George Jackson

List of Publications by Year
in descending order

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265 papers	22,040 citations	13854 67 h-index	9334 143 g-index
281 all docs	281 docs citations	281 times ranked	9360 citing authors

#	Article	IF	Citations
1	Molecular theory of the static dielectric constant of dipolar fluids. Journal of Chemical Physics, 2022, 156, 154111.	1.2	6
2	Ab initio development of generalized Lennard-Jones (Mie) force fields for predictions of thermodynamic properties in advanced molecular-based SAFT equations of state. Journal of Chemical Physics, 2022, 156, 154106.	1.2	6
3	Phase behaviour and pH-solubility profile prediction of aqueous buffered solutions of ibuprofen and ketoprofen. Fluid Phase Equilibria, 2022, 560, 113504.	1.4	6
4	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
5	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
6	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
7	Keith E. Gubbins: A retrospective. AICHE Journal, 2021, 67, e17191.	1.8	0
8	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
9	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
10	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
11	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
12	Gerhard Findenegg (1938â€“2019). Molecular Physics, 2021, 119, .	0.8	0
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	Announcement of the winner of the Longuet-Higgins Early Career Researcher Prize 2020. Molecular Physics, 2021, 119, .	0.8	0
16	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
17	Computer-aided Solvent Mixture Design for the Crystallisation and Isolation of Mefenamic Acid. Computer Aided Chemical Engineering, 2020, 48, 649-654.	0.3	3
18	Thermodynamics 2019 Conferenceâ€“Punta UmbrÃa, Costa de la Luz, Huelva, Spain, 26â€“28 June 2019. Molecular Physics, 2020, 118, e1771043.	0.8	1

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19	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
20	Modeling the Fluid-Phase Equilibria of Semifluorinated Alkanes and Mixtures of (n-Alkanes +) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 & Engineering Data, 2020, 65, 5909-5919.	1.0	4
21	Announcement of the winner of the Longuet-Higgins Early Career Researcher Prize 2019. Molecular Physics, 2020, 118, .	0.8	0
22	A tensorial fundamental measure density functional theory for the description of adsorption in substrates of arbitrary three-dimensional geometry. Journal of Chemical Physics, 2020, 152, .	1.2	4
23	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
24	A comparative study of multi-objective optimization methodologies for molecular and process design. Computers and Chemical Engineering, 2020, 136, 106802.	2.0	17
25	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
26	Announcement of the winner of the Longuet-Higgins Early Career Researcher Prize 2018. Molecular Physics, 2020, 118, e1717103.	0.8	0
27	Modelling the thermodynamic properties and fluid-phase equilibria of n-perfluoroalkanes and their binary mixtures with the SAFT-Î³ Mie group contribution equation of state. Molecular Physics, 2020, 118, e1722270.	0.8	2
28	A comparison of the performance of multi-objective optimization methodologies for solvent design. Computer Aided Chemical Engineering, 2019, 46, 37-42.	0.3	5
29	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
30	Modelling adsorption using an augmented two-dimensional statistical associating fluid theory: 2D-SAFT-VR Mie. Molecular Physics, 2019, 117, 3770-3782.	0.8	7
31	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
32	The formation of biaxial nematic phases in binary mixtures of thermotropic liquid-crystals composed of uniaxial molecules. Molecular Physics, 2019, 117, 2830-2845.	0.8	6
33	Aggregation Behavior of Model Asphaltenes Revealed from Large-Scale Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2019, 123, 2380-2396.	1.2	29
34	Intramolecular bonding in a statistical associating fluid theory of ring aggregates. Molecular Physics, 2019, 117, 3884-3912.	0.8	7
35	A tribute to Alan Soper â€“ foreword by the editors. Molecular Physics, 2019, 117, 3195-3196.	0.8	0
36	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

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37	Optimal design of post combustion CO2 capture processes based on phase-change solvents. Computer Aided Chemical Engineering, 2019, , 463-468.	0.3	4
38	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
39	Daan Frenkel â€" An entropic career. Molecular Physics, 2018, 116, 2737-2741.	0.8	0
40	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
41	Demixing, surface nematization, and competing adsorption in binary mixtures of hard rods and hard spheres under confinement. Journal of Chemical Physics, 2018, 148, 164701.	1.2	13
42	Thermodynamics 2017 Conference â€" Edinburgh, Scotland, 5â€"8 September 2017. Molecular Physics, 2018, 116, 1909-1914.	0.8	2
43	Announcement of the winner of the Longuet-Higgins early career researcher prize 2017. Molecular Physics, 2018, 116, 2143-2144.	0.8	0
44	Nanorings in planar confinement: the role of repulsive surfaces on the formation of lacuna smectics. Molecular Physics, 2018, 116, 2901-2910.	0.8	11
45	Simulation of Asphaltene Aggregation through Molecular Dynamics: Insights and Limitations. Energy & Fuels, 2017, 31, 1108-1125.	2.5	170
46	Structure and Interfacial Tension of a Hard-Rod Fluid in Planar Confinement. Langmuir, 2017, 33, 11754-11770.	1.6	22
47	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
48	Predicting the Fluid-Phase Behavior of Aqueous Solutions of ELP (VPGVG) Sequences Using SAFT-VR. Langmuir, 2017, 33, 11733-11745.	1.6	5
49	Perturbation Theory versus Thermodynamic Integration. Beyond a Mean-Field Treatment of Pair Correlations in a Nematic Model Liquid Crystal. Langmuir, 2017, 33, 11345-11365.	1.6	14
50	Announcement of the winner of the Longuetâ€"Higgins Early Career Researcher Prize 2016. Molecular Physics, 2017, 115, 2903-2904.	0.8	0
51	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.	2.2	32
52	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
53	Nonequilibrium study of the intrinsic free-energy profile across a liquid-vapour interface. Journal of Chemical Physics, 2016, 144, 044703.	1.2	19
54	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

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55	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
56	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.	3.3	39
57	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.	0.8	41
58	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
59	Outer approximation algorithm with physical domain reduction for computerâ€aided molecular and separation process design. AICHE Journal, 2016, 62, 3484-3504.	1.8	47
60	Editors of Molecular Physics 1958â€“2016. Molecular Physics, 2016, 114, 3420-3425.	0.8	2
61	Predicting the adsorption of n-perfluorohexane in BAM-P109 standard activated carbon by molecular simulation using SAFT-Î³ Mie coarse-grained force fields. Adsorption Science and Technology, 2016, 34, 64-78.	1.5	12
62	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
63	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
64	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
65	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.	1.0	71
66	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
67	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
68	Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics. Journal of Chemical Physics, 2015, 143, 244709.	1.2	14
69	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
70	Surface thermodynamics of planar, cylindrical, and spherical vapour-liquid interfaces of water. Journal of Chemical Physics, 2015, 142, 114701.	1.2	53
71	Modeling of Fouling from Molecular to Plant Scale. , 2015, , 179-320.		1
72	Aspects of Asphaltene Aggregation Obtained from Coarse-Grained Molecular Modeling. Energy & Fuels, 2015, 29, 556-566.	2.5	24

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73	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
74	Toward Sustainable Solvent-Based Postcombustion CO2 Capture. Computer Aided Chemical Engineering, 2015, , 279-310.	0.3	20
75	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
76	Jean-Pierre Hansen â€“ a stimulating history of simulating fluids. Molecular Physics, 2015, 113, 2363-2375.	0.8	1
77	Orientational ordering and phase behaviour of binary mixtures of hard spheres and hard spherocylinders. Journal of Chemical Physics, 2015, 143, 044906.	1.2	21
78	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.	0.8	72
79	Molecules Matter. Computer Aided Chemical Engineering, 2014, , 55-64.	0.3	33
80	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
81	Adsorption and separation of CO2/CH4 mixtures using nanoporous adsorbents by molecular simulation. Fluid Phase Equilibria, 2014, 362, 227-234.	1.4	49
82	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.	3.3	141
83	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.	1.3	33
84	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
85	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
86	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
87	Understanding and Describing the Liquid-Crystalline States of Polypeptide Solutions: A Coarse-Grained Model of PBLG in DMF. Macromolecules, 2014, 47, 1482-1493.	2.2	15
88	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	1.2	382
89	New methods for calculating the free energy of charged defects in solid electrolytes. Journal of Physics Condensed Matter, 2013, 25, 395001.	0.7	2
90	Modelling and understanding of the vapourâ€“liquid and liquidâ€“liquid interfacial properties for the binary mixture of n-heptane and perfluoro-n-hexane. Journal of Molecular Liquids, 2013, 185, 36-43.	2.3	9

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91	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
92	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
93	On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness. Journal of Chemical Physics, 2013, 139, 144701.	1.2	57
94	Liquid Crystal Phase Behaviour of Attractive Disc-Like Particles. International Journal of Molecular Sciences, 2013, 14, 16414-16442.	1.8	8
95	Editorial â€“ Topical Review. Molecular Physics, 2013, 111, 825-826.	0.8	0
96	The Use of SAFT in Obtaining Force Fields for Molecular Simulation of Thermodynamic, Interfacial and Transport Properties: The SAFT-Î³ Approach. Chemie-Ingenieur-Technik, 2013, 85, 1360-1360.	0.4	0
97	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
98	A generalisation of the Onsager trial function approach: Describing nematic liquid crystals with an algebraic equation of state. Molecular Physics, 2012, 110, 3107-3107.	0.8	3
99	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
100	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
101	A perspective on the interfacial properties of nanoscopic liquid drops. Journal of Physics Condensed Matter, 2012, 24, 464121.	0.7	81
102	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
103	Viscosity of liquid mixtures: The Vesovic-Wakeham method for chain molecules. Journal of Chemical Physics, 2012, 136, 074514.	1.2	26
104	A generic equation of state for liquid crystalline phases of hard-oblate particles. Molecular Physics, 2012, 110, 1269-1288.	0.8	16
105	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
106	Thermodynamics 2011 Conference Athens, Greece, 31 Augustâ€“3 September 2011 http://www.thermodynamics2011.org/. Molecular Physics, 2012, 110, 1053-1056.	0.8	5
107	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
108	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	0.8	44

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109	The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state. Computers and Chemical Engineering, 2012, 36, 99-118.	2.0	29
110	Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem. Heat Transfer Engineering, 2011, 32, 197-215.	1.2	62
111	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
112	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
113	A study of steric chirality: the chiral nematic phase of a system of chiral two-site HGO molecules. Molecular Physics, 2011, 109, 1313-1330.	0.8	10
114	8th Liblice Conference on the Statistical Mechanics of Liquids â€“ Brno, Czech Republic, 13â€“18 June 2010. Molecular Physics, 2011, 109, 1-2.	0.8	1
115	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
116	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
117	Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation. Fluid Phase Equilibria, 2011, 306, 129-136.	1.4	35
118	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.	0.8	27
119	Cholesteric order in systems of helical Yukawa rods. Journal of Physics Condensed Matter, 2011, 23, 194107.	0.7	31
120	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
121	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
122	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
123	Integrated solvent and process design for the reactive separation of CO2 from flue gas. Computer Aided Chemical Engineering, 2010, , 1231-1236.	0.3	26
124	Monte Carlo Simulations of the Liquidâ^'Vapor Interface of Lennardâ^'Jones Diatomics for the Direct Determination of the Interfacial Tension Using the Test-Area Method. Journal of Chemical & Engineering Data, 2010, 55, 4306-4314.	1.0	11
125	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
126	An overview of CO2 capture technologies. Energy and Environmental Science, 2010, 3, 1645.	15.6	1,376

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127	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
128	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.	1.2	80
129	Robust algorithms for the calculation of phase equilibrium. Computer Aided Chemical Engineering, 2010, 28, 79-84.	0.3	1
130	Generalized van der Waals theory for the twist elastic modulus and helical pitch of cholesterics. Journal of Chemical Physics, 2009, 130, 234911.	1.2	49
131	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 79-94.	1.4	11
132	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 95-104.	1.4	11
133	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
134	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.	0.8	33
135	Liquid Crystal Phase Transitions in Systems of Colloidal Platelets with Bimodal Shape Distribution. Journal of Physical Chemistry B, 2009, 113, 13476-13484.	1.2	25
136	Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures. Fluid Phase Equilibria, 2008, 266, 105-128.	1.4	131
137	A generalisation of the SAFT- group contribution method for groups comprising multiple spherical segments. Fluid Phase Equilibria, 2008, 274, 85-104.	1.4	128
138	Vapor Pressure and Density of Thermotropic Liquid Crystals:â€‰ MBBA, 5CB, and Novel Fluorinated Mesogens. Journal of Physical Chemistry B, 2008, 112, 3918-3926.	1.2	47
139	Many-fluid Onsager density functional theories for orientational ordering in mixtures of anisotropic hard-body fluids. Journal of Chemical Physics, 2008, 129, 144504.	1.2	18
140	A kinetic theory description of the viscosity of dense fluids consisting of chain molecules. Journal of Chemical Physics, 2008, 128, 204901.	1.2	38
141	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
142	A heteronuclear group contribution method for associating chain molecules (SAFT-Î³). Computer Aided Chemical Engineering, 2008, 25, 871-876.	0.3	0
143	A generalisation of the Onsager trial-function approach: describing nematic liquid crystals with an algebraic equation of state. Molecular Physics, 2008, 106, 649-678.	0.8	53
144	Vapor-liquid interfacial properties of fully flexible Lennard-Jones chains. Journal of Chemical Physics, 2008, 129, 144703.	1.2	87

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145	Thermotropic Biaxial Liquid Crystalline Phases in a Mixture of Attractive Uniaxial Rod and Disk Particles. Physical Review Letters, 2008, 101, 237802.	2.9	51
146	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
147	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.	1.5	84
148	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
149	Surface tension of the Widom-Rowlinson model. Journal of Chemical Physics, 2007, 127, 034707.	1.2	19
150	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.	0.8	48
151	Study of the pitch of fluids of electrostatically chiral anisotropic molecules: mean-field theory and simulation. Molecular Physics, 2006, 104, 3681-3691.	0.8	30
152	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
153	7th Liblice Conference on the Statistical Mechanics of Liquids Lednice, Czech Republic June 11â€“16 2006 http://www.icpf.cas.cz/theory/Liblice. Molecular Physics, 2006, 104, 3387-3388.	0.8	2
154	Integrating advanced thermodynamics and process and solvent design for gas separation. Computer Aided Chemical Engineering, 2006, 21, 743-748.	0.3	0
155	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
156	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
157	The nature of the calculation of the pressure in molecular simulations of continuous models from volume perturbations. Journal of Chemical Physics, 2006, 125, 164109.	1.2	94
158	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.	1.2	297
159	Nematic Phase Transitions in Mixtures of Thin and Thick Colloidal Rods. Physical Review Letters, 2005, 94, 057801.	2.9	75
160	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
161	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.	1.2	116
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