Amparo Galindo

List of Publications by Year
in descending order

177 papers	12,758 citations	39113 52 h-index	28425 109 g-index
193 all docs	193 docs citations	193 times ranked	8904 citing authors

#	Article	IF	Citations
1	Systematic study of the effect of the co-solvent on the performance of amine-based solvents for CO2 capture. Separation and Purification Technology, 2022, 282, 120093.	3.9	23
2	Molecular theory of the static dielectric constant of dipolar fluids. Journal of Chemical Physics, 2022, 156, 154111.	1.2	6
3	Temperature dependence and short-range electrolytic interactions within the e-PPC-SAFT framework. Fluid Phase Equilibria, 2022, 560, 113486.	1.4	7
4	Phase behaviour and pH-solubility profile prediction of aqueous buffered solutions of ibuprofen and ketoprofen. Fluid Phase Equilibria, 2022, 560, 113504.	1.4	6
5	Molecular engineering of sustainable phase-change solvents: From digital design to scaling-up for CO2 capture. Chemical Engineering Journal, 2021, 420, 127624.	6.6	15
6	Mechanism, kinetics and selectivity of a Williamson ether synthesis: elucidation under different reaction conditions. Reaction Chemistry and Engineering, 2021, 6, 1195-1211.	1.9	10
7	On the liquid demixing of water + elastin-like polypeptide mixtures: bimodal re-entrant phase behaviour. Physical Chemistry Chemical Physics, 2021, 23, 5936-5944.	1.3	2
8	An approach for simultaneous computer-aided solvent design and process design for CO2 chemical absorption processes. Computer Aided Chemical Engineering, 2021, , 167-172.	0.3	1
9	Description of the thermodynamic properties and fluidâ€phase behavior of aqueous solutions of linear, branched, and cyclic amines. AICHE Journal, 2021, 67, e17194.	1.8	14
10	Solubility of water in mixtures of (n-alkanes + n-perfluoroalkanes) and in n-perfluoroalkylalkanes: experiments and modelling with the SAFT-Î³ Mie group-contribution approach. Molecular Physics, 2021, 119, .	0.8	1
11	Computer Aided Design of Solvent Blends for Hybrid Cooling and Antisolvent Crystallization of Active Pharmaceutical Ingredients. Organic Process Research and Development, 2021, 25, 1123-1142.	1.3	18
12	Monte Carlo Molecular Simulation Study of Carbon Dioxide Sequestration into Dry and Wet Calcite Pores Containing Methane. Energy & Fuels, 2021, 35, 11393-11402.	2.5	7
13	Extending the SAFT-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mi>Î³</mml:mi></mml:math> Mie approach to model benzoic acid, diphenylamine, and mefenamic acid: Solubility prediction and experimental measurement. Fluid Phase Equilibria, 2021, 540, 113002.	1.4	10
14	Special issue in honour of Michael L. Klein FRS. Molecular Physics, 2021, 119, .	0.8	0
15	Beyond a heuristic analysis: integration of process and working-fluid design for organic Rankine cycles. Molecular Systems Design and Engineering, 2020, 5, 493-510.	1.7	20
16	Computer-aided Solvent Mixture Design for the Crystallisation and Isolation of Mefenamic Acid. Computer Aided Chemical Engineering, 2020, 48, 649-654.	0.3	3
17	Thermodynamics 2019 Conferenceâ€“Punta UmbrÃa, Costa de la Luz, Huelva, Spain, 26â€“28 June 2019. Molecular Physics, 2020, 118, e1771043.	0.8	1
18	Expanding the Applications of the SAFT-Î³ Mie Group-Contribution Equation of State: Prediction of Thermodynamic Properties and Phase Behavior of Mixtures. Journal of Chemical & Engineering Data, 2020, 65, 5862-5890.	1.0	32

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19	Modeling the Fluid-Phase Equilibria of Semifluorinated Alkanes and Mixtures of (n-Alkanes +) Tj ETQq1 1 0.784314 rgBT /Overlock & Engineering Data, 2020, 65, 5909-5919.	1.0	4
20	Predictive models for the phase behaviour and solution properties of weak electrolytes: nitric, sulphuric, and carbonic acids. Physical Chemistry Chemical Physics, 2020, 22, 15248-15269.	1.3	13
21	A comparative study of multi-objective optimization methodologies for molecular and process design. Computers and Chemical Engineering, 2020, 136, 106802.	2.0	17
22	An approach for simultaneous computer-aided molecular design with holistic sustainability assessment: Application to phase-change CO2 capture solvents. Computers and Chemical Engineering, 2020, 135, 106769.	2.0	31
23	A comparison of the performance of multi-objective optimization methodologies for solvent design. Computer Aided Chemical Engineering, 2019, 46, 37-42.	0.3	5
24	An investigation of free-energy-averaged (coarse-grained) potentials for fluid adsorption on heterogeneous solid surfaces. Physical Chemistry Chemical Physics, 2019, 21, 25558-25568.	1.3	9
25	Computer-aided Design of Solvent Blends for the Cooling and Anti-solvent Crystallisation of Ibuprofen. Computer Aided Chemical Engineering, 2019, , 949-954.	0.3	9
26	Hybrid QSPR models for the prediction of the free energy of solvation of organic solute/solvent pairs. Physical Chemistry Chemical Physics, 2019, 21, 13706-13720.	1.3	33
27	Intramolecular bonding in a statistical associating fluid theory of ring aggregates. Molecular Physics, 2019, 117, 3884-3912.	0.8	7
28	Modelling and prediction of the thermophysical properties of aqueous mixtures of choline geranate and geranic acid (CAGE) using SAFT-Î³ Mie. RSC Advances, 2019, 9, 38017-38031.	1.7	12
29	Optimal design of post combustion CO2 capture processes based on phase-change solvents. Computer Aided Chemical Engineering, 2019, , 463-468.	0.3	4
30	On the equilibrium contact angle of sessile liquid drops from molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 164704.	1.2	28
31	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
32	Daan Frenkel â€" An entropic career. Molecular Physics, 2018, 116, 2737-2741.	0.8	0
33	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 5. Hetero-Group Coarse-Grained Models of Linear Alkanes and the Importance of Intramolecular Interactions. Journal of Physical Chemistry B, 2018, 122, 9161-9177.	1.2	37
34	Multi-Objective Computer-Aided Solvent Design for Selectivity and Rate in Reactions. Computer Aided Chemical Engineering, 2018, , 2437-2442.	0.3	4
35	Development of Predictive Models of the Kinetics of a Hydrogen Abstraction Reaction Combining Quantum-Mechanical Calculations and Experimental Data. Industrial & Engineering Chemistry Research, 2017, 56, 815-831.	1.8	8
36	Predicting the Solvation of Organic Compounds in Aqueous Environments: From Alkanes and Alcohols to Pharmaceuticals. Industrial & Engineering Chemistry Research, 2017, 56, 10856-10876.	1.8	43

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37	Predicting the Fluid-Phase Behavior of Aqueous Solutions of ELP (VPGVG) Sequences Using SAFT-VR. Langmuir, 2017, 33, 11733-11745.	1.6	5
38	A QM-CAMD approach to solvent design for optimal reaction rates. Chemical Engineering Science, 2017, 159, 69-83.	1.9	39
39	A feasibility-based algorithm for Computer Aided Molecular and Process Design of solvent-based separation systems. Computer Aided Chemical Engineering, 2016, 38, 73-78.	0.3	3
40	On the use of molecular-based thermodynamic models to assess the performance of solvents for CO₂ capture processes: monoethanolamine solutions. Faraday Discussions, 2016, 192, 337-390.	1.6	12
41	Computer-aided molecular design and selection of CO₂ capture solvents based on thermodynamics, reactivity and sustainability. Molecular Systems Design and Engineering, 2016, 1, 313-334.	1.7	56
42	Development of intermolecular potential models for electrolyte solutions using an electrolyte SAFT-VR Mie equation of state. Molecular Physics, 2016, 114, 2724-2749.	0.8	40
43	Outer approximation algorithm with physical domain reduction for computerâ€aided molecular and separation process design. AICHE Journal, 2016, 62, 3484-3504.	1.8	47
44	Application of the SAFT-Î³ Mie group contribution equation of state to fluids of relevance to the oil and gas industry. Fluid Phase Equilibria, 2016, 416, 104-119.	1.4	62
45	Modelling the phase and chemical equilibria of aqueous solutions of alkanolamines and carbon dioxide using the SAFT-Î³ SW group contribution approach. Fluid Phase Equilibria, 2016, 407, 280-297.	1.4	37
46	The development of unlike induced association-site models to study the phase behaviour of aqueous mixtures comprising acetone, alkanes and alkyl carboxylic acids with the SAFT-Î³ Mie group contribution methodology. Fluid Phase Equilibria, 2016, 407, 39-57.	1.4	32
47	Interfacial tensions of systems comprising water, carbon dioxide and diluent gases at high pressures: Experimental measurements and modelling with SAFT-VR Mie and square-gradient theory. Fluid Phase Equilibria, 2016, 407, 159-176.	1.4	47
48	A hierarchical method to integrated solvent and process design of physical <scp>CO</scp>₂ absorption using the <scp>SAFT</scp>â€Î³ <scp>M</scp>ie approach. AICHE Journal, 2015, 61, 3249-3269.	1.8	120
49	The A in SAFT: developing the contribution of association to the Helmholtz free energy within a Wertheim TPT1 treatment of generic Mie fluids. Molecular Physics, 2015, 113, 948-984.	0.8	114
50	Experimental and Modeling Study of the Phase Behavior of (Heptane + Carbon Dioxide + Water) Mixtures. Journal of Chemical & Engineering Data, 2015, 60, 3670-3681.	1.0	24
51	Aspects of Asphaltene Aggregation Obtained from Coarse-Grained Molecular Modeling. Energy & Fuels, 2015, 29, 556-566.	2.5	24
52	High-temperature vapourâ€“liquid equilibrium for ethanolâ€“1-propanol mixtures and modeling with SAFT-VR. Fluid Phase Equilibria, 2015, 398, 5-9.	1.4	4
53	Fluidâ€“fluid coexistence in an athermal colloidâ€“polymer mixture: thermodynamic perturbation theory and continuum molecular-dynamics simulation. Molecular Physics, 2015, 113, 2608-2628.	0.8	12
54	Toward Sustainable Solvent-Based Postcombustion CO2 Capture. Computer Aided Chemical Engineering, 2015, , 279-310.	0.3	20

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55	A corresponding-states framework for the description of the Mie family of intermolecular potentials. Molecular Physics, 2015, 113, 932-947.	0.8	63
56	Developing intermolecularâ€potential models for use with the <scp>SAFT</scp>â€<scp>VR</scp><scp>M</scp>ie equation of state. AICHE Journal, 2015, 61, 2891-2912.	1.8	68
57	Molecules Matter. Computer Aided Chemical Engineering, 2014, , 55-64.	0.3	33
58	Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. Journal of Chemical Physics, 2014, 140, 054107.	1.2	225
59	Nonequilibrium molecular dynamics simulation of diffusion at the liquid-liquid interface. Journal of Chemical Physics, 2014, 141, 154101.	1.2	13
60	Thermodynamics 2013 Conference, Manchester, UK, 3â€“6 September 2013. Molecular Physics, 2014, 112, 2199-2202.	0.8	4
61	Working fluid selection for a two-phase thermofluidic oscillator: Effect of thermodynamic properties. Applied Energy, 2014, 124, 167-185.	5.1	30
62	Prediction of Thermodynamic Properties and Phase Behavior of Fluids and Mixtures with the SAFT-Î³ Mie Group-Contribution Equation of State. Journal of Chemical & Engineering Data, 2014, 59, 3272-3288.	1.0	107
63	On the impact of using volume as an independent variable for the solution of P â€“ T fluid-phase equilibrium with equations of state. Computers and Chemical Engineering, 2014, 71, 67-76.	2.0	12
64	Modelling of the thermodynamic and solvation properties of electrolyte solutions with the statistical associating fluid theory for potentials of variable range. Molecular Physics, 2014, 112, 2339-2364.	0.8	65
65	Foreword: Modeling and Simulation of Real Systems. Journal of Chemical & Engineering Data, 2014, 59, 2927-2927.	1.0	1
66	On the optimal design of gas-expanded liquids based on process performance. Chemical Engineering Science, 2014, 115, 19-30.	1.9	30
67	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	1.2	382
68	New methods for calculating the free energy of charged defects in solid electrolytes. Journal of Physics Condensed Matter, 2013, 25, 395001.	0.7	2
69	Computer-aided molecular design of solvents for accelerated reaction kinetics. Nature Chemistry, 2013, 5, 952-957.	6.6	141
70	Application of the statistical associating fluid theory for potentials of variable range (SAFT-VR) coupled with renormalisation-group (RG) theory to model the phase equilibria and second-derivative properties of pure fluids. Fluid Phase Equilibria, 2013, 337, 274-287.	1.4	23
71	Experimental and molecular modelling study of the three-phase behaviour of (propane+carbon) Tj ETQq1 1 0.784314 rgBT /Overlock	1.6	13
72	High-temperature vapourâ€“liquid equilibrium for the (water+alcohol) systems and modelling with SAFT-VR: 2. Water-1-propanol. Journal of Chemical Thermodynamics, 2013, 60, 15-18.	1.0	11

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73	The role of heat exchange on the behaviour of an oscillatory two-phase low-grade heat engine. Applied Thermal Engineering, 2013, 53, 177-187.	3.0	26
74	Validation of a Process Model of CO2 Capture in an Aqueous Solvent, Using an Implicit Molecular Based Treatment of The Reactions. Energy Procedia, 2013, 37, 1566-1571.	1.8	1
75	SAFT-Î³ Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Greenhouse Gases, Refrigerants, and Long Alkanes. Journal of Physical Chemistry B, 2013, 117, 2717-2733.	1.2	126
76	High-temperature vapourâ€“liquid equilibrium for the waterâ€“alcohol systems and modeling with SAFT-VR: 1. Waterâ€“ethanol. Fluid Phase Equilibria, 2013, 341, 48-53.	1.4	16
77	Modeling of Strong Electrolytes with ePPC-SAFT up to High Temperatures. Industrial & Engineering Chemistry Research, 2013, 52, 9979-9994.	1.8	67
78	Modelling of a two-phase thermofluidic oscillator for low-grade heat utilisation: Accounting for irreversible thermal losses. Applied Energy, 2013, 106, 337-354.	5.1	37
79	SAFT-Î³force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models ofn-decylbenzene. Molecular Physics, 2012, 110, 1189-1203.	0.8	82
80	Anomalous columnar order of charged colloidal platelets. Journal of Chemical Physics, 2012, 136, 034901.	1.2	17
81	Modelling the fluid phase behaviour of aqueous mixtures of multifunctional alkanolamines and carbon dioxide using transferable parameters with the SAFT-VR approach. Molecular Physics, 2012, 110, 1325-1348.	0.8	83
82	Application of the SAFT-VR density functional theory to the prediction of the interfacial properties of mixtures of relevance to reservoir engineering. Fluid Phase Equilibria, 2012, 336, 137-150.	1.4	61
83	Modelling the effect of methanol, glycol inhibitors and electrolytes on the equilibrium stability of hydrates with the SAFT-VR approach. Molecular Physics, 2012, 110, 1223-1240.	0.8	27
84	Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules. Journal of Chemical Physics, 2012, 137, 144505.	1.2	93
85	Validation of an absorber model of carbon dioxide capture in an aqueous amine solvent developed based on the SAFT-VR framework. Computer Aided Chemical Engineering, 2012, , 930-934.	0.3	5
86	Dynamic modelling of a two-phase thermofluidic oscillator for efficient low grade heat utilization: Effect of fluid inertia. Applied Energy, 2012, 89, 156-163.	5.1	43
87	The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state. Computers and Chemical Engineering, 2012, 36, 99-118.	2.0	29
88	Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem. Heat Transfer Engineering, 2011, 32, 197-215.	1.2	62
89	Transferable SAFT-VR Models for the Calculation of the Fluid Phase Equilibria in Reactive Mixtures of Carbon Dioxide, Water, and n-Alkylamines in the Context of Carbon Capture. Journal of Physical Chemistry B, 2011, 115, 8155-8168.	1.2	79
90	Experimental and Molecular Modeling Study of the Three-Phase Behavior of (n-Decane + Carbon) Tj ETQq0 0 0 rgBT /Overlock 10	1.2	33

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91	Application of a renormalization-group treatment to the statistical associating fluid theory for potentials of variable range (SAFT-VR). Journal of Chemical Physics, 2011, 134, 154102.	1.2	42
92	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 1. A Single-Site Coarse Grained Model of Carbon Dioxide. Journal of Physical Chemistry B, 2011, 115, 11154-11169.	1.2	200
93	Simultaneous prediction of vapourâ€“liquid and liquidâ€“liquid equilibria (VLE and LLE) of aqueous mixtures with the SAFT-Î³ group contribution approach. Fluid Phase Equilibria, 2011, 306, 82-96.	1.4	55
94	Integrated solvent and process design using a SAFT-VR thermodynamic description: High-pressure separation of carbon dioxide and methane. Computers and Chemical Engineering, 2011, 35, 474-491.	2.0	83
95	Solidâ€“liquid equilibrium using the SAFT-VR equation of state: Solubility of naphthalene and acetic acid in binary mixtures and calculation of phase diagrams. Fluid Phase Equilibria, 2011, 306, 137-147.	1.4	8
96	Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation. Fluid Phase Equilibria, 2011, 306, 129-136.	1.4	35
97	Simultaneous prediction of phase behaviour and second derivative properties with a group contribution approach (SAFT-Î³ Mie). Computer Aided Chemical Engineering, 2011, , 1593-1597.	0.3	0
98	Integrated Design of a Reactor and a Gas-Expanded Solvent. Computer Aided Chemical Engineering, 2011, , 316-320.	0.3	2
99	Interfacial tension measurements and modelling of (carbon dioxide+n-alkane) and (carbon) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T Fluids, 2010, 55, 743-754.	1.6	120
100	A duality-based optimisation approach for the reliable solution of (P, T) phase equilibrium in volume-composition space. Fluid Phase Equilibria, 2010, 299, 1-23.	1.4	32
101	Solvent design for a Menschutkin reaction by using CAMD and DFT calculations. Computer Aided Chemical Engineering, 2010, 28, 1291-1296.	0.3	2
102	Integrated solvent and process design for the reactive separation of CO2 from flue gas. Computer Aided Chemical Engineering, 2010, , 1231-1236.	0.3	26
103	Modeling the Fluid Phase Behavior of Carbon Dioxide in Aqueous Solutions of Monoethanolamine Using Transferable Parameters with the SAFT-VR Approach. Industrial & Engineering Chemistry Research, 2010, 49, 1883-1899.	1.8	129
104	An overview of CO2 capture technologies. Energy and Environmental Science, 2010, 3, 1645.	15.6	1,376
105	Classical density functional theory for the prediction of the surface tension and interfacial properties of fluids mixtures of chain molecules based on the statistical associating fluid theory for potentials of variable range. Journal of Chemical Physics, 2010, 133, 024704.	1.2	78
106	The Use of Anisotropic Potentials in Modeling Water and Free Energies of Hydration. Journal of Chemical Theory and Computation, 2010, 6, 1590-1607.	2.3	31
107	Robust algorithms for the calculation of phase equilibrium. Computer Aided Chemical Engineering, 2010, 28, 79-84.	0.3	1
108	SAFT Associating Fluids and Fluid Mixtures. , 2010, , 215-279.		61

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109	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 79-94.	1.4	11
110	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 95-104.	1.4	11
111	Application of the generalised SAFT-VR approach for long-ranged square-well potentials to model the phase behaviour of real fluids. Fluid Phase Equilibria, 2009, 276, 116-126.	1.4	33
112	Integrated Modeling of Mixture Fluid Phase Equilibrium Experiments Using SAFT-VR Applied to Xenon + Diborane, Xenon + Cyclopropane, Xenon + Boron Trifluoride. Industrial & Engineering Chemistry Research, 2009, 48, 2188-2198.	1.8	2
113	Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures. Fluid Phase Equilibria, 2008, 266, 105-128.	1.4	131
114	A generalisation of the SAFT- group contribution method for groups comprising multiple spherical segments. Fluid Phase Equilibria, 2008, 274, 85-104.	1.4	128
115	Modeling and Understanding Closed-Loop Liquidâ^'Liquid Immiscibility in Aqueous Solutions of Poly(ethylene glycol) Using the SAFT-VR Approach with Transferable Parameters. Macromolecules, 2008, 41, 6582-6595.	2.2	48
116	A heteronuclear group contribution method for associating chain molecules (SAFT-Î³). Computer Aided Chemical Engineering, 2008, 25, 871-876.	0.3	0
117	Thermotropic Biaxial Liquid Crystalline Phases in a Mixture of Attractive Uniaxial Rod and Disk Particles. Physical Review Letters, 2008, 101, 237802.	2.9	51
118	Examining the effect of chain length polydispersity on the phase behavior of polymer solutions with the statistical associating fluid theory (Wertheim TPT1) using discrete and continuous distributions. Journal of Chemical Physics, 2007, 127, 154906.	1.2	11
119	Phase equilibrium of liquid mixtures: Experimental and modeled data using statistical associating fluid theory for potential of variable range approach. Journal of Chemical Physics, 2007, 127, 144513.	1.2	11
120	A group contribution method for associating chain molecules based on the statistical associating fluid theory (SAFT-Î³). Journal of Chemical Physics, 2007, 127, 234903.	1.2	213
121	Surface ordering and capillary phenomena of confined hard cut-sphere particles. Soft Matter, 2007, 3, 768-778.	1.2	36
122	Phase Equilibria, Excess Properties, and Henry's Constants of the Water + Carbon Dioxide Binary Mixture. Journal of Physical Chemistry C, 2007, 111, 15924-15934.	1.5	47
123	Phase Equilibrium of Binary Mixtures of Cyclic Ethers + Chlorobutane Isomers:â€‰ Experimental Measurements and SAFT-VR Modeling. Journal of Physical Chemistry B, 2007, 111, 9588-9597.	1.2	16
124	Investigation of the Salting Out of Methane from Aqueous Electrolyte Solutions Using Computer Simulations. Journal of Physical Chemistry B, 2007, 111, 8993-9000.	1.2	36
125	Intermolecular potential model parameters for cyclic ethers and chloroalkanes in the SAFT-VR approach. Fluid Phase Equilibria, 2007, 255, 200-206.	1.4	15
126	Modelling the phase equilibria and excess properties of the waterâ€‰+â€‰carbon dioxide binary mixture. Fluid Phase Equilibria, 2007, 261, 359-365.	1.4	48

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127	A study of Wertheim's thermodynamic perturbation theory (TPT1) for associating fluids with dispersive interactions: the importance of the association range. Molecular Physics, 2006, 104, 3551-3560.	0.8	12
128	Developing optimal Wertheim-like models of water for use in Statistical Associating Fluid Theory (SAFT) and related approaches. Molecular Physics, 2006, 104, 3561-3581.	0.8	170
129	Design of polyolefin reactor mixtures. Computer Aided Chemical Engineering, 2006, 22, 301-332.	0.3	2
130	Integrating advanced thermodynamics and process and solvent design for gas separation. Computer Aided Chemical Engineering, 2006, 21, 743-748.	0.3	0
131	Predicting enhanced absorption of light gases in polyethylene using simplified PC-SAFT and SAFT-VR. Fluid Phase Equilibria, 2006, 243, 74-91.	1.4	36
132	The derivation of size parameters for the SAFTâ€“VR equation of state from quantum mechanical calculations. Computer Aided Chemical Engineering, 2006, , 143-159.	0.3	6
133	A potential model for methane in water describing correctly the solubility of the gas and the properties of the methane hydrate. Journal of Chemical Physics, 2006, 125, 074510.	1.2	139
134	Modeling electrolyte solutions with the SAFT-VR equation using Yukawa potentials and the mean-spherical approximation. Fluid Phase Equilibria, 2005, 236, 241-255.	1.4	51
135	Application of the simplex simulated annealing technique to nonlinear parameter optimization for the SAFT-VR equation of state. Chemical Engineering Science, 2005, 60, 6607-6621.	1.9	25
136	Density functional theory and simulation of the columnar phase of a system of parallel hard ellipsoids with attractive interactions. Physical Review E, 2005, 72, 051707.	0.8	19
137	Nematic Phase Transitions in Mixtures of Thin and Thick Colloidal Rods. Physical Review Letters, 2005, 94, 057801.	2.9	75
138	Nematic-nematic phase separation in binary mixtures of thick and thin hard rods: Results from Onsager-like theories. Physical Review E, 2005, 72, 051704.	0.8	41
139	Generalized equation of state for square-well potentials of variable range. Molecular Physics, 2005, 103, 129-139.	0.8	64
140	Phase behavior of carbon dioxide mixtures with n-alkanes and n-perfluoroalkanes. Fluid Phase Equilibria, 2004, 222-223, 77-85.	1.4	41
141	Molecular modeling of flexible molecules. Vaporâ€“liquid and fluidâ€“solid equilibria. Journal of Molecular Liquids, 2004, 113, 37-51.	2.3	12
142	Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: Comparison with flexible models. Journal of Chemical Physics, 2004, 120, 3957-3968.	1.2	27
143	Modeling the Cloud Curves and the Solubility of Gases in Amorphous and Semicrystalline Polyethylene with the SAFT-VR Approach and Flory Theory of Crystallization. Industrial & Engineering Chemistry Research, 2004, 43, 6871-6889.	1.8	85
144	The phase behavior of a binary mixture of rodlike and disclike mesogens: Monte Carlo simulation, theory, and experiment. Journal of Chemical Physics, 2003, 119, 5216-5225.	1.2	54

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145	Prediction of the Salting-Out Effect of Strong Electrolytes on Water + Alkane Solutions. Industrial & Engineering Chemistry Research, 2003, 42, 3809-3823.	1.8	102
146	Anomalies in the Solubility of Alkanes in Near-Critical Water. Journal of Physical Chemistry B, 2003, 107, 12307-12314.	1.2	49
147	Fluidâ€“solid equilibria of flexible and linear rigid tangent chains from Wertheimâ€™s thermodynamic perturbation theory. Journal of Chemical Physics, 2003, 119, 10958-10971.	1.2	17
148	New types of phase behaviour in binary mixtures of hard rod-like particles. Molecular Physics, 2003, 101, 817-825.	0.8	41
149	Understanding liquid-liquid immiscibility and LCST behaviour in polymer solutions with a Wertheim TPT1 description. Molecular Physics, 2003, 101, 2575-2600.	0.8	52
150	The phase diagram of the two center Lennard-Jones model as obtained from computer simulation and Wertheimâ€™s thermodynamic perturbation theory. Journal of Chemical Physics, 2003, 118, 10696-10706.	1.2	33
151	Study of the solid-liquid-vapour phase equilibria of flexible chain molecules using Wertheim's thermodynamic perturbation theory. Molecular Physics, 2003, 101, 449-458.	0.8	27
152	Towards the identification of optimal solvents for long chain alkanes with the SAFT equation of state. Computer Aided Chemical Engineering, 2003, 14, 137-142.	0.3	2
153	Ordering transitions, biaxiality, and demixing in the symmetric binary mixture of rod and plate molecules described with the Onsager theory. Physical Review E, 2002, 66, 011707.	0.8	44
154	Extending Wertheimâ€™s perturbation theory to the solid phase of Lennard-Jones chains: Determination of the global phase diagram. Journal of Chemical Physics, 2002, 116, 7645-7655.	1.2	35
155	Global fluid phase behavior in binary mixtures of rodlike and platelike molecules. Journal of Chemical Physics, 2002, 117, 7207-7221.	1.2	34
156	Phase behavior of symmetric rodâ€“plate mixtures revisited: Biaxiality versus demixing. Journal of Chemical Physics, 2002, 117, 10412-10424.	1.2	31
157	Improved models for the phase behaviour of hydrogen fluoride: chain and ring aggregates in the SAFT approach and the AEOS model. Molecular Physics, 2002, 100, 2241-2259.	0.8	49
158	Study of the high pressure phase behaviour of CO2+n-alkane mixtures using the SAFT-VR approach with transferable parameters. Fluid Phase Equilibria, 2002, 194-197, 501-509.	1.4	85
159	Recent advances in the use of the SAFT approach in describing electrolytes, interfaces, liquid crystals and polymers. Fluid Phase Equilibria, 2002, 194-197, 87-96.	1.4	117
160	Theoretical Examination of the Global Fluid Phase Behavior and Critical Phenomena in Carbon Dioxide +n-Alkane Binary Mixtures. Journal of Physical Chemistry B, 2002, 106, 4503-4515.	1.2	110
161	A statistical associating fluid theory for electrolyte solutions (SAFT-VRE). Molecular Physics, 2001, 99, 531-546.	0.8	84
162	Examining the Adsorption (Vaporâ^'Liquid Equilibria) of Short-Chain Hydrocarbons in Low-Density Polyethylene with the SAFT-VR Approach. Industrial & Engineering Chemistry Research, 2001, 40, 3835-3842.	1.8	71

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