Clare McCabe

List of Publications by Year
in descending order

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153 papers	5,628 citations	66234 42 h-index	106150 65 g-index
158 all docs	158 docs citations	158 times ranked	3962 citing authors

#	Article	IF	Citations
1	Improvement of Quality in Publication of Experimental Thermophysical Property Data: Challenges, Assessment Tools, Global Implementation, and Online Support. Journal of Chemical & Engineering Data, 2013, 58, 2699-2716.	1.0	236
2	Oscillatory Behavior of Double-Walled Nanotubes under Extension:â€‰ A Simple Nanoscale Damped Spring. Nano Letters, 2003, 3, 1001-1005.	4.5	171
3	Molecular simulations of liquid-liquid interfacial properties: Waterâ€“n-alkane and water-methanolâ€“n-alkane systems. Physical Review E, 2003, 67, 011603.	0.8	149
4	Derivation of coarse-grained potentials via multistate iterative Boltzmann inversion. Journal of Chemical Physics, 2014, 140, 224104.	1.2	146
5	SAFT-VR modelling of the phase equilibrium of long-chain n-alkanes. Physical Chemistry Chemical Physics, 1999, 1, 2057-2064.	1.3	142
6	Coarse-grained molecular models of water: a review. Molecular Simulation, 2012, 38, 671-681.	0.9	128
7	Comparison of Nonequilibrium Molecular Dynamics with Experimental Measurements in the Nonlinear Shear-Thinning Regime. Physical Review Letters, 2002, 88, 058302.	2.9	124
8	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.	1.2	115
9	Multiple Functions of Aromatic-Carbohydrate Interactions in a Processive Cellulase Examined with Molecular Simulation. Journal of Biological Chemistry, 2011, 286, 41028-41035.	1.6	108
10	The oscillatory damped behaviour of incommensurate double-walled carbon nanotubes. Nanotechnology, 2005, 16, 186-198.	1.3	106
11	Developing a predictive group-contribution-based SAFT-VR equation of state. Fluid Phase Equilibria, 2009, 277, 131-144.	1.4	106
12	Application of Crossover Theory to the SAFT-VR Equation of State:â€‰ SAFT-VRX for Pure Fluids. Industrial & Engineering Chemistry Research, 2004, 43, 2839-2851.	1.8	96
13	The O-Glycosylated Linker from the Trichoderma reesei Family 7 Cellulase Is a Flexible, Disordered Protein. Biophysical Journal, 2010, 99, 3773-3781.	0.2	96
14	A crossover SAFT-VR equation of state for pure fluids: preliminary results for light hydrocarbons. Fluid Phase Equilibria, 2004, 219, 3-9.	1.4	83
15	Predicting the High-Pressure Phase Equilibria of Methane +n-Hexane Using the SAFT-VR Approach. Journal of Physical Chemistry B, 1998, 102, 4183-4188.	1.2	78
16	Simulation Study of the Structure and Phase Behavior of Ceramide Bilayers and the Role of Lipid Headgroup Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 5116-5126.	2.3	72
17	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
18	The thermodynamics of heteronuclear molecules formed from bonded square-well (BSW) segments using the SAFT-VR approach. Molecular Physics, 1999, 97, 551-558.	0.8	66

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19	On the Investigation of Coarse-Grained Models for Water: Balancing Computational Efficiency and the Retention of Structural Properties. Journal of Physical Chemistry B, 2010, 114, 4590-4599.	1.2	66
20	Examining the rheology of 9-octylheptadecane to giga-pascal pressures. Journal of Chemical Physics, 2001, 114, 1887-1891.	1.2	64
21	Evaluation of Force Fields for Molecular Simulation of Polyhedral Oligomeric Silsesquioxanes. Journal of Physical Chemistry B, 2006, 110, 2502-2510.	1.2	64
22	Computational Investigation of Glycosylation Effects on a Family 1 Carbohydrate-binding Module. Journal of Biological Chemistry, 2012, 287, 3147-3155.	1.6	64
23	Molecular dynamics study of the nano-rheology ofn-dodecane confined between planar surfaces. Journal of Chemical Physics, 2003, 118, 8941-8944.	1.2	63
24	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + Ethane) and (Xenon + Propane). Journal of Physical Chemistry B, 2000, 104, 1315-1321.	1.2	62
25	Predicting Mixture Phase Equilibria and Critical Behavior Using the SAFT-VRX Approach. Journal of Physical Chemistry B, 2005, 109, 9047-9058.	1.2	61
26	SAFT Associating Fluids and Fluid Mixtures. , 2010, , 215-279.		61
27	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.	1.0	60
28	Thermodynamic and Transport Properties of Polyhedral Oligomeric Sislesquioxanes in Poly(dimethylsiloxane). Journal of Physical Chemistry B, 2005, 109, 14300-14307.	1.2	57
29	Tribological Durability of Silane Monolayers on Silicon. Langmuir, 2011, 27, 5909-5917.	1.6	57
30	Binding Site Dynamics and Aromaticâ€“Carbohydrate Interactions in Processive and Non-Processive Family 7 Glycoside Hydrolases. Journal of Physical Chemistry B, 2013, 117, 4924-4933.	1.2	57
31	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + n-Butane) and (Xenon +) Tj ETQq1 1 0.784314 rgBT /Overl	1.2	53
32	Layering Behavior and Axial Phase Equilibria of Pure Water and Water + Carbon Dioxide Inside Single Wall Carbon Nanotubes. Nano Letters, 2002, 2, 1427-1431.	4.5	53
33	Modelling the phase behaviour and excess properties of alkane + perfluoroalkane binary mixtures with the SAFTâ€“VR approach. Fluid Phase Equilibria, 2005, 228-229, 389-393.	1.4	53
34	Liquid Phase Behavior of Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2007, 111, 2856-2863.	1.2	52
35	Calculation of Viscous EHL Traction for Squalane Using Molecular Simulation and Rheometry. Tribology Letters, 2002, 13, 251-254.	1.2	51
36	Anomalies in the Solubility of Alkanes in Near-Critical Water. Journal of Physical Chemistry B, 2003, 107, 12307-12314.	1.2	49

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37	Predicting adsorption isotherms using a two-dimensional statistical associating fluid theory. Journal of Chemical Physics, 2007, 126, 074707.	1.2	48
38	Measurement and prediction of high-pressure vaporâ€“liquid equilibria for binary mixtures of carbon dioxide+n-octane, methanol, ethanol, and perfluorohexane. Journal of Supercritical Fluids, 2010, 55, 682-689.	1.6	47
39	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose Iî². Cellulose, 2008, 15, 261-273.	2.4	46
40	Predicting the Phase Behavior of Polymer Systems with the GC-SAFT-VR Approach. Industrial & Engineering Chemistry Research, 2010, 49, 1378-1394.	1.8	46
41	Predicting the Phase Behavior of Nitrogen +n-Alkanes for Enhanced Oil Recovery from the SAFT-VR Approach:Â Examining the Effect of the Quadrupole Moment. Journal of Physical Chemistry B, 2006, 110, 24083-24092.	1.2	43
42	Extending the GC-SAFT-VR approach to associating functional groups: Alcohols, aldehydes, amines and carboxylic acids. Fluid Phase Equilibria, 2011, 306, 97-111.	1.4	43
43	A study of mechanical shear bands in liquids at high pressure. Tribology International, 2004, 37, 783-789.	3.0	42
44	Viscosity of Liquid Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 9130-9139.	1.2	42
45	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. Molecular Physics, 2002, 100, 2547-2553.	0.8	40
46	Tribology of Monolayer Films: Comparison between n-Alkanethiols on Gold and n-Alkyl Trichlorosilanes on Silicon. Langmuir, 2009, 25, 9995-10001.	1.6	40
47	Molecular Dynamics Study of Alkylsilane Monolayers on Realistic Amorphous Silica Surfaces. Langmuir, 2015, 31, 3086-3093.	1.6	39
48	Effective Interactions between Polyhedral Oligomeric Sislesquioxanes Dissolved in Normal Hexadecane from Molecular Simulation. Macromolecules, 2005, 38, 8950-8959.	2.2	38
49	On the thermodynamics of diblock chain fluids from simulation and heteronuclear statistical associating fluid theory for potentials of variable range. Molecular Physics, 2006, 104, 571-586.	0.8	38
50	Coarse-grained force field for simulating polymer-tethered silsesquioxane self-assembly in solution. Journal of Chemical Physics, 2007, 127, 114102.	1.2	38
51	Characterizing the viscosityâ€“temperature dependence of lubricants by molecular simulation. Fluid Phase Equilibria, 2001, 183-184, 363-370.	1.4	37
52	Organic-inorganic telechelic molecules: Solution properties from simulations. Journal of Chemical Physics, 2006, 125, 104904.	1.2	37
53	Development of an equation of state for electrolyte solutions by combining the statistical associating fluid theory and the mean spherical approximation for the nonprimitive model. Journal of Chemical Physics, 2007, 126, 244503.	1.2	37
54	Predicting the phase equilibria of petroleum fluids with the SAFT-VR approach. AICHE Journal, 2007, 53, 720-731.	1.8	37

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55	Frictional Dynamics of Alkylsilane Monolayers on SiO₂: Effect of 1-n-Butyl-3-methylimidazolium Nitrate as a Lubricant. Langmuir, 2009, 25, 5103-5110.	1.6	37
56	Predicting the Newtonian viscosity of complex fluids from high strain rate molecular simulations. Journal of Chemical Physics, 2002, 116, 3339-3342.	1.2	36
57	A Hierarchical, Component Based Approach to Screening Properties of Soft Matter. Molecular Modeling and Simulation, 2016, , 79-92.	0.2	36
58	Effect of Ceramide Tail Length on the Structure of Model Stratum Corneum Lipid Bilayers. Biophysical Journal, 2018, 114, 113-125.	0.2	36
59	Phase behavior of dipolar fluids from a modified statistical associating fluid theory for potentials of variable range. Journal of Chemical Physics, 2006, 125, 104504.	1.2	35
60	Solution Behavior of Perfluoroalkanes and Perfluoroalkylalkane Surfactants in n-Octane. Journal of Physical Chemistry C, 2007, 111, 15962-15968.	1.5	34
61	Deposition and Wettability of [bmim][triflate] on Self-Assembled Monolayers. Journal of Physical Chemistry C, 2009, 113, 2384-2392.	1.5	34
62	Systems Involving Hydrogenated and Fluorinated Chains: Volumetric Properties of Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 15013-15023.	1.2	34
63	Application of SAFTâ€“VRX to binary phase behaviour: alkanes. Fluid Phase Equilibria, 2005, 228-229, 275-282.	1.4	33
64	Ab Initio Analysis of the Structural Properties of Alkyl-Substituted Polyhedral Oligomeric Silsesquioxanes. Journal of Physical Chemistry A, 2007, 111, 3577-3584.	1.1	32
65	A coarse-grained model for amorphous and crystalline fatty acids. Journal of Chemical Physics, 2010, 132, 134505.	1.2	31
66	Prediction of viscosity for molecular fluids at experimentally accessible shear rates using the transient time correlation function formalism. Journal of Chemical Physics, 2006, 125, 194527.	1.2	30
67	A molecular dynamics study of the Gibbs free energy of solvation of fullerene particles in octanol and water. Carbon, 2009, 47, 2865-2874.	5.4	30
68	Vapor Pressure of Perfluoroalkylalkanes: The Role of the Dipole. Journal of Physical Chemistry B, 2015, 119, 1623-1632.	1.2	30
69	Frictional Properties of Mixed Fluorocarbon/Hydrocarbon Silane Monolayers: A Simulation Study. Langmuir, 2012, 28, 14218-14226.	1.6	29
70	Formalizing atom-typing and the dissemination of force fields with foyer. Computational Materials Science, 2019, 167, 215-227.	1.4	29
71	Is xenon an â€œennobledâ€•alkane?. Physical Chemistry Chemical Physics, 2002, 4, 1618-1621.	1.3	28
72	Perfluoroalkanes and perfluoroalkylalkane surfactants in solution: Partial molar volumes in n-octane and hetero-SAFT-VR modelling. Fluid Phase Equilibria, 2011, 306, 76-81.	1.4	28

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73	Gibbs ensemble computer simulation and SAFT-VR theory of non-conformal square-well monomerâ€“dimer mixtures. Chemical Physics Letters, 1999, 303, 27-36.	1.2	27
74	Molecular simulation evidence for processive motion of Trichoderma reesei Cel7A during cellulose depolymerization. Chemical Physics Letters, 2008, 460, 284-288.	1.2	27
75	A Structurally Relevant Coarse-Grained Model for Cholesterol. Biophysical Journal, 2010, 99, 2896-2905.	0.2	27
76	Predicting the thermodynamic properties and dielectric behavior of electrolyte solutions using the SAFTâ€VR+DE equation of state. AICHE Journal, 2015, 61, 3053-3072.	1.8	27
77	Operator splitting algorithm for isokinetic SLLOD molecular dynamics. Journal of Chemical Physics, 2005, 122, 094114.	1.2	26
78	Phase behavior of dipolar associating fluids from the SAFT-VR+D equation of state. Journal of Chemical Physics, 2007, 127, 084514.	1.2	26
79	A simulation study of the self-assembly of coarse-grained skin lipids. Soft Matter, 2012, 8, 4802.	1.2	26
80	Coexistence Densities of Methane and Propane by Canonical Molecular Dynamics and Gibbs Ensemble Monte Carlo Simulations. Molecular Simulation, 2003, 29, 463-470.	0.9	25
81	On the development of a general force field for the molecular simulation of perfluoroethers. Molecular Physics, 2003, 101, 2157-2169.	0.8	25
82	Frictional performance of silica microspheres. Tribology International, 2011, 44, 180-186.	3.0	25
83	On the liquid mixtures of xenon, alkanes and perfluorinated compounds. Physical Chemistry Chemical Physics, 2001, 3, 2852-2855.	1.3	24
84	Surface and Frictional Properties of Two-Component Alkylsilane Monolayers and Hydroxyl-Terminated Monolayers on Silicon. Journal of Physical Chemistry C, 2009, 113, 14972-14977.	1.5	24
85	Multiscale Simulation of the Synthesis, Assembly and Properties of Nanostructured Organic/Inorganic Hybrid Materials. Journal of Computational and Theoretical Nanoscience, 2004, 1, 265-279.	0.4	24
86	Examining the frictional forces between mixed hydrophobic â€“ hydrophilic alkylsilane monolayers. Journal of Chemical Physics, 2012, 136, 244701.	1.2	23
87	Investigating Alkylsilane Monolayer Tribology at a Single-Asperity Contact with Molecular Dynamics Simulation. Langmuir, 2017, 33, 11270-11280.	1.6	23
88	Phase equilibrium in aqueous two-phase systems containing ethylene oxideâ€“propylene oxide block copolymers and dextran. Fluid Phase Equilibria, 2004, 218, 221-228.	1.4	22
89	Viscosity of liquid systems involving hydrogenated and fluorinated substances: Liquid mixtures of (hexane+perfluorohexane). Fluid Phase Equilibria, 2013, 358, 161-165.	1.4	22
90	Tunable transition from hydration to monomer-supported lubrication in zwitterionic monolayers revealed by molecular dynamics simulation. Soft Matter, 2015, 11, 3340-3346.	1.2	22

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91	Investigating the Structure of Multicomponent Gel-Phase Lipid Bilayers. Biophysical Journal, 2016, 111, 813-823.	0.2	22
92	MoSDeF, a Python Framework Enabling Large-Scale Computational Screening of Soft Matter: Application to Chemistry-Property Relationships in Lubricating Monolayer Films. Journal of Chemical Theory and Computation, 2020, 16, 1779-1793.	2.3	22
93	Towards molecular simulations that are transparent, reproducible, usable by others, and extensible (TRUE). Molecular Physics, 2020, 118, e1742938.	0.8	22
94	Thermodynamics of Liquid (Xenon + Methane) Mixtures. Journal of Physical Chemistry B, 2004, 108, 7377-7381.	1.2	21
95	Modeling the phase behavior, excess enthalpies and Henry's constants of the H2O+H2S binary mixture using the SAFT-VR+D approach. Fluid Phase Equilibria, 2010, 290, 137-147.	1.4	21
96	Modeling the Phase Behavior of H₂S + n-Alkane Binary Mixtures Using the SAFT-VR+D Approach. Journal of Physical Chemistry B, 2008, 112, 9417-9427.	1.2	20
97	Predicting the phase behavior of fatty acid methyl esters and their mixtures using the GC-SAFT-VR approach. Fluid Phase Equilibria, 2016, 411, 43-52.	1.4	20
98	Transport Properties of Perfluoroalkanes Using Molecular Dynamics Simulation:Â Comparison of United- and Explicit-Atom Models. Industrial & Engineering Chemistry Research, 2003, 42, 6956-6961.	1.8	19
99	Molecular dynamics simulations of stratum corneum lipid mixtures: A multiscale perspective. Biochemical and Biophysical Research Communications, 2018, 498, 313-318.	1.0	19
100	Liquidâ€“vapour equilibrium of {xBF3 + (1 â^' x)n-butane} at 195.49 K. Fluid Phase Equilibria, 2003, 205, 163-170.	1.4	18
101	Examining the phase transition behavior of amphiphilic lipids in solution using statistical temperature molecular dynamics and replica-exchange Wang-Landau methods. Journal of Chemical Physics, 2013, 139, 054505.	1.2	18
102	A Coarse-Grained Model of Stratum Corneum Lipids: Free Fatty Acids and Ceramide NS. Journal of Physical Chemistry B, 2016, 120, 9944-9958.	1.2	18
103	Development of a force field for molecular simulation of the phase equilibria of perfluoromethylpropyl ether. Molecular Physics, 2002, 100, 265-272.	0.8	17
104	Equation of state and liquid-vapor equilibria of one- and two-Yukawa hard-sphere chain fluids: Theory and simulation. Journal of Chemical Physics, 2004, 121, 8128.	1.2	17
105	Molecular simulation and theoretical modeling of polyhedral oligomeric silsesquioxanes. Molecular Physics, 2007, 105, 261-272.	0.8	17
106	Vapor pressure and liquid density of fluorinated alcohols: Experimental, simulation and GC-SAFT-VR predictions. Fluid Phase Equilibria, 2016, 425, 297-304.	1.4	17
107	Perfluoropolyethers: Development of an All-Atom Force Field for Molecular Simulations and Validation with New Experimental Vapor Pressures and Liquid Densities. Journal of Physical Chemistry B, 2017, 121, 6588-6600.	1.2	16
108	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16

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109	Discriminating between Correlations of Experimental Viscosity Data for Perfluorobutane Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2001, 40, 473-475.	1.8	15
110	Non-equilibrium molecular dynamics simulation study of the behavior of hydrocarbon-isomers in silicalite. Fluid Phase Equilibria, 2002, 194-197, 309-317.	1.4	15
111	Aggregation of POSS Monomers in Liquid Hexane:â€‰ A Molecular-Simulation Study. Journal of Physical Chemistry B, 2007, 111, 12248-12256.	1.2	15
112	Adsorption of Chain Molecules in Slit-Shaped Pores: Development of a SAFT-FMT-DFT Approach. Journal of Physical Chemistry C, 2013, 117, 21337-21350.	1.5	15
113	Composition Dependence of Water Permeation Across Multicomponent Gel-Phase Bilayers. Journal of Physical Chemistry B, 2018, 122, 3113-3123.	1.2	15
114	Prediction of n-Alkane Adsorption on Activated Carbon Using the SAFTâ€“FMTâ€“DFT Approach. Journal of Physical Chemistry C, 2015, 119, 1457-1463.	1.5	14
115	A SAFT-VR+DE equation of state based approach for the study of mixed dipolar solvent electrolytes. Fluid Phase Equilibria, 2016, 416, 72-82.	1.4	14
116	Predicting the thermodynamic properties of experimental mixed-solvent electrolyte systems using the SAFT-VR+DE equation of state. Fluid Phase Equilibria, 2018, 460, 105-118.	1.4	14
117	Structural and thermodynamic properties of a multicomponent freely jointed hard sphere multi-Yukawa chain fluid. Molecular Physics, 2002, 100, 2499-2517.	0.8	13
118	Molecular Dynamics Study of the Behavior of Selected Nanoscale Building Blocks in a Gel-Phase Lipid Bilayer. Journal of Physical Chemistry B, 2010, 114, 9165-9172.	1.2	13
119	Accurately modeling benzene and alkylbenzenes using a group contribution based SAFT approach. Fluid Phase Equilibria, 2014, 362, 242-251.	1.4	13
120	Influence of Surface Morphology on the Shear-Induced Wear of Alkylsilane Monolayers: Molecular Dynamics Study. Langmuir, 2016, 32, 2348-2359.	1.6	13
121	Influence of Single-Stranded DNA Coatings on the Interaction between Graphene Nanoflakes and Lipid Bilayers. Journal of Physical Chemistry B, 2019, 123, 7711-7721.	1.2	13
122	Predicting the phase behavior of fluorinated organic molecules using the GC-SAFT-VR equation of state. Fluid Phase Equilibria, 2017, 440, 111-121.	1.4	13
123	Fourier space approach to the classical density functional theory for multi-Yukawa and square-well fluids. Journal of Chemical Physics, 2012, 137, 104104.	1.2	12
124	Simulating Phase Equilibria using Wang-Landau-Transition Matrix Monte Carlo. Journal of Physics: Conference Series, 2014, 487, 012002.	0.3	11
125	Investigation of the Impact of Cross-Polymerization on the Structural and Frictional Properties of Alkylsilane Monolayers Using Molecular Simulation. Nanomaterials, 2019, 9, 639.	1.9	11
126	Thermodynamic properties of freely-jointed hard-sphere multi-Yukawa chain fluids: theory and simulation. Fluid Phase Equilibria, 2002, 194-197, 185-196.	1.4	10

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127	Square-well chain molecules: a semi-empirical equation of state and Monte Carlo simulation data. Fluid Phase Equilibria, 2004, 221, 63-72.	1.4	10
128	Examining the aggregation behavior of polymer grafted nanoparticles using molecular simulation and theory. Journal of Chemical Physics, 2015, 143, 054904.	1.2	10
129	Liquid Mixtures of Xenon with Fluorinated Species:Â Xenon + Sulfur Hexafluoride. Journal of Physical Chemistry B, 2007, 111, 5284-5289.	1.2	8
130	Development of a Coarse-Grained Water Forcefield via Multistate Iterative Boltzmann Inversion. Molecular Modeling and Simulation, 2016, 2016, 37-52.	0.2	8
131	A Transferable, Multi-Resolution Coarse-Grained Model for Amorphous Silica Nanoparticles. Journal of Chemical Theory and Computation, 2019, 15, 3260-3271.	2.3	8
132	Tribological characterization of gradient monolayer films from trichlorosilanes on silicon. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 412, 57-63.	2.3	7
133	Comparison of several classical density functional theories for the adsorption of flexible chain molecules into cylindrical nanopores. Journal of Chemical Physics, 2013, 139, 234902.	1.2	7
134	Web- and Cloud-based Software Infrastructure for Materials Design. Procedia Computer Science, 2014, 29, 2034-2044.	1.2	7
135	Examination of the phase transition behavior of nano-confined fluids by statistical temperature molecular dynamics. Journal of Chemical Physics, 2015, 143, 054504.	1.2	7
136	Structural Properties of Phospholipid-based Bilayers with Long-Chain Alcohol Molecules in the Gel Phase. Journal of Physical Chemistry B, 2016, 120, 12863-12871.	1.2	7
137	Multiscale Simulation of Ternary Stratum Corneum Lipid Mixtures: Effects of Cholesterol Composition. Langmuir, 2022, 38, 7496-7511.	1.6	7
138	Transient time correlation function calculation of the viscosity of a molecular fluid at low shear rates: a comparison of stress tensors. Molecular Physics, 2009, 107, 1423-1429.	0.8	6
139	Modeling the thermodynamic properties and phase behaviour of organic sulfur molecules with a group contribution based statistical associating fluid theory approach (GC-SAFT-VR). Fluid Phase Equilibria, 2017, 446, 46-54.	1.4	6
140	On the Behavior of Solutions of Xenon in Liquid n-Alkanes: Solubility of Xenon in n-Pentane and n-Hexane. Journal of Physical Chemistry B, 2010, 114, 15897-15904.	1.2	5
141	On the prediction of ternary mixture phase behavior from the GC-SAFT-VR approach: 1-Pentanol+dibutyl ether+n-nonane. Fluid Phase Equilibria, 2011, 302, 161-168.	1.4	5
142	Effect of Roughness on the Microscale Friction of Hydrocarbon Films. Journal of Physical Chemistry C, 2012, 116, 21795-21801.	1.5	5
143	Vapor-liquid equilibria for binary systems carbon dioxideÂ+Â1,1,1,2,3,3-hexafluoro-3-(2,2,2-trifluoroethoxy)propane or 1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluorobutane at 303.15â€“323.15ÂK. Fluid Phase Equilibria, 2020, 524, 112814.	1.4	5
144	High-throughput screening of tribological properties of monolayer films using molecular dynamics and machine learning. Journal of Chemical Physics, 2022, 156, 154902.	1.2	5

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145	Energy Storage in Cellulase Linker Peptides?. ACS Symposium Series, 2010, , 119-134.	0.5	4
146	A Wang-Landau study of a lattice model for lipid bilayer self-assembly. Journal of Chemical Physics, 2012, 137, 144901.	1.2	4
147	Incorporating configurational-bias Monte Carlo into the Wang-Landau algorithm for continuous molecular systems. Journal of Chemical Physics, 2012, 137, 204105.	1.2	4
148	Examining Tail and Headgroup Effects on Binary and Ternary Gel-Phase Lipid Bilayer Structure. Journal of Physical Chemistry B, 2020, 124, 3043-3053.	1.2	3
149	Examining the self-assembly of patchy alkane-grafted silica nanoparticles using molecular simulation. Journal of Chemical Physics, 2021, 154, 034903.	1.2	2
150	Third Foundations of Molecular Modeling and Simulation Conference FOMMS 2006. Molecular Physics, 2007, 105, 137-137.	0.8	1
151	Aqueous solutions: Bulk fluids and interfaces. Fluid Phase Equilibria, 2016, 407, 1.	1.4	1
152	Third Foundations of Molecular Modeling and Simulation Conference FOMMS 2006. Molecular Simulation, 2007, 33, 277-277.	0.9	0
153	Effective Interaction Potentials for Coarse-Grained Simulations of Polymer-Tethered Nanoparticle Self-Assembly in Solution. , 2008, , 415-431.		0