George Jackson

List of Publications by Year
in descending order

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266 papers	22,040 citations	13865 67 h-index	9345 143 g-index
281 all docs	281 docs citations	281 times ranked	9360 citing authors

#	Article	IF	Citations
1	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	30.8	2,378
2	New reference equation of state for associating liquids. Industrial & Engineering Chemistry Research, 1990, 29, 1709-1721.	3.7	1,799
3	An overview of CO2 capture technologies. Energy and Environmental Science, 2010, 3, 1645.	30.8	1,376
4	SAFT: Equation-of-state solution model for associating fluids. Fluid Phase Equilibria, 1989, 52, 31-38.	2.5	1,275
5	Phase equilibria of associating fluids. Molecular Physics, 1988, 65, 1-31.	1.7	1,107
6	Phase equilibria of associating fluids. Molecular Physics, 1988, 65, 1057-1079.	1.7	1,102
7	Statistical associating fluid theory for chain molecules with attractive potentials of variable range. Journal of Chemical Physics, 1997, 106, 4168-4186.	3.0	932
8	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	3.0	382
9	A reâ€examination of the phase diagram of hard spherocylinders. Journal of Chemical Physics, 1996, 104, 6755-6771.	3.0	351
10	The thermodynamics of mixtures and the corresponding mixing rules in the SAFT-VR approach for potentials of variable range. Molecular Physics, 1998, 93, 241-252.	1.7	323
11	Phase equilibria and critical behavior of squareâ€well fluids of variable width by Gibbs ensemble Monte Carlo simulation. Journal of Chemical Physics, 1992, 96, 2296-2305.	3.0	307
12	Test-area simulation method for the direct determination of the interfacial tension of systems with continuous or discontinuous potentials. Journal of Chemical Physics, 2005, 123, 134703.	3.0	297
13	Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. Journal of Chemical Physics, 2014, 140, 054107.	3.0	225
14	A group contribution method for associating chain molecules based on the statistical associating fluid theory (SAFT-Î³). Journal of Chemical Physics, 2007, 127, 234903.	3.0	213
15	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.	2.6	200
16	SAFT-VRE:Â Phase Behavior of Electrolyte Solutions with the Statistical Associating Fluid Theory for Potentials of Variable Range. Journal of Physical Chemistry B, 1999, 103, 10272-10281.	2.6	199
17	Developing optimal Wertheim-like models of water for use in Statistical Associating Fluid Theory (SAFT) and related approaches. Molecular Physics, 2006, 104, 3561-3581.	1.7	170
18	Simulation of Asphaltene Aggregation through Molecular Dynamics: Insights and Limitations. Energy & Fuels, 2017, 31, 1108-1125.	5.1	170

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19	Predicting the High-Pressure Phase Equilibria of Water +n-Alkanes Using a Simplified SAFT Theory with Transferable Intermolecular Interaction Parameters. The Journal of Physical Chemistry, 1996, 100, 6781-6792.	2.9	142
20	SAFT-VR modelling of the phase equilibrium of long-chain n-alkanes. Physical Chemistry Chemical Physics, 1999, 1, 2057-2064.	2.8	142
21	Force-Field Parameters from the SAFT-Î³ Equation of State for Use in Coarse-Grained Molecular Simulations. Annual Review of Chemical and Biomolecular Engineering, 2014, 5, 405-427.	6.8	141
22	Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures. Fluid Phase Equilibria, 2008, 266, 105-128.	2.5	131
23	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.	3.7	129
24	A generalisation of the SAFT- group contribution method for groups comprising multiple spherical segments. Fluid Phase Equilibria, 2008, 274, 85-104.	2.5	128
25	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.	2.6	126
26	Interfacial tension measurements and modelling of (carbon dioxide+n-alkane) and (carbon) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 Td Fluids, 2010, 55, 743-754.	3.2	120
27	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.	3.6	120
28	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.	2.5	117
29	An accurate density functional theory for the vapor-liquid interface of associating chain molecules based on the statistical associating fluid theory for potentials of variable range. Journal of Chemical Physics, 2004, 121, 12740.	3.0	116
30	Predicting the High-Pressure Phase Equilibria of Binary Mixtures of Perfluoro-n-alkanes +n-Alkanes Using the SAFT-VR Approach. Journal of Physical Chemistry B, 1998, 102, 8060-8069.	2.6	115
31	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.	1.7	114
32	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.	1.9	107
33	Vapourâ€"liquid equilibrium of the square-well fluid of variable range via a hybrid simulation approach. Molecular Physics, 2002, 100, 2531-2546.	1.7	104
34	The nature of the calculation of the pressure in molecular simulations of continuous models from volume perturbations. Journal of Chemical Physics, 2006, 125, 164109.	3.0	94
35	Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules. Journal of Chemical Physics, 2012, 137, 144505.	3.0	93
36	Thermodynamic perturbation theory for association into chains and rings. Physical Review E, 1994, 50, 386-394.	2.1	88

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37	Bonded hardâ€sphere (BHS) theory for the equation of state of fused hardâ€sphere polyatomic molecules and their mixtures. Journal of Chemical Physics, 1992, 96, 4604-4618.	3.0	87
38	Vapor-liquid interfacial properties of fully flexible Lennard-Jones chains. Journal of Chemical Physics, 2008, 129, 144703.	3.0	87
39	Computer simulation of mixtures of hard spheres. The Journal of Physical Chemistry, 1987, 91, 4907-4912.	2.9	86
40	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.	3.7	85
41	Mixtures of associating spherical and chain molecules. Pure and Applied Chemistry, 1989, 61, 1021-1026.	1.9	84
42	A statistical associating fluid theory for electrolyte solutions (SAFT-VRE). Molecular Physics, 2001, 99, 531-546.	1.7	84
43	Prediction of the Vaporâ^'Liquid Interfacial Tension of Nonassociating and Associating Fluids with the SAFT-VR Density Functional Theory. Journal of Physical Chemistry C, 2007, 111, 15513-15522.	3.1	84
44	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.	3.8	83
45	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.	1.7	83
46	Theory of closed-loop liquid-liquid immiscibility in mixtures of molecules with directional attractive forces. Molecular Physics, 1991, 72, 1365-1385.	1.7	82
47	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.	1.7	82
48	A SAFTâ€“DFT approach for the vapourâ€“liquid interface of associating fluids. Fluid Phase Equilibria, 2002, 194-197, 521-530.	2.5	81
49	A perspective on the interfacial properties of nanoscopic liquid drops. Journal of Physics Condensed Matter, 2012, 24, 464121.	1.8	81
50	Title is missing!. International Journal of Thermophysics, 1998, 19, 675-686.	2.1	80
51	An examination of the vapour-liquid interface of associating fluids using a SAFT-DFT approach. Molecular Physics, 2001, 99, 1851-1865.	1.7	80
52	Communications: Evidence for the role of fluctuations in the thermodynamics of nanoscale drops and the implications in computations of the surface tension. Journal of Chemical Physics, 2010, 132, 141101.	3.0	80
53	Predicting the Phase Equilibria of Mixtures of Hydrogen Fluoride with Water, Difluoromethane (HFC-32), and 1,1,1,2-Tetrafluoroethane (HFC-134a) Using a Simplified SAFT Approach. Journal of Physical Chemistry B, 1997, 101, 2082-2091.	2.6	79
54	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.	2.6	79

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55	Predicting the High-Pressure Phase Equilibria of Methane +n-Hexane Using the SAFT-VR Approach. Journal of Physical Chemistry B, 1998, 102, 4183-4188.	2.6	78
56	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.	3.0	78
57	BHS theory and computer simulations of linear heteronuclear triatomic hard-sphere molecules. Molecular Physics, 1991, 74, 191-210.	1.7	77
58	An Examination of the Cloud Curves of Liquidâ^'Liquid Immiscibility in Aqueous Solutions of Alkyl Polyoxyethylene Surfactants Using the SAFT-HS Approach with Transferable Parameters. Journal of the American Chemical Society, 1998, 120, 4191-4199.	13.7	77
59	Prediction of Phase Equilibria for Refrigerant Mixtures of Difluoromethane (HFC-32), 1,1,1,2-Tetrafluoroethane (HFC-134a), and Pentafluoroethane (HFC-125a) Using SAFT-VR. Journal of Physical Chemistry B, 1998, 102, 7632-7639.	2.6	77
60	Liquid crystalline phase behavior in systems of hard-sphere chains. Journal of Chemical Physics, 1998, 108, 10294-10302.	3.0	76
61	Nematic Phase Transitions in Mixtures of Thin and Thick Colloidal Rods. Physical Review Letters, 2005, 94, 057801.	7.8	75
62	SAFT-Î³ force field for the simulation of molecular fluids: 4. A single-site coarse-grained model of water applicable over a wide temperature range. Molecular Physics, 2015, 113, 1228-1249.	1.7	72
63	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.	3.7	71
64	SAFT- Î³ force field for the simulation of molecular fluids 6: Binary and ternary mixtures comprising water, carbon dioxide, and n -alkanes. Journal of Chemical Thermodynamics, 2016, 93, 320-336.	2.0	71
65	Theory and computer simulations of heteronuclear diatomic hard-sphere molecules (hard dumbbells). Molecular Physics, 1991, 73, 881-896.	1.7	70
66	Chain and ring structures in smectic phases of molecules with transverse dipoles. Chemical Physics Letters, 1997, 269, 441-447.	2.6	70
67	The theoretical prediction of the cricital points of alkanes, perfluoroalkanes, and their mixtures using bonded hard-sphere (BHS) theory. International Journal of Thermophysics, 1996, 17, 201-211.	2.1	68
68	Study of the demixing transition in model athermal mixtures of colloids and flexible self-excluding polymers using the thermodynamic perturbation theory of Wertheim. Journal of Chemical Physics, 2003, 118, 8525-8536.	3.0	68
69	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.	3.6	68
70	Vaporâ€"liquid and liquidâ€"liquid phase equilibria of mixtures containing squareâ€well molecules by Gibbs ensemble Monte Carlo simulation. Journal of Chemical Physics, 1994, 101, 3190-3204.	3.0	67
71	The thermodynamics of heteronuclear molecules formed from bonded square-well (BSW) segments using the SAFT-VR approach. Molecular Physics, 1999, 97, 551-558.	1.7	66
72	An analytical equation of state for chain molecules formed from Yukawa segments. Journal of Chemical Physics, 1999, 111, 8659-8665.	3.0	65

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73	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.	1.7	65
74	The effect of dipolar interactions on the liquid crystalline phase transitions of hard spherocylinders with central longitudinal dipoles. Molecular Physics, 1998, 95, 657-673.	1.7	63
75	Island of Vapor-Liquid Coexistence in Dipolar Hard-Core Systems. Physical Review Letters, 1996, 76, 4183-4186.	7.8	62
76	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + Ethane) and (Xenon + Propane). Journal of Physical Chemistry B, 2000, 104, 1315-1321.	2.6	62
77	Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem. Heat Transfer Engineering, 2011, 32, 197-215.	1.9	62
78	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.	2.5	62
79	Reaction-field and Ewald summation methods in Monte Carlo simulations of dipolar liquid crystals. Molecular Physics, 1997, 92, 723-734.	1.7	61
80	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.	2.5	61
81	Thermodynamic perturbation theory for association with bond cooperativity. Journal of Chemical Physics, 1996, 105, 1113-1120.	3.0	60
82	Predicting the High-Pressure Phase Equilibria of Binary Mixtures of n-Alkanes Using the SAFT-VR Approach. International Journal of Thermophysics, 1998, 19, 1511-1522.	2.1	60
83	On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness. Journal of Chemical Physics, 2013, 139, 144701.	3.0	57
84	Predicting the high-pressure phase equilibria of binary aqueous solutions of 1-butanol, n-butoxyethanol and n-decylpentaoxyethylene ether (C10E5) using the SAFT-HS approach. Molecular Physics, 1998, 93, 57-71.	1.7	57
85	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.	3.4	56
86	The liquid-crystalline phase behaviour of hard spherocylinders with terminal point dipoles. Journal of Physics Condensed Matter, 1996, 8, 9649-9655.	1.8	55
87	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.	2.5	55
88	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.	3.0	54
89	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + n-Butane) and (Xenon +) Tj ETQq1 1 0.784314 rgBT /Overl	2.6	53
90	A generalisation of the Onsager trial-function approach: describing nematic liquid crystals with an algebraic equation of state. Molecular Physics, 2008, 106, 649-678.	1.7	53

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91	Surface thermodynamics of planar, cylindrical, and spherical vapour-liquid interfaces of water. Journal of Chemical Physics, 2015, 142, 114701.	3.0	53
92	Understanding liquid-liquid immiscibility and LCST behaviour in polymer solutions with a Wertheim TPT1 description. Molecular Physics, 2003, 101, 2575-2600.	1.7	52
93	Thermotropic Biaxial Liquid Crystalline Phases in a Mixture of Attractive Uniaxial Rod and Disk Particles. Physical Review Letters, 2008, 101, 237802.	7.8	51
94	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.	1.7	49
95	Generalized van der Waals theory for the twist elastic modulus and helical pitch of cholesterics. Journal of Chemical Physics, 2009, 130, 234911.	3.0	49
96	Adsorption and separation of CO2/CH4 mixtures using nanoporous adsorbents by molecular simulation. Fluid Phase Equilibria, 2014, 362, 227-234.	2.5	49
97	Detailed examination of the calculation of the pressure in simulations of systems with discontinuous interactions from the mechanical and thermodynamic perspectives. Molecular Physics, 2006, 104, 3717-3734.	1.7	48
98	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.	4.8	48
99	Hydrogen-bonding and Phase Biaxiality in Nematic Rod-Plate Mixtures. Molecular Crystals and Liquid Crystals, 1998, 323, 199-209.	0.3	47
100	Vapor Pressure and Density of Thermotropic Liquid Crystals:â€‰ MBBA, 5CB, and Novel Fluorinated Mesogens. Journal of Physical Chemistry B, 2008, 112, 3918-3926.	2.6	47
101	Outer approximation algorithm with physical domain reduction for computerâ€aided molecular and separation process design. AIChE Journal, 2016, 62, 3484-3504.	3.6	47
102	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.	2.5	47
103	Excluded volume for a pair of linear chains of tangent hard spheres with an arbitrary relative orientation. Molecular Physics, 1995, 86, 819-836.	1.7	46
104	Theory of phase equilibria and closedâ€loop liquidâ€“liquid immiscibility for model aqueous solutions of associating chain molecules: Waterâ€‰+alkanol mixtures. Journal of Chemical Physics, 1992, 97, 8672-8691.	3.0	45
105	Theory for the phase behavior of a mixture of a rodlike colloid and a rodlike polymer. Journal of Chemical Physics, 1995, 103, 8684-8693.	3.0	44
106	Simulation study of the phase behavior of a primitive model for thermotropic liquid crystals: Rodlike molecules with terminal dipoles and flexible tails. Journal of Chemical Physics, 2000, 112, 9092-9104.	3.0	44
107	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.	2.1	44
108	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	2.1	44

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109	Predicting the Solvation of Organic Compounds in Aqueous Environments: From Alkanes and Alcohols to Pharmaceuticals. Industrial & Engineering Chemistry Research, 2017, 56, 10856-10876.	3.7	43
110	Theory of phase equilibria for model aqueous solutions of chain molecules: water + alkane mixtures. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1395.	1.7	42
111	New types of phase behaviour in binary mixtures of hard rod-like particles. Molecular Physics, 2003, 101, 817-825.	1.7	41
112	Nematic-nematic phase separation in binary mixtures of thick and thin hard rods: Results from Onsager-like theories. Physical Review E, 2005, 72, 051704.	2.1	41
113	SAFT-Î³ force field for the simulation of molecular fluids: 8. Hetero-segmented coarse-grained models of perfluoroalkylalkanes assessed with new vapourâ€“liquid interfacial tension data. Molecular Physics, 2016, 114, 2597-2614.	1.7	41
114	Theory and computer simulation of hard-sphere site models of ring molecules. Molecular Physics, 1994, 81, 801-811.	1.7	40
115	Development of intermolecular potential models for electrolyte solutions using an electrolyte SAFT-VR Mie equation of state. Molecular Physics, 2016, 114, 2724-2749.	1.7	40
116	Assembly of porous smectic structures formed from interlocking high-symmetry planar nanorings. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9699-9703.	7.1	39
117	A kinetic theory description of the viscosity of dense fluids consisting of chain molecules. Journal of Chemical Physics, 2008, 128, 204901.	3.0	38
118	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.	2.5	37
119	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.	2.6	37
120	Phase equilibria in model mixtures of spherical molecules of different sizes. Journal of the Chemical Society Faraday Transactions I, 1986, 82, 3461.	1.0	36
121	Predicting enhanced absorption of light gases in polyethylene using simplified PC-SAFT and SAFT-VR. Fluid Phase Equilibria, 2006, 243, 74-91.	2.5	36
122	Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation. Fluid Phase Equilibria, 2011, 306, 129-136.	2.5	35
123	Global fluid phase behavior in binary mixtures of rodlike and platelike molecules. Journal of Chemical Physics, 2002, 117, 7207-7221.	3.0	34
124	Thermodynamic perturbation theory for association into doubly bonded dimers. Molecular Physics, 1994, 82, 1033-1048.	1.7	33
125	Advances in generalised van der Waals approaches for the isotropicâ€“nematic fluid phase equilibria of thermotropic liquid crystalsâ€“an algebraic equation of state for attractive anisotropic particles with the Onsager trial function. Molecular Physics, 2009, 107, 2329-2358.	1.7	33
126	Molecules Matter. Computer Aided Chemical Engineering, 2014, , 55-64.	0.5	33

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127	Effective coarse-grained solidâ€“fluid potentials and their application to model adsorption of fluids on heterogeneous surfaces. Physical Chemistry Chemical Physics, 2014, 16, 19165-19180.	2.8	33
128	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.	2.5	32
129	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.	2.5	32
130	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.	1.9	32
131	Group Contribution Coarse-Grained Molecular Simulations of Polystyrene Melts and Polystyrene Solutions in Alkanes Using the SAFT-Î³ Force Field. Macromolecules, 2017, 50, 4840-4853.	4.8	32
132	Phase behavior of symmetric rodâ€“plate mixtures revisited: Biaxiality versus demixing. Journal of Chemical Physics, 2002, 117, 10412-10424.	3.0	31
133	Cholesteric order in systems of helical Yukawa rods. Journal of Physics Condensed Matter, 2011, 23, 194107.	1.8	31
134	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.	3.8	31
135	Bonded hard-sphere theory and computer simulations of polyatomic hard-sphere models of alkanes and their derivatives. Molecular Physics, 1993, 80, 777-788.	1.7	30
136	Simulation of the macroscopic pitch of a chiral nematic phase of a model chiral mesogen. Chemical Physics Letters, 2003, 377, 6-12.	2.6	30
137	Study of the pitch of fluids of electrostatically chiral anisotropic molecules: mean-field theory and simulation. Molecular Physics, 2006, 104, 3681-3691.	1.7	30
138	The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state. Computers and Chemical Engineering, 2012, 36, 99-118.	3.8	29
139	Aggregation Behavior of Model Asphaltenes Revealed from Large-Scale Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2019, 123, 2380-2396.	2.6	29
140	Is xenon an â€œennobledâ€•alkane?. Physical Chemistry Chemical Physics, 2002, 4, 1618-1621.	2.8	28
141	Gibbs ensemble computer simulation and SAFT-VR theory of non-conformal square-well monomerâ€“dimer mixtures. Chemical Physics Letters, 1999, 303, 27-36.	2.6	27
142	Subtleties in the calculation of the pressure and pressure tensor of anisotropic particles from volume-perturbation methods and the apparent asymmetry of the compressive and expansive contributions. Molecular Physics, 2011, 109, 169-189.	1.7	27
143	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.	1.7	27
144	Simulation Study of the Link between Molecular Association and Reentrant Miscibility for a Mixture of Molecules with Directional Interactions. Physical Review Letters, 1999, 82, 5285-5288.	7.8	26

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145	Effect of polymer chain-length polydispersity on the phase behavior of model athermal mixtures of colloids and flexible self-excluding polymers. Chemical Physics Letters, 2004, 398, 489-494.	2.6	26
146	Integrated solvent and process design for the reactive separation of CO2 from flue gas. Computer Aided Chemical Engineering, 2010, , 1231-1236.	0.5	26
147	Viscosity of liquid mixtures: The Vesovic-Wakeham method for chain molecules. Journal of Chemical Physics, 2012, 136, 074514.	3.0	26
148	The condition of microscopic reversibility in Gibbs ensemble Monte Carlo simulations of phase equilibria. Molecular Physics, 1995, 85, 435-447.	1.7	25
149	The liquid crystalline phase behavior of dimerizing hard spherocylinders. Journal of Chemical Physics, 1997, 106, 7315-7330.	3.0	25
150	Liquid Crystal Phase Transitions in Systems of Colloidal Platelets with Bimodal Shape Distribution. Journal of Physical Chemistry B, 2009, 113, 13476-13484.	2.6	25
151	Computer simulation of the interface between two liquid crystalline phases in rodâ€“plate binary mixtures. Chemical Physics Letters, 2000, 325, 631-638.	2.6	24
152	On the liquid mixtures of xenon, alkanes and perfluorinated compounds. Physical Chemistry Chemical Physics, 2001, 3, 2852-2855.	2.8	24
153	Aspects of Asphaltene Aggregation Obtained from Coarse-Grained Molecular Modeling. Energy & Fuels, 2015, 29, 556-566.	5.1	24
154	Monte Carlo annealing technique for the minimization of the Onsager free energy functional. Molecular Physics, 1994, 83, 603-611.	1.7	23
155	Theory for hydrogen-bonding nematic liquid crystals. Molecular Physics, 1994, 82, 473-485.	1.7	22
156	A study of orientational ordering in a fluid of dipolar Gayâ€“Berne molecules using density-functional theory. Journal of Chemical Physics, 2002, 116, 9107-9119.	3.0	22
157	Structure and Interfacial Tension of a Hard-Rod Fluid in Planar Confinement. Langmuir, 2017, 33, 11754-11770.	3.5	22
158	Stability of the nematic phase of a mixture of aligned cylinders with respect to the smectic and columnar phases. Journal of Chemical Physics, 1995, 102, 2622-2627.	3.0	21
159	Orientational ordering and phase behaviour of binary mixtures of hard spheres and hard spherocylinders. Journal of Chemical Physics, 2015, 143, 044906.	3.0	21
160	Computer simulation of dipolar liquid crystals. Journal of Molecular Liquids, 1998, 76, 171-181.	4.9	20
161	Phase equilibria of a square-well monomer-dimer mixture: Gibbs ensemble computer simulation and statistical associating fluid theory for potentials of variable range. Physical Review E, 1998, 57, 2035-2044.	2.1	20
162	Toward Sustainable Solvent-Based Postcombustion CO2 Capture. Computer Aided Chemical Engineering, 2015, , 279-310.	0.5	20

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