Frederico Wanderley Tavares

List of Publications by Year
in descending order

183	3,396	185998 28	189595 50
papers	citations	h-index	g-index

190	190	190	2796
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A new high-pressure cell for equilibrium measurements of systems with fluid and solid phases. Journal of Supercritical Fluids, 2022, 179, 105420.	1.6	3
2	PCP-SAFT Density Functional Theory as a much-improved approach to obtain confined fluid isotherm data applied to sub and supercritical conditions. Chemical Engineering Science, 2022, 247, 116905.	1.9	5
3	Physicalâ€“Chemical Properties of Compressible Clathrates: A Natural Pressure Shift by Extending the van der Waals and Platteeuw Model. Journal of Physical Chemistry C, 2022, 126, 2839-2856.	1.5	0
4	Synthesis of polyglobalide by enzymatic ring opening polymerization using pressurized fluids. Journal of Supercritical Fluids, 2022, 186, 105588.	1.6	6
5	A First Approach towards Adsorption-Oriented Physics-Informed Neural Networks: Monoclonal Antibody Adsorption Performance on an Ion-Exchange Column as a Case Study. ChemEngineering, 2022, 6, 21.	1.0	7
6	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes? 2. A systematic study considering different chain lengths. Journal of Molecular Liquids, 2022, 354, 118829.	2.3	5
7	Revisiting the birth of NaCl crystals using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2022, 115, 108202.	1.3	0
8	The impact of the adsorbent energy heterogeneities by multidimensional-multicomponent PC-SAFT-DFT. Fluid Phase Equilibria, 2022, 562, 113546.	1.4	10
9	Molecular Thermodynamics for Aggregation of Surfactants with Alkylbenzene or Branched Alkane Tails: An Experimental-Modeling Approach. Fluid Phase Equilibria, 2021, 532, 112918.	1.4	2
10	Helmholtz Scaling: An Alternative Approach to Calculate Viscosity with the PCP-SAFT Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 9231-9245.	1.8	4
11	Exploring the multiple solutions of the classical density functional theory using metadynamics based method. Adsorption, 2021, 27, 1023-1034.	1.4	5
12	A self-consistent perturbative density functional theory for hard-core fluids: phase diagrams, structural and interfacial properties. Fluid Phase Equilibria, 2021, 542-543, 113095.	1.4	1
13	Molecular dynamics of dissolution of a 36-chain cellulose Iî² microfibril at different temperatures above the critical pressure of water. Journal of Molecular Liquids, 2021, 336, 116271.	2.3	5
14	Asphaltenes at the water-oil interface using DPD/COSMO-SAC. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 625, 126828.	2.3	12
15	The binding interaction of protein on a charged surface using Poissonâ€“Boltzmann equation: lysozyme adsorption onto SBA-15. Adsorption, 2021, 27, 1137-1148.	1.4	4
16	Electro-rheological investigation on W/O emulsions morphology under electric fields. Journal of Dispersion Science and Technology, 2020, 41, 1465-1470.	1.3	0
17	Self-diffusion coefficients of methane/n-hexane mixtures at high pressures: An evaluation of the finite-size effect and a comparison of force fields. Journal of Supercritical Fluids, 2020, 155, 104639.	1.6	14
18	Renormalization group theory applied to the CPA equation of state: Impacts on phase equilibrium and derivative properties. Fluid Phase Equilibria, 2020, 506, 112365.	1.4	5

#	Article	IF	Citations
19	Phase Equilibria Data and Thermodynamic Analysis for Liquidâ€“Hydrateâ€“Vapor (LHV) with High Ethanol Concentrations. Journal of Chemical & Engineering Data, 2020, 65, 349-359.	1.0	8
20	A computational tool for parameter estimation in EoS: New methodologies and natural gas phase equilibria calculations. Chemical Engineering Science, 2020, 215, 115437.	1.9	6
21	Development of Coalescence and Capture Kernels for the Electrocoalescence Process Based on Batch Experiments. Industrial & Engineering Chemistry Research, 2020, 59, 1277-1297.	1.8	5
22	Concentration and Solvent Effects on Structural, Dynamical, and Rheological Properties of Asphaltene Suspensions. Energy & Fuels, 2020, 34, 1071-1081.	2.5	12
23	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes?. Journal of Molecular Modeling, 2020, 26, 296.	0.8	21
24	Experimental high-pressure phase equilibria of carbon dioxide/n-alkanes mixtures and model-parameters for solid-phase obtained from DSC thermograms. Fluid Phase Equilibria, 2020, 526, 112802.	1.4	4
25	Quenched solid density functional theory coupled with PC-SAFT for the adsorption modeling on nanopores. Fluid Phase Equilibria, 2020, 521, 112700.	1.4	8
26	Sixty Years of the van der Waals and Platteeuw Model for Clathrate Hydratesâ€”A Critical Review from Its Statistical Thermodynamic Basis to Its Extensions and Applications. Chemical Reviews, 2020, 120, 13349-13381.	23.0	29
27	Modified clustering algorithm for molecular simulation. Molecular Simulation, 2020, 46, 1453-1466.	0.9	5
28	Inferring kinetic dissolution of NaCl in aqueous glycol solution using a lowâ€cost apparatus and population balance model. Canadian Journal of Chemical Engineering, 2020, 98, 2435-2450.	0.9	0
29	Current status of Lattice Boltzmann Methods applied to aerodynamic, aeroacoustic, and thermal flows. Progress in Aerospace Sciences, 2020, 115, 100616.	6.3	38
30	Anomalous diffusion and sorption-desorption process in complex fluid systems. Communications in Nonlinear Science and Numerical Simulation, 2020, 90, 105411.	1.7	2
31	Phase behavior of systems with high CO2 content: Experiments and thermodynamic modeling. Fluid Phase Equilibria, 2020, 515, 112574.	1.4	6
32	Thermophysical Properties of Amorphousâ€Paracrystalline Celluloses by Molecular Dynamics. Macromolecular Theory and Simulations, 2020, 29, 2000007.	0.6	4
33	Microscope analysis and evaluation of the destabilization process of water-in-oil emulsions under application of electric field. IEEE Transactions on Dielectrics and Electrical Insulation, 2020, 27, 873-881.	1.8	2
34	Lattice Boltzmann Methods for Industrial Applications. Industrial & Engineering Chemistry Research, 2019, 58, 16205-16234.	1.8	25
35	Adsorption of Gases on Zeolitic Imidazolate Frameworks: Modeling with Equations of State for Confined Fluids and Pore Size Distribution Estimation. Industrial & Engineering Chemistry Research, 2019, 58, 19702-19708.	1.8	4
36	Reconstruction of the pore size distribution of porous materials: The influence of uncertainties in the gaseous adsorption experimental data. Fluid Phase Equilibria, 2019, 494, 93-102.	1.4	5

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37	A molecular dynamics study of the solvation of carbon dioxide and other compounds in the ionic liquids [emim][B(CN)4] and [emim][NTf2]. Fluid Phase Equilibria, 2019, 491, 1-11.	1.4	11
38	Amorphous paracrystalline structures from native crystalline cellulose: A molecular dynamics protocol. Fluid Phase Equilibria, 2019, 491, 56-76.	1.4	25
39	Pore size distributions from extended Peng-Robinson equations of state for fluids confined in cylindrical and slit pores. Fluid Phase Equilibria, 2019, 493, 67-77.	1.4	8
40	Wax appearance and prevention in two-phase flow using the multi-solid and drift-flux model. Journal of Petroleum Science and Engineering, 2019, 177, 374-383.	2.1	5
41	Wettability of rock, oil and brine system based on density functional theory. Fluid Phase Equilibria, 2019, 479, 99-105.	1.4	2
42	A new simple and efficient flash algorithm for T-v specifications. Fluid Phase Equilibria, 2018, 464, 32-39.	1.4	13
43	Phenomenological modeling for elemental mercury capture on hydroxyapatite-based adsorbents: An experimental validation. Fuel, 2018, 225, 509-518.	3.4	6
44	High pressure phase equilibria of carbon dioxideÂ+Ân-alkanes mixtures: Experimental data and modeling. Fluid Phase Equilibria, 2018, 463, 114-120.	1.4	8
45	Cubic equations of state extended to confined fluids: New mixing rules and extension to spherical pores. Chemical Engineering Science, 2018, 184, 52-61.	1.9	19
46	Accurate thermodynamic description of vaporâ€“liquid and solidâ€“liquid equilibria of THF, water and gas hydrates with a unique set of parameters. Journal of Chemical Thermodynamics, 2018, 117, 60-67.	1.0	11
47	Molecular dynamics simulation and experimental validation by X-ray data of hydroxyapatite crystalline structures. Fluid Phase Equilibria, 2018, 470, 60-67.	1.4	5
48	A modified Poisson-Boltzmann equation applied to protein adsorption. Journal of Chromatography A, 2018, 1531, 74-82.	1.8	9
49	Emulsion phase inversion of model and crude oil systems detected by near-infrared spectroscopy and principal component analysis. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2018, 538, 565-573.	2.3	16
50	Heat of dissociation from Statistical Thermodynamics: Using calorimetric data to estimate gas hydrate parameters. Journal of Chemical Thermodynamics, 2018, 117, 164-179.	1.0	3
51	CHEMICAL POTENTIALS OF HARD-CORE MOLECULES BY A STEPWISE INSERTION METHOD. Brazilian Journal of Chemical Engineering, 2018, 35, 277-288.	0.7	4
52	Laser-induced wettability alteration in limestone rocks. Materials Today Communications, 2018, 17, 332-340.	0.9	2
53	Representative elementary volume in limestone sample. Journal of Instrumentation, 2018, 13, C10003-C10003.	0.5	8
54	Cascaded Lattice Boltzmann Method application in forced and natural convection. Journal of Physics: Conference Series, 2018, 1101, 012040.	0.3	2

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55	Natural convection heat transfer modeling by the cascaded thermal lattice Boltzmann method. International Journal of Thermal Sciences, 2018, 134, 552-564.	2.6	16
56	Paraffin solubility curves of diesel fuels from thermodynamic model adjusted through experimental DSC thermograms. Fuel, 2018, 230, 266-273.	3.4	4
57	Laser-induced alteration of microstructural and microscopic transport properties in porous materials: Experiment, modeling and analysis. Materials and Design, 2018, 155, 307-316.	3.3	4
58	Stability studies of high-stable water-in-oil model emulsions. Journal of Dispersion Science and Technology, 2017, 38, 82-88.	1.3	19
59	Machine learning model and optimization of a PSA unit for methane-nitrogen separation. Computers and Chemical Engineering, 2017, 104, 377-391.	2.0	51
60	New Cascaded Thermal Lattice Boltzmann Method for simulations of advection-diffusion and convective heat transfer. International Journal of Thermal Sciences, 2017, 118, 259-277.	2.6	26
61	Evaluation of Microwave and Conventional Heating for Electrostatic Treatment of a Water-in-Oil Model Emulsion in a Pilot Plant. Energy & Fuels, 2017, 31, 6587-6597.	2.5	14
62	Crude Oil Electrical Conductivity Measurements at High Temperatures: Introduction of Apparatus and Methodology. Energy & Fuels, 2017, 31, 3669-3674.	2.5	9
63	Non-isothermal population balance model of the formation and dissociation of gas hydrates. Chemical Engineering Science, 2017, 163, 234-254.	1.9	8
64			

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73	Alternative EoS-based model for predicting water content, metastable phases and hydrate formation in natural gas systems. Journal of Natural Gas Science and Engineering, 2016, 36, 550-562.	2.1	6
74	Equation of state based on the hole-lattice theory and surface-charge density (COSMO): Part B â€“ Vaporâ€“liquid equilibrium for mixtures. Fluid Phase Equilibria, 2016, 419, 1-10.	1.4	2
75	Extending an equation of state to confined fluids with basis on molecular simulations. Chemical Engineering Science, 2016, 153, 212-220.	1.9	22
76	Investigation of the PIT emulsification mechanism by NIR and conductometry. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 506, 566-575.	2.3	4
77	Methane/nitrogen separation through pressure swing adsorption process from nitrogen-rich streams. Chemical Engineering and Processing: Process Intensification, 2016, 103, 70-79.	1.8	33
78	Molecular Dynamic Simulation of Oxaliplatin Diffusion in Poly(lactic acid-co -glycolic acid). Part A: Parameterization and Validation of the Force-Field CVFF. Macromolecular Theory and Simulations, 2016, 25, 45-62.	0.6	34
79	Phase diagrams for hydrates beyond incipient condition â€" Complex behavior in methane/propane and carbon dioxide/iso-butane hydrates. Fluid Phase Equilibria, 2016, 426, 75-82.	1.4	6
80	Equation of state based on the hole-lattice theory and surface-charge density (COSMO): Part A â€“ Pure compounds. Fluid Phase Equilibria, 2016, 409, 472-481.	1.4	6
81	Simultaneous multiphase flash and stability analysis calculations including hydrates. Fluid Phase Equilibria, 2016, 413, 196-208.	1.4	11
82	A lowâ€disturbance nonequilibrium molecular dynamics algorithm applied to the determination of thermal conductivities. AICHE Journal, 2015, 61, 2881-2890.	1.8	4
83	NON-EQUILIBRIUM MOLECULAR DYNAMICS USED TO OBTAIN SORET COEFFICIENTS OF BINARY HYDROCARBON MIXTURES. Brazilian Journal of Chemical Engineering, 2015, 32, 683-698.	0.7	11
84	Cubic Plus Association Equation of State for Flow Assurance Projects. Industrial & Engineering Chemistry Research, 2015, 54, 6812-6824.	1.8	15
85	Modelling of Hg⁰ Removal from Gaseous Streams and its Fixation in Hydroxyapatite-Based Adsorbents Modified with Copper Sulphide. Adsorption Science and Technology, 2015, 33, 175-190.	1.5	2
86	The electrostatic behavior of the bacterial cell wall using a smoothing function to describe the charge-regulated volume charge density profile. Colloids and Surfaces B: Biointerfaces, 2015, 134, 447-452.	2.5	8
87	Membrane Potential and Ion Partitioning in an Erythrocyte Using the Poissonâ€“Boltzmann Equation. Journal of Physical Chemistry B, 2015, 119, 6379-6388.	1.2	9
88	Modeling MEA with the CPA equation of state: A parameter estimation study adding local search to PSO algorithm. Fluid Phase Equilibria, 2015, 400, 76-86.	1.4	7
89	Influence of Commercial Anti-agglomerants and Ammonium Quaternary Compounds on the Stability of Waxy Crude Oil Emulsion. Energy & Fuels, 2015, 29, 2211-2218.	2.5	6
90	Studies on transitional emulsion phase inversion using the steady state protocol. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 484, 424-433.	2.3	10

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91	Modeling Water Saturation Points in Natural Gas Streams Containing CO₂ and H₂Sâ€"Comparisons with Different Equations of State. Industrial & Engineering Chemistry Research, 2015, 54, 743-757.	1.8	5
92	Effects of electrostatic correlations on ion dynamics in alternating current voltages. Electrochimica Acta, 2015, 152, 84-92.	2.6	11
93	A modified multi-site occupancy model: evaluation of azeotropelike behavior in adsorption. Adsorption, 2015, 21, 3-16.	1.4	6
94	STEADY STATE AND PSEUDO-TRANSIENT ELECTRIC POTENTIAL USING THE POISSONBOLTZMANN EQUATION. Brazilian Journal of Chemical Engineering, 2015, 32, 293-302.	0.7	1
95	Investigation of adsorption-enhanced reaction process of mercury removal from simulated natural gas by mathematical modeling. Fuel, 2014, 129, 129-137.	3.4	30
96	Phase equilibrium of fluids confined in porous media from an extended Pengâ€"Robinson equation of state. Fluid Phase Equilibria, 2014, 362, 335-341.	1.4	122
97	Steric effects on ion dynamics near charged electrodes. Fluid Phase Equilibria, 2014, 362, 177-186.	1.4	9
98	Transitional Phase Inversion of Emulsions Monitored by in Situ Near-Infrared Spectroscopy. Langmuir, 2013, 29, 5995-6003.	1.6	13
99	Thermodynamic Properties of 1:1 Salt Aqueous Solutions with the Electrolattice Equation of State. Oil and Gas Science and Technology, 2013, 68, 255-270.	1.4	21
100	Double layer interaction between charged parallel plates using a modified Poissonâ€"Boltzmann equation to include size effects and ion specificity. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 412, 29-35.	2.3	18
101	Vaporâ^'Liquid Equilibrium Calculations of Aqueous and Nonaqueous Binary Systems Using the Mattediâ^'Tavaresâ^'Castier Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 102-110.	1.8	4
102	High-Pressure Experimental Data of CO₂ + Mitotane and CO₂ + Ethanol + Mitotane Mixtures. Journal of Chemical & Engineering Data, 2011, 56, 4333-4341.	1.0	31
103	Parameter estimation of kinetic cure using DSC non-isothermal data. Journal of Thermal Analysis and Calorimetry, 2011, 103, 495-499.	2.0	10
104	Attractive double-layer forces between neutral hydrophobic and neutral hydrophilic surfaces. Physical Review E, 2011, 84, 061903.	0.8	8
105	Vaporâ€"liquid equilibrium calculations for refrigerant mixtures with the Mattediâ€"Tavaresâ€"Castier EOS. Fluid Phase Equilibria, 2010, 296, 133-139.	1.4	6
106	High-pressure phase diagram of the drug mitotane in compressed and/or supercritical CO2. Journal of Chemical Thermodynamics, 2010, 42, 286-290.	1.0	15
107	Ion-specific thermodynamic properties of colloids and proteins. Fluid Phase Equilibria, 2010, 296, 99-105.	1.4	3
108	Critical behavior of pure confined fluids from an extension of the van der Waals equation of state. Journal of Supercritical Fluids, 2010, 55, 455-461.	1.6	101

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109	Thermodynamic modeling of confined fluids using an extension of the generalized van der Waals theory. Chemical Engineering Science, 2010, 65, 3088-3099.	1.9	135
110	Ion-specific thermodynamical properties of aqueous proteins. Anais Da Academia Brasileira De Ciencias, 2010, 82, 109-126.	0.3	3
111	Inner segment radial distribution functions at contact point for chain-like molecules. Journal of Molecular Liquids, 2009, 147, 198-210.	2.3	2
112	Ion specific forces between charged self-assembled monolayers explained by modified DLVO theory. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2009, 346, 11-15.	2.3	11
113	Modifying the Poissonâ€“Boltzmann Approach to Model Specific Ion Effects. , 2009, , 293-309.		1
114	Anion-Specific Partitioning in Two-Phase Finite Volume Systems: Possible Implications for Mechanisms of Ion Pumps. Journal of Physical Chemistry B, 2009, 113, 8124-8127.	1.2	14
115	Phase transition of waterâ€“inâ€“oil emulsions over influence of an external electric field. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 326, 10-17.	2.3	14
116	Forces between air-bubbles in electrolyte solution. Chemical Physics Letters, 2008, 458, 299-302.	1.2	8
117	Cure kinetic parameter estimation of thermosetting resins with isothermal data by using particle swarm optimization. European Polymer Journal, 2008, 44, 2678-2686.	2.6	21
118	Specific ion effects: Interaction between nanoparticles in electrolyte solutions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 319, 98-102.	2.3	18
119	Rheological Behavior of an Epoxy Resin with Hollow Glass Microspheres. AIP Conference Proceedings, 2008, , .	0.3	0
120	Co-Ion and Ion Competition Effects:â€‰ Ion Distributions Close to a Hydrophobic Solid Surface in Mixed Electrolyte Solutions. Langmuir, 2008, 24, 3944-3948.	1.6	25
121	Specific Ion Adsorption and Surface Forces in Colloid Science. Journal of Physical Chemistry B, 2008, 112, 1580-1585.	1.2	48
122	The influence of ion binding and ion specific potentials on the double layer pressure between charged bilayers at low salt concentrations. Journal of Chemical Physics, 2008, 128, 135104.	1.2	23
123	Ion-specific potential of mean force between two aqueous proteins. Computer Aided Chemical Engineering, 2008, , 865-870.	0.3	0
124	Osmotic Second Virial Coefficients and Phase Diagrams for Aqueous Proteins from a Much-Improved Poissonâ^'Boltzmann Equationâ€. Journal of Physical Chemistry C, 2007, 111, 16055-16059.	1.5	36
125	Finite volume solution of the modified Poissonâ€“Boltzmann equation for two colloidal particles. Physical Chemistry Chemical Physics, 2007, 9, 3174-3180.	1.3	26
126	Ion-Specific Forces between a Colloidal Nanoprobe and a Charged Surface. Langmuir, 2007, 23, 7456-7458.	1.6	7

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127	Adsorption equilibrium of light hydrocarbon mixtures by monte carlo simulation. Brazilian Journal of Chemical Engineering, 2007, 24, 597-610.	0.7	4
128	Effect of the ion-protein dispersion interactions on the protein-surface and protein-protein interactions. Journal of the Brazilian Chemical Society, 2007, 18, 223-230.	0.6	16
129	Evaluation of mixing and combining rules for asymmetric Lennardâ€"Jones chain mixtures: Effect of segment diameter, energy interaction, and chain length. Fluid Phase Equilibria, 2007, 259, 123-134.	1.4	3
130	Effect of Salt Identity on the Phase Diagram for a Globular Protein in Aqueous Electrolyte Solution. Journal of Physical Chemistry B, 2006, 110, 24757-24760.	1.2	44
131	Phase behavior of olive and soybean oils in compressed propane and n-butane. Brazilian Journal of Chemical Engineering, 2006, 23, 405-415.	0.7	48
132	Hofmeister effects: Why protein charge, pH titration and protein precipitation depend on the choice of background salt solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2006, 282-283, 457-463.	2.3	58
133	Phase behavior of soybean oil, castor oil and their fatty acid ethyl esters in carbon dioxide at high pressures. Journal of Supercritical Fluids, 2006, 37, 29-37.	1.6	98
134	Ion Specific Interactions Between Pairs of Nanometer Sized Particles in Aqueous Solutions. , 2006, , 74-77.		1
135	Thermodynamic equilibrium of adsorbed phases. Fluid Phase Equilibria, 2005, 233, 66-72.	1.4	7
136	Phase behavior of castor oil in compressed propane and n-butane. Journal of Supercritical Fluids, 2005, 34, 215-221.	1.6	30
137	Why forces between proteins follow different Hofmeister series for pH above and below pI. Biophysical Chemistry, 2005, 117, 217-224.	1.5	194
138	Thermodynamic equilibrium in systems with multiple adsorbed and bulk phases. Chemical Engineering Science, 2005, 60, 1773-1782.	1.9	22
139	Centrifugation equilibrium of natural gas. Chemical Engineering Science, 2005, 60, 2927-2935.	1.9	9
140	Self- and mutual diffusion coefficient equation for pure fluids, liquid mixtures and polymeric solutions. Chemical Engineering Science, 2005, 60, 4581-4592.	1.9	19
141	Centrifugation equilibrium for spheres and spherocylinders. Journal of Colloid and Interface Science, 2005, 281, 360-367.	5.0	5
142	Phase equilibrium calculations for confined fluids, including surface tension prediction models. Brazilian Journal of Chemical Engineering, 2005, 22, 93-104.	0.7	6
143	Specific Ion Effects in Solutions of Globular Proteins:Â Comparison between Analytical Models and Simulation. Journal of Physical Chemistry B, 2005, 109, 24489-24494.	1.2	52
144	Vapor Pressure Data of Soybean Oil, Castor Oil, and Their Fatty Acid Ethyl Ester Derivatives. Journal of Chemical & Engineering Data, 2005, 50, 330-333.	1.0	34

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145	Mutual diffusion coefficient models for polymer-solvent systems based on the Chapman-Enskog theory. Brazilian Journal of Chemical Engineering, 2004, 21, 611-619.	0.7	2
146	Phase behavior of aqueous solutions containing dipolar proteins from second-order perturbation theory. Journal of Chemical Physics, 2004, 120, 9859-9869.	1.2	33
147	Analytic calculation of phase diagrams for solutions containing colloids or globular proteins. Colloid and Polymer Science, 2004, 282, 620-632.	1.0	41
148	Thermodynamics of fluid-phase equilibria for standard chemical engineering operations. AICHE Journal, 2004, 50, 739-761.	1.8	183
149	Molecular dynamics simulation data of self-diffusion coefficient for Lennardâ€“Jones chain fluids. Fluid Phase Equilibria, 2004, 221, 25-33.	1.4	22
150	The role of saltâ€“macroion van der Waals interactions in the colloidâ€“colloid potential of mean force. Current Opinion in Colloid and Interface Science, 2004, 9, 81-86.	3.4	27
151	Ion-Specific Effects in the Colloidâ^'Colloid or Proteinâ^'Protein Potential of Mean Force:Â Role of Saltâ^'Macroion van der Waals Interactions. Journal of Physical Chemistry B, 2004, 108, 9228-9235.	1.2	142
152	Influence of particle shape on the packing and on the segregation of spherocylinders via Monte Carlo simulations. Powder Technology, 2003, 134, 167-180.	2.1	165
153	Monte Carlo simulation of adsorption using 2-D models of heterogeneous solids. AICHE Journal, 2003, 49, 753-763.	1.8	7
154	Shear viscosity calculated by perturbation theory and molecular dynamics for dense fluids. International Journal of Quantum Chemistry, 2003, 95, 79-87.	1.0	7
155	Monte Carlo Simulations of the Adsorption of Chainlike Molecules on Two-Dimensional Heterogeneous Surfaces. Langmuir, 2003, 19, 1429-1438.	1.6	14
156	Analytic calculation of phase diagrams for charged dipolar colloids with orientation-averaged pair potentials. Physical Chemistry Chemical Physics, 2003, 5, 4851.	1.3	15
157	Role of attractive forces in self-diffusion and mutual diffusion in dense simple fluids and real substances. Fluid Phase Equilibria, 2002, 194-197, 1131-1140.	1.4	12
158	High pressure phase equilibrium calculations for hydrocarbon systems using an equation of state based on the lattice fluid theory. Fluid Phase Equilibria, 2002, 194-197, 599-607.	1.4	3
159	Improving the SAFT-EOS by using an effective WCA segment diameter. Fluid Phase Equilibria, 2002, 194-197, 531-539.	1.4	3
160	An Equation of State for Polymers and Normal Fluids Using the Square-Well Potential of Variable Well Width. Industrial & Engineering Chemistry Research, 2001, 40, 1748-1754.	1.8	10
161	An analytic equation-of-state for mixture of square-well chain fluids of variable well width. Fluid Phase Equilibria, 2001, 179, 231-243.	1.4	9
162	Square-well chain mixture: analytic equation of state and Monte Carlo simulation data. Fluid Phase Equilibria, 2001, 179, 245-267.	1.4	12

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163	Phase behavior of isotactic polypropylene/C4-solvents at high pressure. Experimental data and SAFT modeling. Journal of Supercritical Fluids, 2001, 21, 93-103.	1.6	18
164	Phase equilibria of polypropylene samples with hydrocarbon solvents at high pressures. Journal of Applied Polymer Science, 2001, 81, 3044-3055.	1.3	26
165	Calculation of sedimentation equilibrium using a modified flash algorithm. Chemical Engineering Science, 2001, 56, 3771-3779.	1.9	2
166	Phase equilibria of binary mixtures by molecular simulation and cubic equations of state. Brazilian Journal of Chemical Engineering, 2001, 18, 149-161.	0.7	5
167	MONTE CARLO SIMULATIONS OF THE ADSORPTION OF DIMERS ON STRUCTURED HETEROGENEOUS SURFACES. Brazilian Journal of Chemical Engineering, 2001, 18, 385-397.	0.7	2
168	Calculations of thermodynamic equilibrium in systems subject to gravitational fields. Chemical Engineering Science, 2000, 55, 3495-3504.	1.9	35
169	Phase Equilibrium Calculations for Semicontinuous Mixtures Subject to Gravitational Fields. Industrial & Engineering Chemistry Research, 2000, 39, 4415-4421.	1.8	3
170	A comparison of simulated annealing algorithms in the scheduling of multiproduct serial batch plants. Brazilian Journal of Chemical Engineering, 2000, 17, 199-209.	0.7	1
171	Calculation of mixture critical diagrams using an equation of state based on the lattice fluid theory. Brazilian Journal of Chemical Engineering, 2000, 17, 771-784.	0.7	3
172	A phase stability analysis of the combinatorial term of the UNIQUAC model. Chemical Engineering Science, 1999, 54, 893-896.	1.9	5
173	Liquid film flow and area generation in structured packed columns. Powder Technology, 1999, 104, 84-94.	2.1	31
174	Dense fluid self-diffusion coefficient calculations using perturbation theory and molecular dynamics. Brazilian Journal of Chemical Engineering, 1999, 16, 319-329.	0.7	12
175	A Monte Carlo simulation of the packing and segregation of spheres in cylinders. Brazilian Journal of Chemical Engineering, 1999, 16, 395-405.	0.7	12
176	Monte Carlo simulation of particle segregation. Powder Technology, 1998, 97, 200-207.	2.1	15
177	Group contribution equation of state based on the lattice fluid theory: Alkaneâ€“alkanol systems. Fluid Phase Equilibria, 1998, 142, 33-54.	1.4	29
178	GROUP CONTRIBUTION LATTICE FLUID EQUATION OF STATE: APPLICATION TO POLYMER+SOLVENT SYSTEMS. Brazilian Journal of Chemical Engineering, 1998, 15, 313-319.	0.7	5
179	A completely analytic equation of state for the square-well chain fluid of variable well width. Fluid Phase Equilibria, 1997, 140, 129-143.	1.4	50
180	Vapour-liquid equilibria of exponential-six fluids. Molecular Physics, 1996, 87, 1471-1476.	0.8	10

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181	RESEARCH NOTE Vapour-liquid equilibria of exponential-six fluids. Molecular Physics, 1996, 87, 1471-1476.	0.8	16
182	Equation of state for the square-well chain fluid based on the dimer version of Wertheim's perturbation theory. Molecular Physics, 1995, 86, 1451-1471.	0.8	68
183	Equations of state for chainlike polar fluids: a comparison of reference terms. Fluid Phase Equilibria, 1994, 99, 87-103.	1.4	6