

Joachim Groß

List of Publications by Year in descending order

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145
papers

8,808
citations

109321

35
h-index

43889

91
g-index

150
all docs

150
docs citations

150
times ranked

3125
citing authors

#	ARTICLE	IF	CITATIONS
1	Dielectric constant of mixed solvents based on perturbation theory. <i>Fluid Phase Equilibria</i> , 2022, 555, 113346.	2.5	7
2	Equation of state and Helmholtz energy functional for fused heterosegmented hard chains. <i>Physical Review E</i> , 2022, 105, 034110.	2.1	1
3	Perturbation theories for fluids with short-ranged attractive forces: A case study of the Lennard-Jones spline fluid. <i>Journal of Chemical Physics</i> , 2022, 156, 104504.	3.0	6
4	Modeling Subsurface Hydrogen Storage With Transport Properties From Entropy Scaling Using the PC-SAFT Equation of State. <i>Water Resources Research</i> , 2022, 58, .	4.2	10
5	Influence of layer slipping on adsorption of light gases in covalent organic frameworks: A combined experimental and computational study. <i>Microporous and Mesoporous Materials</i> , 2022, 336, 111796.	4.4	6
6	Towards optimal mixtures of working fluids: Integrated design of processes and mixtures for Organic Rankine Cycles. <i>Renewable and Sustainable Energy Reviews</i> , 2021, 135, 110179.	16.4	23
7	Accurate first-order perturbation theory for fluids: ϵ -theory. <i>Journal of Chemical Physics</i> , 2021, 154, 041102.	3.0	11
8	Modified Stokes-Einstein Equation for Molecular Self-Diffusion Based on Entropy Scaling. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 4453-4459.	3.7	16
9	Free-Energy-Averaged Potentials for Adsorption in Heterogeneous Slit Pores Using PC-SAFT Classical Density Functional Theory. <i>Langmuir</i> , 2021, 37, 3538-3549.	3.5	15
10	Surfactant Modeling Using Classical Density Functional Theory and a Group Contribution PC-SAFT Approach. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 7111-7123.	3.7	17
11	Predicting solvation free energies in non-polar solvents using classical density functional theory based on the PC-SAFT equation of state. <i>Journal of Chemical Physics</i> , 2021, 154, 244106.	3.0	6
12	Adsorption of light gases in covalent organic frameworks: comparison of classical density functional theory and grand canonical Monte Carlo simulations. <i>Microporous and Mesoporous Materials</i> , 2021, 324, 111263.	4.4	13
13	Hydrodynamic density functional theory for mixtures from a variational principle and its application to droplet coalescence. <i>Journal of Chemical Physics</i> , 2021, 155, 134101.	3.0	7
14	Accurate thermodynamics of simple fluids and chain fluids based on first-order perturbation theory and second virial coefficients: ϵ -theory. <i>Journal of Chemical Physics</i> , 2021, 155, 244501.	3.0	11
15	Guide to efficient solution of PC-SAFT classical Density Functional Theory in various Coordinate Systems using fast Fourier and similar Transforms. <i>Fluid Phase Equilibria</i> , 2020, 504, 112306.	2.5	21
16	Nonprimitive Model Electrolyte Solutions: Comprehensive Data from Monte Carlo Simulations. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 634-639.	1.9	4
17	Transferable Anisotropic Mie-Potential Force Field for n -Alcohols: Static and Dynamic Fluid Properties of Pure Substances and Binary Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 919-929.	3.7	8
18	Perturbation approaches for describing dipolar fluids and electrolyte solutions. <i>Journal of Chemical Physics</i> , 2020, 153, 044102.	3.0	4

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19	Multiobjective Optimization of PCP-SAFT Parameters for Water and Alcohols Using Surface Tension Data. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 5698-5707.	1.9	22
20	Force Fields with Fixed Bond Lengths and with Flexible Bond Lengths: Comparing Static and Dynamic Fluid Properties. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 1583-1593.	1.9	4
21	On the Selection of Boundary Conditions for Droplet Evaporation and Condensation at high Pressure and Temperature Conditions from interfacial Transport Resistivities. <i>International Journal of Heat and Mass Transfer</i> , 2020, 151, 119450.	4.8	26
22	A fast inverse Hankel Transform of first Order for computing vector-valued weight Functions appearing in Fundamental Measure Theory in cylindrical Coordinates. <i>Fluid Phase Equilibria</i> , 2020, 511, 112500.	2.5	3
23	Transferable Anisotropic United-Atom Mie (TAMie) Force Field: Transport Properties from Equilibrium Molecular Dynamic Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 8855-8869.	3.7	7
24	Prediction of Adsorption Isotherms and Selectivities: Comparison between Classical Density Functional Theory Based on the Perturbed-Chain Statistical Associating Fluid Theory Equation of State and Ideal Adsorbed Solution Theory. <i>Langmuir</i> , 2019, 35, 11690-11701.	3.5	30
25	Direct numerical simulation of sublimating ice particles. <i>International Journal of Thermal Sciences</i> , 2019, 145, 105953.	4.9	8
26	Extension of Wertheim's thermodynamic perturbation theory to include higher order graph integrals. <i>Journal of Chemical Physics</i> , 2019, 150, 244902.	3.0	1
27	Thermal Conductivity from Entropy Scaling: A Group-Contribution Method. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 20441-20449.	3.7	30
28	An equation of state for Stockmayer fluids based on a perturbation theory for dipolar hard spheres. <i>Journal of Chemical Physics</i> , 2019, 151, 104102.	3.0	2
29	Thermal Conductivity via Entropy Scaling: An Approach That Captures the Effect of Intramolecular Degrees of Freedom. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 18432-18438.	3.7	22
30	Dipolar Hard Spheres: Comprehensive Data from Monte Carlo Simulations. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 827-832.	1.9	8
31	Phase Equilibria of Solid and Fluid Phases from Molecular Dynamics Simulations with Equilibrium and Nonequilibrium Free Energy Methods. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3778-3792.	5.3	4
32	On the use of transport properties to discriminate Mie-type molecular models for 1-propanol optimized against VLE data. <i>European Physical Journal: Special Topics</i> , 2019, 227, 1529-1545.	2.6	5
33	Particle methods in natural science and engineering. <i>European Physical Journal: Special Topics</i> , 2019, 227, 1493-1499.	2.6	2
34	Polarizable Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibria: Ethers, <i>n</i> -Alkanes, and Nitrogen. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2561-2573.	5.3	3
35	Reply to Comment on "Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules". <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 5744-5745.	3.7	14
36	Phase equilibria of binary mixtures with alkanes, ketones, and esters based on the Transferable Anisotropic Mie force field. <i>Fluid Phase Equilibria</i> , 2019, 490, 123-132.	2.5	3

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37	A Modified Shifted Force Approach to the Wolf Summation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 572-583.	5.3	8
38	Individualized force fields for alkanes, olefins, ethers and ketones based on the transferable anisotropic Mie potential. <i>Fluid Phase Equilibria</i> , 2018, 470, 101-108.	2.5	8
39	Pure Substance and Mixture Viscosities Based on Entropy Scaling and an Analytic Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 4095-4114.	3.7	76
40	Surface tension of droplets and Tolman lengths of real substances and mixtures from density functional theory. <i>Journal of Chemical Physics</i> , 2018, 148, 164703.	3.0	23
41	Modification of the Wolf Method and Evaluation for Molecular Simulation of Vapor-Liquid Equilibria. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2198-2206.	5.3	7
42	Transferability of cross-interaction pair potentials: Vapor-liquid phase equilibria of n-alkane/nitrogen mixtures using the TAMie force field. <i>Fluid Phase Equilibria</i> , 2018, 456, 124-130.	2.5	10
43	Characterisation of acid-base surface free energy components of urea-water solutions. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2018, 538, 774-780.	4.7	14
44	Modeling properties of the one-dimensional vapor-liquid interface: Application of classical density functional and density gradient theory. <i>Fluid Phase Equilibria</i> , 2018, 458, 243-252.	2.5	31
45	Germany's next top molecule: Predictive Thermodynamik als Schlüssel der simultanen Optimierung von Prozess und Lösungsmittel. <i>Chemie-Ingenieur-Technik</i> , 2018, 90, 1304-1304.	0.8	0
46	Predictive density gradient theory based on nonlocal density functional theory. <i>Physical Review E</i> , 2018, 98, .	2.1	15
47	Prediction of Contact Angles and Density Profiles of Sessile Droplets Using Classical Density Functional Theory Based on the PCP-SAFT Equation of State. <i>Langmuir</i> , 2018, 34, 12519-12531.	3.5	26
48	On the importance of non-equilibrium models for describing the coupling of heat and mass transfer at high pressure. <i>International Communications in Heat and Mass Transfer</i> , 2018, 98, 49-58.	5.6	23
49	Self-Diffusion Coefficients from Entropy Scaling Using the PCP-SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 12942-12950.	3.7	44
50	A classical density functional theory for vapor-liquid interfaces consistent with the heterosegmented group-contribution perturbed-chain polar statistical associating fluid theory. <i>Fluid Phase Equilibria</i> , 2018, 472, 117-127.	2.5	14
51	An improved group contribution method for PC-SAFT applied to branched alkanes: Data analysis and parameterization. <i>Fluid Phase Equilibria</i> , 2018, 473, 183-191.	2.5	7
52	A third and fourth order perturbation theory for dipolar hard spheres. <i>Journal of Chemical Physics</i> , 2018, 149, 044901.	3.0	3
53	Identifying Pure-Component Parameters of an Analytic Equation of State Using Experimental Surface Tension or Molecular Simulations with a Transferable Force Field. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 12254-12263.	3.7	4
54	1-stage CoMT-CAMD: An approach for integrated design of ORC process and working fluid using PC-SAFT. <i>Chemical Engineering Science</i> , 2017, 159, 217-230.	3.8	74

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55	Modeling of interfacial properties of multicomponent systems using density gradient theory and PCP-SAFT. <i>Fluid Phase Equilibria</i> , 2017, 439, 31-42.	2.5	43
56	Three-body effects in triplets of capped gold nanocrystals. <i>Molecular Physics</i> , 2017, 115, 1031-1040.	1.7	13
57	From molecules to dollars: integrating molecular design into thermo-economic process design using consistent thermodynamic modeling. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 301-320.	3.4	54
58	Heat release at the wetting front during capillary filling of cellulosic micro-substrates. <i>Journal of Colloid and Interface Science</i> , 2017, 504, 751-757.	9.4	13
59	Thermal Conductivity of Real Substances from Excess Entropy Scaling Using PCP-SAFT. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 4527-4538.	3.7	74
60	Numerical aspects of classical density functional theory for one-dimensional vapor-liquid interfaces. <i>Fluid Phase Equilibria</i> , 2017, 444, 1-12.	2.5	32
61	Classical Density Functional Theory for Liquid-Fluid Interfaces and Confined Systems: A Functional for the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 4119-4135.	3.7	77
62	Integrating working fluid design into the thermo-economic design of ORC processes using PC-SAFT. <i>Energy Procedia</i> , 2017, 129, 121-128.	1.8	8
63	Integrated design of ORC process and working fluid using process flowsheeting software and PC-SAFT. <i>Energy Procedia</i> , 2017, 129, 129-136.	1.8	20
64	A critical evaluation of perturbation theories by Monte Carlo simulation of the first four perturbation terms in a Helmholtz energy expansion for the Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 2017, 147, 014503.	3.0	27
65	Integrated thermo-economic design of ORC process, working fluid and equipment using PC-SAFT. <i>Computer Aided Chemical Engineering</i> , 2017, , 1795-1800.	0.5	2
66	Non-Equilibrium Thermodynamics for Engineers. , 2017, , .		18
67	One-stage approach for the integrated design of ORC processes and working fluid using PC-SAFT. <i>Computer Aided Chemical Engineering</i> , 2016, 38, 1335-1340.	0.5	2
68	Theory of model electrolyte solutions: Assessing the short- and long-ranged contributions by molecular simulations. <i>Fluid Phase Equilibria</i> , 2016, 430, 195-206.	2.5	7
69	Detailed pedagogical review and analysis of Wertheim's thermodynamic perturbation theory. <i>Fluid Phase Equilibria</i> , 2016, 428, 121-152.	2.5	30
70	Bayesian Model Selection Helps To Choose Objectively between Thermodynamic Models: A Demonstration of Selecting a Viscosity Model Based on Entropy Scaling. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 10191-10207.	3.7	14
71	Chemical potential of model electrolyte solutions consisting of hard sphere ions and hard dipoles from molecular simulations. <i>Fluid Phase Equilibria</i> , 2016, 429, 205-213.	2.5	5
72	Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibria: Aldehydes, Ketones, and Small Cyclic Alkanes. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 12123-12132.	3.7	23

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73	A new equation of state for linear hard chains: Analysis of a third-order expansion of Wertheim's Thermodynamic Perturbation Theory. <i>Fluid Phase Equilibria</i> , 2016, 416, 18-26.	2.5	10
74	Estimation of the binary interaction parameter k of the PC-SAFT Equation of State based on pure component parameters using a QSPR method. <i>Fluid Phase Equilibria</i> , 2016, 416, 138-149.	2.5	18
75	Different ways of looking at the force between two nanocrystals. <i>Journal of Chemical Physics</i> , 2015, 143, 244115.	3.0	2
76	Grand Canonical Monte Carlo Simulations Guided by an Analytic Equation of State—Transferable Anisotropic Mie Potentials for Ethers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7087-7099.	2.6	34
77	Computer-aided molecular design in the continuous-molecular targeting framework using group-contribution PC-SAFT. <i>Computers and Chemical Engineering</i> , 2015, 81, 278-287.	3.8	97
78	Effective potentials between gold nano crystals — functional dependence on temperature. <i>Molecular Simulation</i> , 2015, 41, 1153-1158.	2.0	9
79	Group Contribution Method for Viscosities Based on Entropy Scaling Using the Perturbed-Chain Polar Statistical Associating Fluid Theory. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 7942-7952.	3.7	113
80	Density Functional Theory for Liquid—Liquid Interfaces of Mixtures Using the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 4633-4642.	3.7	30
81	Analysis of Interfacial Transport Resistivities of Pure Components and Mixtures Based on Density Functional Theory. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 11483-11492.	3.7	23
82	On the vapor-liquid equilibrium of attractive chain fluids with variable degree of molecular flexibility. <i>Journal of Chemical Physics</i> , 2015, 142, 224504.	3.0	5
83	Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibrium Calculations: n-Alkanes and n-Olefins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11695-11707.	2.6	46
84	An analytical equation of state for describing isotropic-nematic phase equilibria of Lennard-Jones chain fluids with variable degree of molecular flexibility. <i>Journal of Chemical Physics</i> , 2015, 142, 244903.	3.0	11
85	Computer-aided Molecular Design of ORC Working Fluids using PC-SAFT. <i>Computer Aided Chemical Engineering</i> , 2014, , 357-362.	0.5	13
86	An equation of state for the isotropic phase of linear, partially flexible and fully flexible tangent hard-sphere chain fluids. <i>Molecular Physics</i> , 2014, 112, 919-928.	1.7	12
87	The isotropic-nematic and nematic-nematic phase transition of binary mixtures of tangent hard-sphere chain fluids: An analytical equation of state. <i>Journal of Chemical Physics</i> , 2014, 140, 034504.	3.0	5
88	Continuous Molecular Targeting—Computer-Aided Molecular Design (CoMT—CAMD) for Simultaneous Process and Solvent Design for CO ₂ Capture. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 18029-18041.	3.7	79
89	Comparison between a Homo- and a Heterosegmented Group Contribution Approach Based on the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 14854-14864.	3.7	76
90	A new perturbation theory for electrolyte solutions. <i>Journal of Chemical Physics</i> , 2014, 141, 054103.	3.0	12

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91	Physically-based Thermodynamic Models in Integrated Process and Molecular Design. Computer Aided Chemical Engineering, 2014, 33, 67-72.	0.5	0
92	Chemical osmosis in two-phase flow and salinity-dependent capillary pressures in rocks with microporosity. Water Resources Research, 2014, 50, 763-789.	4.2	5
93	Simultaneous Optimization of Working Fluid and Process for Organic Rankine Cycles Using PC-SAFT. Industrial & Engineering Chemistry Research, 2014, 53, 8821-8830.	3.7	108
94	A Density Functional Theory for Vapor-Liquid Interfaces of Mixtures Using the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. Industrial & Engineering Chemistry Research, 2014, 53, 6169-6178.	3.7	48
95	The isotropic-nematic phase transition of tangent hard-sphere chain fluids—Pure components. Journal of Chemical Physics, 2013, 139, 034505.	3.0	16
96	Grand canonical Monte Carlo simulations of vapor-liquid equilibria using a bias potential from an analytic equation of state. Journal of Chemical Physics, 2013, 138, 234106.	3.0	8
97	An analytical approximation for the orientation-dependent excluded volume of tangent hard sphere chains of arbitrary chain length and flexibility. Journal of Chemical Physics, 2012, 137, 044906.	3.0	13
98	Acceleration of Monte-Carlo molecular simulations on hybrid computing architectures. , 2012, , .		6
99	Simultaneous process and working fluid optimisation for Organic Rankine Cycles (ORC) using PC-SAFT. Computer Aided Chemical Engineering, 2012, , 572-576.	0.5	25
100	On the Treatment of Electrostatic Interactions of Non-spherical Molecules in Equation of State Models. Soft Materials, 2012, 10, 81-105.	1.7	6
101	Phase Behavior of the System Linear Polyglycerol + Methanol + Carbon Dioxide. Journal of Chemical & Engineering Data, 2011, 56, 2927-2931.	1.9	7
102	Determining Force Field Parameters Using a Physically Based Equation of State. Journal of Physical Chemistry B, 2011, 115, 7872-7880.	2.6	33
103	Using an Analytic Equation of State to Obtain Quantitative Solubilities of CO ₂ by Molecular Simulation. Journal of Physical Chemistry Letters, 2011, 2, 393-396.	4.6	7
104	Integration of process and solvent design towards a novel generation of CO ₂ absorption capture systems. Energy Procedia, 2011, 4, 282-290.	1.8	20
105	Developments in the pre-combustion CO ₂ capture pilot plant at the Buggenum IGCC. Energy Procedia, 2011, 4, 1214-1221.	1.8	31
106	Two performance indicators for the characterization of the entropy production in a process unit. Energy, 2011, 36, 3727-3732.	8.8	14
107	Modeling the phase equilibria of hydrogen sulfide and carbon dioxide in mixture with hydrocarbons and water using the PC-SAFT equation of state. Fluid Phase Equilibria, 2010, 293, 11-21.	2.5	64
108	Equation of state for aqueous electrolyte systems based on the semirestricted non-primitive mean spherical approximation. Fluid Phase Equilibria, 2010, 297, 23-33.	2.5	38

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109	Density functional theory for calculating surface tensions with a simple renormalization formalism for the critical point. <i>Journal of Supercritical Fluids</i> , 2010, 55, 735-742.	3.2	24
110	Phase behavior of the system hyperbranched polyglycerol+methanol+carbon dioxide. <i>Fluid Phase Equilibria</i> , 2010, 299, 252-258.	2.5	15
111	Continuous-Molecular Targeting for Integrated Solvent and Process Design. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 2834-2840.	3.7	126
112	Renormalization-Group Corrections to the Perturbed-Chain Statistical Associating Fluid Theory for Binary Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 9436-9444.	3.7	30
113	Application of Infinite Dilution Activity Coefficients for Determining Binary Equation of State Parameters. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 7646-7653.	3.7	21
114	A Continuous Targeting Approach for Integrated Solvent and Process Design Based on Molecular Thermodynamic Models. <i>Computer Aided Chemical Engineering</i> , 2009, 27, 813-818.	0.5	8
115	A density functional theory for vapor-liquid interfaces using the PCP-SAFT equation of state. <i>Journal of Chemical Physics</i> , 2009, 131, 204705.	3.0	98
116	A non-equilibrium thermodynamics approach to model mass and heat transport for water pervaporation through a zeolite membrane. <i>Journal of Membrane Science</i> , 2009, 330, 388-398.	8.2	37
117	Performance and stability of multi-channel MFI zeolite membranes detemplated by calcination and ozonation in ethanol/water pervaporation. <i>Journal of Membrane Science</i> , 2009, 339, 261-274.	8.2	49
118	Detemplation of [B]MFI zeolite crystals by ozonation. <i>Microporous and Mesoporous Materials</i> , 2009, 120, 35-38.	4.4	24
119	Detemplation of DDR type zeolites by ozonation. <i>Microporous and Mesoporous Materials</i> , 2009, 120, 12-18.	4.4	38
120	Tuning the framework polarity in MFI membranes by deboronation: Effect on mass transport. <i>Microporous and Mesoporous Materials</i> , 2009, 125, 39-45.	4.4	5
121	Modeling the phase equilibria of CO ₂ and H ₂ S in aqueous electrolyte systems at elevated pressure. <i>Energy Procedia</i> , 2009, 1, 1807-1814.	1.8	7
122	Phase Behavior of Hyperbranched Polymer Systems: Experiments and Application of the Perturbed-Chain Polar SAFT Equation of State. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1022-1029.	2.6	36
123	Efficient Conversion of Thermal Energy into Hydrogen: Comparing Two Methods to Reduce Exergy Losses in a Sulfuric Acid Decomposition Reactor. <i>Industrial & Engineering Chemistry Research</i> , 2009, 48, 8500-8507.	3.7	23
124	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14290-14301.	3.1	69
125	Dehydration performance of a hydrophobic DD3R zeolite membrane. <i>Journal of Membrane Science</i> , 2008, 321, 344-349.	8.2	69
126	Nonequilibrium thermodynamics of interfaces using classical density functional theory. <i>Journal of Chemical Physics</i> , 2008, 129, 184703.	3.0	27

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127	Vapor-Liquid Equilibria Simulation and an Equation of State Contribution for Dipole-Quadrupole Interactions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 51-60.	2.6	91
128	Investigating mass transport in zeolite pores by tuning the framework polarity. <i>Studies in Surface Science and Catalysis</i> , 2007, , 942-948.	1.5	5
129	On the Driving Force of Methanol Pervaporation through a Microporous Methylated Silica Membrane. <i>Industrial & Engineering Chemistry Research</i> , 2007, 46, 4091-4099.	3.7	22
130	Basic parameter study for the separation of an isopropanol-water mixture by using FricDiff technology. <i>Chemical Engineering and Processing: Process Intensification</i> , 2007, 46, 810-817.	3.6	10
131	An equation-of-state contribution for polar components: Dipolar molecules. <i>AIChE Journal</i> , 2006, 52, 1194-1204.	3.6	321
132	An equation of state contribution for polar components: Polarizable dipoles. <i>AIChE Journal</i> , 2006, 52, 1951-1961.	3.6	109
133	Thermodynamic modeling of complex systems using PC-SAFT. <i>Fluid Phase Equilibria</i> , 2005, 228-229, 89-98.	2.5	122
134	An equation-of-state contribution for polar components: Quadrupolar molecules. <i>AIChE Journal</i> , 2005, 51, 2556-2568.	3.6	249
135	Perturbed-Chain-SAFT. , 2004, , 295-322.		4
136	Reactive Phase Equilibria in Silica Aerogel Synthesis: An Experimental Study and Prediction of the Complex Phase Behavior Using the PC-SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2004, 43, 4457-4464.	3.7	31
137	Modeling Copolymer Systems Using the Perturbed-Chain SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2003, 42, 1266-1274.	3.7	191
138	Application of the Perturbed-Chain SAFT Equation of State to Associating Systems. <i>Industrial & Engineering Chemistry Research</i> , 2002, 41, 5510-5515.	3.7	1,016
139	Modeling Polymer Systems Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2002, 41, 1084-1093.	3.7	357
140	Modeling of polymer phase equilibria using Perturbed-Chain SAFT. <i>Fluid Phase Equilibria</i> , 2002, 194-197, 541-551.	2.5	124
141	Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules. <i>Industrial & Engineering Chemistry Research</i> , 2001, 40, 1244-1260.	3.7	2,786
142	Modeling of Solid/Fluid Phase Equilibria in Multicomponent Systems at High Pressure. <i>Chemical Engineering and Technology</i> , 2001, 24, 607-612.	1.5	25
143	Berechnung von Fest/Fluid-Phasengleichgewichten bei erhöhten Drücken. <i>Chemie-Ingenieur-Technik</i> , 2000, 72, 722-727.	0.8	0
144	Application of perturbation theory to a hard-chain reference fluid: an equation of state for square-well chains. <i>Fluid Phase Equilibria</i> , 2000, 168, 183-199.	2.5	294

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145	Experimental Investigation of Droplet Injections in the Vicinity of the Critical Point: A comparison of different model approaches. , 0, , .		2