterâ€“polar solvent: review and modeling with the Pengâ€“Robinson equation of state. Journal of Supercritical Fluids, 1998, 12, 185-221.	3.2	86
35	CO₂ Capture for Fossil Fuelâ€Fired Power Plants. Chemical Engineering and Technology, 2011, 34, 163-172.	1.5	85
36	Quantitative NMR Spectroscopy of Complex Liquid Mixtures:Â Methods and Results for Chemical Equilibria in Formaldehydeâ^'Waterâ^'Methanol at Temperatures up to 383 K. Industrial & Engineering Chemistry Research, 2003, 42, 259-266.	3.7	82

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37	Mutual diffusion in the ternary mixture of water + methanol + ethanol and its binary subsystems. Physical Chemistry Chemical Physics, 2013, 15, 3985.	2.8	76
38	Osmotic Virial Coefficients of Aqueous Poly(ethylene glycol) from Laser-Light Scattering and Isopiestic Measurements. Macromolecules, 1995, 28, 3540-3552.	4.8	74
39	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.	6.4	74
40	Comprehensive study of the vapourâ€“liquid equilibria of the pure two-centre Lennardâ€“Jones plus pointquadrupole fluid. Fluid Phase Equilibria, 2001, 179, 339-362.	2.5	73
41	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.	2.1	73
42	Influence of ion-exchange resin catalysts on side reactions of the esterification of <mml:math altimg="si34.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.els. Chemical Engine	3.8	72
43	Development of a new industrial process for trioxane production. Chemical Engineering Science, 2007, 62, 5613-5620.	3.8	71
44	Molecular model for carbon dioxide optimized to vapor-liquid equilibria. Journal of Chemical Physics, 2010, 132, 234512.	3.0	71
45	Contact Angle of Sessile Drops in Lennard-Jones Systems. Langmuir, 2014, 30, 13606-13614.	3.5	71
46	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml56" display="inline" overflow="scroll" altimg="si19.gif"><mml:mi>m</mml:mi><mml:mi>s</mml:mi><mml:mn>2</mml:mn></mml:math>: A molecular simulation tool for thermodynamic properties, release 3.0. Computer Physics Communications, 2017, 221, 343-351.	7.5	70
47	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mi>m</mml:mi><mml:mi>s</mml:mi><mml:mn>2</mml:mn></mml:math>: A molecular simulation tool for thermodynamic properties, new version release. Computer Physics Communications, 2014, 185, 3302-3306.	7.5	67
48	Selection and Pilot Plant Tests of New Absorbents for Post-Combustion Carbon Dioxide Capture. Chemical Engineering Research and Design, 2007, 85, 510-515.	5.6	66
49	The influence of the liquid slab thickness on the planar vaporâ€“liquid interfacial tension. Physica A: Statistical Mechanics and Its Applications, 2013, 392, 2359-2367.	2.6	66
50	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.	1.9	66
51	Phase Equilibrium in Formaldehyde Containing Multicomponent Mixtures:Â Experimental Results for Formaldehyde + Chemistry Research, 2006, 45, 5155-5164.	3.7	65
52	MolMod â€“ an open access database of force fields for molecular simulations of fluids. Molecular Simulation, 2019, 45, 806-814.	2.0	65
53	Pilot plant experiments for post combustion carbon dioxide capture by reactive absorption with novel solvents. Energy Procedia, 2011, 4, 1-8.	1.8	62
54	A set of molecular models for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2012, 136, 084501.	3.0	62

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55	Multi-objective optimization using reduced models in conceptual design of a fuel additive production process. Chemical Engineering Science, 2013, 99, 118-126.	3.8	61
56	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.	3.7	61
57	Equation of state for the Lennard-Jones truncated and shifted fluid with a cut-off radius of 2.5â€‰ïƒ based on perturbation theory and its applications to interfacial thermodynamics. Molecular Physics, 2018, 116, 2083-2094.	1.7	61
58	Vaporâ^'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.	3.1	61
59	Methyl Acetate Hydrolysis in a Reactive Divided Wall Column. Chemical Engineering Research and Design, 2007, 85, 149-154.	5.6	59
60	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.	5.6	58
61	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.	4.6	58
62	Review and comparison of equations of state for the Lennard-Jones fluid. Fluid Phase Equilibria, 2020, 523, 112772.	2.5	58
63	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	56
64	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.	3.8	56
65	Enrichment at vapourâ€“liquid interfaces of mixtures: establishing a link between nanoscopic and macroscopic properties. International Reviews in Physical Chemistry, 2020, 39, 319-349.	2.3	56
66	Experimental study and model of reaction kinetics of heterogeneously catalyzed methylal synthesis. Chemical Engineering Research and Design, 2012, 90, 696-703.	5.6	55
67	Machine Learning in Thermodynamics: Prediction of Activity Coefficients by Matrix Completion. Journal of Physical Chemistry Letters, 2020, 11, 981-985.	4.6	55
68	Vaporâ€“liquid equilibrium of formaldehyde mixtures: New data and model revision. AICHE Journal, 1996, 42, 1741-1752.	3.6	54
69	Online NMR Spectroscopic Study of Species Distribution in MDEAâ^'H₂Oâ^'CO₂ and MDEAâ^'PIPâ^'H₂Oâ^'CO₂. Industrial & Engineering Chemistry Research, 2008, 47, 7917-7926.	3.7	54
70	Molecular models for 267 binary mixtures validated by vaporâ€“liquid equilibria: A systematic approach. Fluid Phase Equilibria, 2009, 279, 120-135.	2.5	54
71	Interfacial properties of binary Lennard-Jones mixtures by molecular simulation and density gradient theory. Journal of Chemical Physics, 2019, 150, 174704.	3.0	53
72	Vaporâ^'Liquid and Liquidâ^'Liquid Equilibria in Binary and Ternary Mixtures of Water, Methanol, and Methylal. Journal of Chemical & Engineering Data, 2001, 46, 897-903.	1.9	52

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73	Self Diffusion and Binary Maxwellâ€“Stefan Diffusion in Simple Fluids with the Greenâ€“Kubo Method. International Journal of Thermophysics, 2004, 25, 175-186.	2.1	52
74	Set of Molecular Models Based on Quantum Mechanical Ab Initio Calculations and Thermodynamic Data. Journal of Physical Chemistry B, 2008, 112, 12710-12721.	2.6	51
75	Comprehensive study of the vapourâ€“liquid equilibria of the pure two-centre Lennardâ€“Jones plus pointdipole fluid. Fluid Phase Equilibria, 2003, 209, 29-53.	2.5	50
76	A short-cut method for assessing absorbents for post-combustion carbon dioxide capture. International Journal of Greenhouse Gas Control, 2011, 5, 413-421.	4.6	50
77	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	50
78	Revised vapor-liquid equilibrium model for multicomponent formaldehyde mixtures. AICHE Journal, 1990, 36, 1807-1814.	3.6	49
79	Chemical potential of quadrupolar two-centre Lennard-Jones fluids by gradual insertion. Chemical Physics Letters, 2002, 356, 431-436.	2.6	49
80	Synthesis of n-hexyl acetate by reactive distillation. Chemical Engineering and Processing: Process Intensification, 2004, 43, 397-409.	3.6	48
81	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.	5.3	48
82	Kinetics of oligomerization reactions in formaldehyde solutions: NMR experiments up to 373K and thermodynamically consistent model. Chemical Engineering and Processing: Process Intensification, 2005, 44, 653-660.	3.6	47
83	Prediction of Jouleâ€“Thomson inversion curves for pure fluids and one mixture by molecular simulation. Cryogenics, 2005, 45, 253-258.	1.7	47
84	Molecular models of unlike interactions in fluid mixtures. Molecular Simulation, 2005, 31, 215-221.	2.0	47
85	Quantitative NMR spectroscopy of complex technical mixtures using a virtual reference: chemical equilibria and reaction kinetics of formaldehydeâ€“waterâ€“1,3,5-trioxane. Analytical and Bioanalytical Chemistry, 2006, 385, 910-917.	3.7	47
86	An optimised molecular model for ammonia. Molecular Physics, 2008, 106, 1039-1046.	1.7	47
87	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.	3.8	47
88	Multiâ€Objective Optimization and Decision Support in Process Engineering â€“ Implementation and Application. Chemie-Ingenieur-Technik, 2014, 86, 1065-1072.	0.8	46
89	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	2.1	44
90	Quantitative and qualitative ¹H,â€‰¹³C, and ¹⁵Nâ€‰NMR spectroscopic investigation of the ureaâ€“formaldehyde resin synthesis. Magnetic Resonance in Chemistry, 2014, 52, 138-162.	1.9	44

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91	TweTriS: Twenty trillion-atom simulation. International Journal of High Performance Computing Applications, 2019, 33, 838-854.	3.7	43
92	Vaporâ€"liquid equilibrium of formaldehyde-containing mixtures at temperatures below 320 K. Fluid Phase Equilibria, 1991, 64, 185-199.	2.5	42
93	Thermodynamics of Phase and Chemical Equilibrium in a Strongly Nonideal Esterification System. Journal of Chemical & Engineering Data, 2005, 50, 92-101.	1.9	42
94	Multicriteria optimization of molecular force fields by Pareto approach. Fluid Phase Equilibria, 2014, 373, 100-108.	2.5	42
95	Quantitative on-line high-resolution NMR spectroscopy in process engineering applications. Analytical and Bioanalytical Chemistry, 2003, 375, 1111-1115.	3.7	41
96	Phase Equlibria for Hexyl Acetate Reactive Distillation. Journal of Chemical & Engineering Data, 2005, 50, 1677-1683.	1.9	41
97	Multiphase high-pressure equilibria of carbon dioxide-water-isopropanol. Journal of Supercritical Fluids, 1993, 6, 211-222.	3.2	40
98	Self-Diffusion and Binary Maxwellâ€"Stefan Diffusion Coefficients of Quadrupolar Real Fluids from Molecular Simulation. International Journal of Thermophysics, 2005, 26, 1389-1407.	2.1	40
99	Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants. Energy Procedia, 2009, 1, 1249-1256.	1.8	40
100	Chemical Equilibrium and Reaction Kinetics of Heterogeneously Catalyzedn-Hexyl Acetate Esterification. Industrial & Engineering Chemistry Research, 2006, 45, 4123-4132.	3.7	38
101	Kinetics of the poly(oxymethylene) glycol formation in aqueous formaldehyde solutions. Industrial & Engineering Chemistry Research, 1991, 30, 2195-2200.	3.7	37
102	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.	1.9	37
103	Jouleâ€"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	37
104	Molecular dispersion energy parameters for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2014, 140, 044504.	3.0	36
105	Development of an Integrated Reactionâ€"Distillation Process for the Production of Methylal. Industrial & Engineering Chemistry Research, 2017, 56, 575-582.	3.7	36
106	Influence of dispersive long-range interactions on properties of vapourâ€"liquid equilibria and interfaces of binary Lennard-Jones mixtures. Molecular Physics, 2020, 118, e1699185.	1.7	36
107	Molecular interactions at vapor-liquid interfaces: Binary mixtures of simple fluids. Physical Review E, 2020, 101, 012802.	2.1	36
108	Mass transfer through vapourâ€"liquid interfaces: a molecular dynamics simulation study. Molecular Physics, 2021, 119, e1810798.	1.7	36

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109	Vaporâ€“liquid equilibria of hydrogen chloride, phosgene, benzene, chlorobenzene, orthoâ€dichlorobenzene, and toluene by molecular simulation. AIChE Journal, 2011, 57, 1043-1060.	3.6	35
110	âˆž/âˆž-Analysis of homogeneous distillation processes. Chemical Engineering Science, 2012, 84, 315-332.	3.8	35
111	Interfacial properties of binary mixtures of simple fluids and their relation to the phase diagram. Physical Chemistry Chemical Physics, 2020, 22, 12544-12564.	2.8	35
112	591 TFLOPS Multi-trillion Particles Simulation on SuperMUC. Lecture Notes in Computer Science, 2013, , 1-12.	1.3	34
113	Parametrization of two-center Lennard-Jones plus point-quadrupole force field models by multicriteria optimization. Fluid Phase Equilibria, 2016, 411, 33-42.	2.5	34
114	Multiâ€criteria optimization for parameterization of SAFTâ€type equations of state for water. AIChE Journal, 2018, 64, 226-237.	3.6	34
115	Solubility of Formaldehyde and Trioxane in Aqueous Solutions. Journal of Chemical & Engineering Data, 2004, 49, 642-646.	1.9	33
116	Molecular Modeling and Simulation of Vaporâ€“Liquid Equilibria of Ethylene Oxide, Ethylene Glycol, and Water as Well as their Binary Mixtures. Industrial & Engineering Chemistry Research, 2012, 51, 7428-7440.	3.7	33
117	Molecular modelling and simulation of the surface tension of real quadrupolar fluids. Chemical Engineering Science, 2015, 121, 110-117.	3.8	32
118	Interfacial and bulk properties of vapor-liquid equilibria in the system tolueneÂ+Âhydrogen chlorideÂ+Âcarbon dioxide by molecular simulation and density gradient theoryÂ+ÂPC-SAFT. Fluid Phase Equilibria, 2016, 427, 219-230.	2.5	32
119	Thermostatted micro-reactor NMR probe head for monitoring fast reactions. Journal of Magnetic Resonance, 2014, 242, 155-161.	2.1	31
120	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	31
121	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	31
122	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. Computer Physics Communications, 2021, 262, 107860.	7.5	31
123	Microcalorimetric study of adsorption of human monoclonal antibodies on cation exchange chromatographic materials. Journal of Chromatography A, 2008, 1205, 1-9.	3.7	30
124	Homogeneous nucleation in supersaturated vapors of methane, ethane, and carbon dioxide predicted by brute force molecular dynamics. Journal of Chemical Physics, 2008, 128, 164510.	3.0	30
125	Microcalorimetric study of the adsorption of PEGylated lysozyme on a strong cation exchange resin. Journal of Chromatography A, 2011, 1218, 4720-4726.	3.7	30
126	Thermodynamic and IR spectroscopic studies of solutions with simultaneous association and solvation. Fluid Phase Equilibria, 2003, 208, 23-51.	2.5	29

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127	Distillation of formaldehyde containing mixtures: laboratory experiments, equilibrium stage modeling and simulation. Chemical Engineering and Processing: Process Intensification, 2005, 44, 687-694.	3.6	29
128	Thermal properties of the metastable supersaturated vapor of the Lennard-Jones fluid. Journal of Chemical Physics, 2005, 122, 144506.	3.0	29
129	New Experimental Results for the Vaporâ"Liquid Equilibrium of the Binary System (Trioxane + Water) and the Ternary System (Formaldehyde + Trioxane + Water). Journal of Chemical & Engineering Data, 2005, 50, 1218-1223.	1.9	29
130	On-line 1H NMR spectroscopic investigation of hydrogen bonding in supercritical and near critical CO2â€"methanol up to 35MPa and 403K. Journal of Supercritical Fluids, 2007, 43, 267-275.	3.2	29
131	A calorimetric study of carbamate formation. Journal of Chemical Thermodynamics, 2011, 43, 664-669.	2.0	29
132	A Set of Molecular Models for Alkaline-Earth Cations in Aqueous Solution. Journal of Physical Chemistry B, 2012, 116, 5448-5457.	2.6	29
133	Hydrogen bonding of ethanol in supercritical mixtures with CO2 by 1H NMR spectroscopy and molecular simulation. Journal of Supercritical Fluids, 2012, 68, 94-103.	3.2	29
134	Design of a Production Process for Poly(oxymethylene) Dimethyl Ethers from Dimethyl Ether and Trioxane. Chemie-Ingenieur-Technik, 2018, 90, 1489-1496.	0.8	29
135	The Influence of Lubrication and the Solidâ€"Fluid Interaction on Thermodynamic Properties in a Nanoscopic Scratching Process. Langmuir, 2019, 35, 16948-16960.	3.5	29
136	Vapor-liquid interfacial properties of the system cyclohexaneÂ+ CO2: Experiments, molecular simulation and density gradient theory. Fluid Phase Equilibria, 2020, 518, 112583.	2.5	29
137	Engineering Molecular Models: Efficient Parameterization Procedure and Cyclohexanol as Case Study. Soft Materials, 2012, 10, 3-25.	1.7	28
138	On-Line NMR Spectroscopic Reaction Kinetic Study of Ureaâ€"Formaldehyde Resin Synthesis. Industrial & Engineering Chemistry Research, 2014, 53, 12602-12613.	3.7	28
139	Characterization of Alkylsilane Self-Assembled Monolayers by Molecular Simulation. Langmuir, 2015, 31, 2630-2638.	3.5	28
140	Solvent activity in electrolyte solutions from molecular simulation of the osmotic pressure. Journal of Chemical Physics, 2016, 144, 084112.	3.0	28
141	Multiphase high-pressure equilibria of carbon dioxide-water-acetone. Journal of Supercritical Fluids, 1994, 7, 245-250.	3.2	27
142	Microcalorimetric Study of the Adsorption of PEGylated Lysozyme and PEG on a Mildly Hydrophobic Resin: Influence of Ammonium Sulfate. Langmuir, 2012, 28, 11376-11383.	3.5	27
143	Pilot plant experiments for two new amine solvents for post-combustion carbon dioxide capture. International Journal of Greenhouse Gas Control, 2013, 18, 305-314.	4.6	27
144	Long-range correction for multi-site Lennard-Jones models and planar interfaces. Molecular Physics, 2014, 112, 2227-2234.	1.7	27

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145	Removal of carbon dioxide from flue gases with aqueous MEA solution containing ethanol. Chemical Engineering and Processing: Process Intensification, 2014, 75, 81-89.	3.6	27
146	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.	8.2	27
147	Molecular dynamics and phase field simulations of droplets on surfaces with wettability gradient. Computer Methods in Applied Mechanics and Engineering, 2020, 361, 112773.	6.6	27
148	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.	1.9	26
149	INES â€“ An Interface Between Experiments and Simulation to Support the Development of Robust Process Designs. Chemie-Ingenieur-Technik, 2015, 87, 1810-1825.	0.8	26
150	Reaction Monitoring by Benchtop NMR Spectroscopy Using a Novel Stationary Flow Reactor Setup. Industrial & Engineering Chemistry Research, 2019, 58, 18125-18133.	3.7	26
151	Application of IR-spectroscopy in thermodynamic investigations of associating solutions. Fluid Phase Equilibria, 2003, 205, 195-214.	2.5	25
152	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.	3.7	25
153	Molecular simulation study of hydrogen bonding mixtures and new molecular models for mono- and dimethylamine. Fluid Phase Equilibria, 2008, 263, 144-159.	2.5	25
154	Contact Angle Dependence on the Fluidâ^'Wall Dispersive Energy. Langmuir, 2010, 26, 10913-10917.	3.5	25
155	Efficient Approach for Calculating Pareto Boundaries under Uncertainties in Chemical Process Design. Industrial & Engineering Chemistry Research, 2017, 56, 12672-12681.	3.7	25
156	Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields. Topics in Current Chemistry, 2011, 307, 201-249.	4.0	24
157	A thermodynamic model for vanadate in aqueous solution â€“ equilibria and reaction enthalpies. Dalton Transactions, 2013, 42, 2622-2628.	3.3	24
158	Vaporâ€“liquid equilibrium and distillation of mixtures containing formaldehdye and poly(oxymethylene) dimethyl ethers. Chemical Engineering and Processing: Process Intensification, 2018, 131, 116-124.	3.6	24
159	Limiting Activity Coefficients in Alcohol-Containing Organic Solutions from Headspace Gas Chromatography. Journal of Chemical & Engineering Data, 1998, 43, 74-80.	1.9	23
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