Erich A MÃ¼ller

List of Publications by Year
in descending order

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159	7,358	66250	71088
papers	citations	44 h-index	80 g-index

162	162	162	5412
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coarseâ€Grained Molecular Simulation of Polymers Supported by the Use of the SAFTâ€Î³$gamma$ Mie Equation of State. Macromolecular Theory and Simulations, 2022, 31, 2100031.	0.6	7
2	Adsorption of Hydrolysed Polyacrylamide onto Calcium Carbonate. Polymers, 2022, 14, 405.	2.0	13
3	Use of Boundary-Driven Nonequilibrium Molecular Dynamics for Determining Transport Diffusivities of Multicomponent Mixtures in Nanoporous Materials. Journal of Physical Chemistry B, 2022, 126, 1085-1100.	1.2	4
4	Water Flow in Single-Wall Nanotubes: Oxygen Makes It Slip, Hydrogen Makes It Stick. ACS Nano, 2022, 16, 10775-10782.	7.3	25
5	Machine learning hybrid approach for the prediction of surface tension profiles of hydrocarbon surfactants in aqueous solution. Journal of Colloid and Interface Science, 2022, 625, 328-339.	5.0	7
6	A simple thermodynamic model for the solubility of thermolabile solids in supercritical fluids. Chemical Engineering Science, 2021, 232, 116268.	1.9	5
7	How does the shape and surface energy of pores affect the adsorption of nanoconfined fluids?. AICHE Journal, 2021, 67, e17011.	1.8	7
8	Coarse-grained molecular dynamics study of the self-assembly of polyphilic bolaamphiphiles using the SAFT-Î³ Mie force field. Molecular Systems Design and Engineering, 2021, 6, 594-608.	1.7	11
9	SGTPy: A Python Code for Calculating the Interfacial Properties of Fluids Based on the Square Gradient Theory Using the SAFT-VR Mie Equation of State. Journal of Chemical Information and Modeling, 2021, 61, 1244-1250.	2.5	27
10	Defect-Dependent Corrugation in Graphene. Nano Letters, 2021, 21, 8143-8150.	4.5	29
11	Machine learning potentials for complex aqueous systems made simple. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	82
12	Phase equilibria and interfacial properties of selected methaneÂ+Ân-alkane binary mixtures. Journal of Molecular Liquids, 2021, 341, 116918.	2.3	6
13	Employing SAFT Coarse-Grained Force Fields for the Molecular Simulation of Thermodynamic and Transport Properties of CO2â€“n-Alkane Mixtures. Journal of Chemical & Engineering Data, 2020, 65, 1159-1171.	1.0	5
14	Generating a Machine-Learned Equation of State for Fluid Properties. Journal of Physical Chemistry B, 2020, 124, 8628-8639.	1.2	25
15	Machine Learning Potential for Hexagonal Boron Nitride Applied to Thermally and Mechanically Induced Rippling. Journal of Physical Chemistry C, 2020, 124, 22278-22290.	1.5	25
16	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
17	Surrogate Models for Studying the Wettability of Nanoscale Natural Rough Surfaces Using Molecular Dynamics. Energies, 2020, 13, 2770.	1.6	11
18	Equation of state and force fields for Feynmanâ€“Hibbs-corrected Mie fluids. II. Application to mixtures of helium, neon, hydrogen, and deuterium. Journal of Chemical Physics, 2020, 152, 074507.	1.2	19

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19	Probing the Interfacial Behavior of Type IIIa Binary Mixtures Along the Three-Phase Line Employing Molecular Thermodynamics. Molecules, 2020, 25, 1499.	1.7	9
20	A Guide to Computing Interfacial Properties of Fluids from Molecular Simulations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	17
21	A GPU Accelerated Lennard-Jones System for Immersive Molecular Dynamics Simulations in Virtual Reality. Lecture Notes in Computer Science, 2020, , 19-34.	1.0	1
22	Equation of state and force fields for Feynmanâ€“Hibbs-corrected Mie fluids. I. Application to pure helium, neon, hydrogen, and deuterium. Journal of Chemical Physics, 2019, 151, .	1.2	23
23	Multiscale Approach Linking Self-Aggregation and Surface Interactions of Synthesized Foulants to Fouling Mitigation Strategies. Energy & Fuels, 2019, 33, 7216-7224.	2.5	4
24	Spreading of aqueous droplets with common and superspreading surfactants. A molecular dynamics study. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 581, 123810.	2.3	13
25	Extension of the SAFT-VR-Mie equation of state for adsorption. Journal of Molecular Liquids, 2019, 294, 111639.	2.3	6
26	Catalogue of Plausible Molecular Models for the Molecular Dynamics of Asphaltenes and Resins Obtained from Quantitative Molecular Representation. Energy & Fuels, 2019, 33, 9779-9795.	2.5	34
27	Molecular Dynamics Simulation of the Superspreading of Surfactant-Laden Droplets. A Review. Fluids, 2019, 4, 176.	0.8	10
28	Extension of the effective solid-fluid Steele potential for Mie force fields. Molecular Physics, 2019, 117, 3840-3851.	0.8	9
29	Fluid-solid phase transition of n-alkane mixtures: Coarse-grained molecular dynamics simulations and diffusion-ordered spectroscopy nuclear magnetic resonance. Scientific Reports, 2019, 9, 1002.	1.6	24
30	Predicting the pressure dependence of the viscosity of 2,2,4-trimethylhexane using the SAFT coarse-grained force field. Fluid Phase Equilibria, 2019, 496, 1-6.	1.4	8
31	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
32	Molecular Simulation of the Adsorption and Diffusion in Cylindrical Nanopores: Effect of Shape and Fluidâ€“Solid Interactions. Molecules, 2019, 24, 608.	1.7	9
33	Machine Learning for Fluid Property Correlations: Classroom Examples with MATLAB. Journal of Chemical Education, 2019, 96, 697-703.	1.1	42
34	Combined Experimental, Theoretical, and Molecular Simulation Approach for the Description of the Fluid-Phase Behavior of Hydrocarbon Mixtures within Shale Rocks. Energy & Fuels, 2018, 32, 5750-5762.	2.5	46
35	Experimental measurements and theoretical modeling of high-pressure mass densities and interfacial tensions of carbon dioxideâ€¯+â€¯n-heptaneâ€¯+â€¯toluene and its carbon dioxide binary systems. Fuel, 2018, 228,3.4 92-102.		13
36	Prediction of the water/oil interfacial tension from molecular simulations using the coarse-grained SAFT-Î³ Mie force field. Fluid Phase Equilibria, 2018, 476, 9-15.	1.4	40

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37	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
38	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
39	Bulk viscosity of molecular fluids. Journal of Chemical Physics, 2018, 148, 174504.	1.2	59
40	Unusual flexibility of mesophase pitch-derived carbon materials: An approach to the synthesis of graphene. Carbon, 2017, 115, 539-545.	5.4	31
41	Extension of the SAFT-VR Mie EoS To Model Homonuclear Rings and Its Parametrization Based on the Principle of Corresponding States. Langmuir, 2017, 33, 11518-11529.	1.6	25
42	Simulation of Asphaltene Aggregation through Molecular Dynamics: Insights and Limitations. Energy & Fuels, 2017, 31, 1108-1125.	2.5	170
43	raaSAFT: A framework enabling coarse-grained molecular dynamics simulations based on the SAFT-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si16.gif" display="inline" overflow="scroll"><mml:mi>Î³</mml:mi></mml:math> Mie force field. Computer Physics Communications, 2017, 212, 161-179.	3.0	8
44	Working-fluid selection and performance investigation of a two-phase single-reciprocating-piston heat-conversion engine. Applied Energy, 2017, 186, 376-395.	5.1	42
45	Multiscale molecular simulations of the formation and structure of polyamide membranes created by interfacial polymerization. Journal of Membrane Science, 2017, 527, 180-190.	4.1	77
46	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
47	Physical insights into the bloodâ€“brain barrier translocation mechanisms. Physical Biology, 2017, 14, 041001.	0.8	27
48	Nonequilibrium study of the intrinsic free-energy profile across a liquid-vapour interface. Journal of Chemical Physics, 2016, 144, 044703.	1.2	19
49	Optimizing Water Transport through Graphene-Based Membranes: Insights from Nonequilibrium Molecular Dynamics. ACS Applied Materials & Interfaces, 2016, 8, 12330-12336.	4.0	110
50	A multiscale method for simulating fluid interfaces covered with large molecules such as asphaltenes. Journal of Computational Physics, 2016, 327, 576-611.	1.9	12
51	Bottled SAFT: A Web App Providing SAFT-Î³ Mie Force Field Parameters for Thousands of Molecular Fluids. Journal of Chemical Information and Modeling, 2016, 56, 1609-1614.	2.5	36
52	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
53	A Langevin model for fluctuating contact angle behaviour parametrised using molecular dynamics. Soft Matter, 2016, 12, 9604-9615.	1.2	18
54	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

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55	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
56	Interfacial tensions of industrial fluids from a molecularâ€based square gradient theory. AIChE Journal, 2016, 62, 1781-1794.	1.8	66
57	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
58	Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics. Journal of Chemical Physics, 2015, 143, 244709.	1.2	14
59	Coarse-Grained Models for Crude Oils: A Direct Link Between Equations of State and Molecular Simulations. , 2015, , .		3
60	Surface thermodynamics of planar, cylindrical, and spherical vapour-liquid interfaces of water. Journal of Chemical Physics, 2015, 142, 114701.	1.2	53
61	In Silico Determination of Gas Permeabilities by Non-Equilibrium Molecular Dynamics: CO2 and He through PIM-1. Membranes, 2015, 5, 99-119.	1.4	44
62	Aspects of Asphaltene Aggregation Obtained from Coarse-Grained Molecular Modeling. Energy & Fuels, 2015, 29, 556-566.	2.5	24
63	Modelling the interfacial behaviour of dilute light-switching surfactant solutions. Journal of Colloid and Interface Science, 2015, 445, 16-23.	5.0	36
64	Superspreading: Mechanisms and Molecular Design. Langmuir, 2015, 31, 2304-2309.	1.6	59
65	Coarse grained force field for the molecular simulation of natural gases and condensates. Fluid Phase Equilibria, 2015, 406, 91-100.	1.4	85
66	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
67	A corresponding-states framework for the description of the Mie family of intermolecular potentials. Molecular Physics, 2015, 113, 932-947.	0.8	63
68	Crude Oil Fouling: Fluid Dynamics, Reactions and Phase Change. Procedia IUTAM, 2015, 15, 186-193.	1.2	11
69	Modelling the superspreading of surfactant-laden droplets with computer simulation. Soft Matter, 2015, 11, 9254-9261.	1.2	37
70	Orientational ordering and phase behaviour of binary mixtures of hard spheres and hard spherocylinders. Journal of Chemical Physics, 2015, 143, 044906.	1.2	21
71	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
72	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

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73	Interface Science for Advanced Materials & Technologies. Adsorption Science and Technology, 2014, 32, i-ii.	1.5	0
74	Nonequilibrium molecular dynamics simulation of diffusion at the liquid-liquid interface. Journal of Chemical Physics, 2014, 141, 154101.	1.2	13
75	Adsorption and separation of CO2/CH4 mixtures using nanoporous adsorbents by molecular simulation. Fluid Phase Equilibria, 2014, 362, 227-234.	1.4	49
76	Use of Equations of State and Coarse Grained Simulations to Complement Experiments: Describing the Interfacial Properties of Carbon Dioxide + Decane and Carbon Dioxide + Eicosane Mixtures. Journal of Chemical & Engineering Data, 2014, 59, 2928-2941.	1.0	85
77	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
78	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
79	Force Fields for Coarse-Grained Molecular Simulations from a Corresponding States Correlation. Industrial & Engineering Chemistry Research, 2014, 53, 4131-4141.	1.8	109
80	High-pressure densities and interfacial tensions of binary systems containing carbon dioxide+n-alkanes: (n-Dodecane, n-tridecane, n-tetradecane). Fluid Phase Equilibria, 2014, 380, 82-92.	1.4	60
81	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
82	Insights into surfactant-assisted superspreading. Current Opinion in Colloid and Interface Science, 2014, 19, 283-289.	3.4	22
83	Resolving Discrepancies in the Measurements of the Interfacial Tension for the CO₂ + H₂O Mixture by Computer Simulation. Journal of Physical Chemistry Letters, 2014, 5, 1267-1271.	2.1	43
84	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	1.2	382
85	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
86	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
87	Purification of water through nanoporous carbon membranes: a molecular simulation viewpoint. Current Opinion in Chemical Engineering, 2013, 2, 223-228.	3.8	27
88	Fundamental Studies of Methyl Iodide Adsorption in DABCO Impregnated Activated Carbons. Langmuir, 2013, 29, 6849-6855.	1.6	16
89	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
90	Liquid Crystal Phase Behaviour of Attractive Disc-Like Particles. International Journal of Molecular Sciences, 2013, 14, 16414-16442.	1.8	8

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91	On the Calculation of Solid-Fluid Contact Angles from Molecular Dynamics. Entropy, 2013, 15, 3734-3745.	1.1	66
92	Professor Ken Sing: A Festschrift. Adsorption Science and Technology, 2013, 31, i-ii.	1.5	0
93	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
94	Modelling Fluid Flow in Nanoporous Membrane Materials via Nonâ€“equilibrium Molecular Dynamics. Procedia Engineering, 2012, 44, 383-385.	1.2	1
95	Effect of Pore Morphology on the Adsorption of Methane/Hydrogen Mixtures on Carbon Micropores. Journal of Physical Chemistry C, 2012, 116, 11820-11829.	1.5	61
96	A generic equation of state for liquid crystalline phases of hard-oblate particles. Molecular Physics, 2012, 110, 1269-1288.	0.8	16
97	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
98	Transport diffusivities of fluids in nanopores by non-equilibrium molecular dynamics simulation. Molecular Simulation, 2012, 38, 540-553.	0.9	61
99	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	0.8	44
100	Liquid crystalline behavior of a coarse-grained model of shape-persistent macrocycles with flexible attractive chains. Soft Matter, 2011, 7, 1694-1701.	1.2	12
101	Global phase behaviour of polyphilic tapered dendrons. Soft Matter, 2011, 7, 7465.	1.2	1
102	Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem. Heat Transfer Engineering, 2011, 32, 197-215.	1.2	62
103	Comparison of United-Atom Potentials for the Simulation of Vaporâ€“Liquid Equilibria and Interfacial Properties of Long-Chainn-Alkanes up ton-C₁₀₀. Journal of Physical Chemistry B, 2011, 115, 12822-12834.	1.2	46
104	Self-Assembly of T-Shaped Polyphilic Molecules in Solvent Mixtures. Journal of Physical Chemistry B, 2011, 115, 4592-4605.	1.2	11
105	The role of the intermolecular potential on the dynamics of ethylene confined in cylindrical nanopores. RSC Advances, 2011, 1, 270.	1.7	10
106	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
107	Jorge (Giorgio) Zgrablich. Adsorption Science and Technology, 2011, 29, 423-424.	1.5	1
108	Molecular Simulation of Hydrogen Physisorption and Chemisorption in Nanoporous Carbon Structures. Adsorption Science and Technology, 2011, 29, 799-817.	1.5	36

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109	Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation. Fluid Phase Equilibria, 2011, 306, 129-136.	1.4	35
110	A Molecular Simulation Study of Propane and Propylene Adsorption onto Single-Walled Carbon Nanotube Bundles. Journal of Nanoscience and Nanotechnology, 2010, 10, 2537-2546.	0.9	7
111	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
112	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
113	Lyotropic self-assembly mechanism of T-shaped polyphilic molecules. Faraday Discussions, 2010, 144, 187-202.	1.6	13
114	Molecular Simulation of Adsorption of Gases on Nanotubes. , 2010, , 41-67.		7
115	Liquid crystalline and antinematic behavior of shape-persistent macrocycles from molecular-dynamics simulations. Physical Review E, 2009, 80, 061702.	0.8	10
116	Behavior of ethylene and ethane within single-walled carbon nanotubes, 2: dynamical properties. Adsorption, 2009, 15, 13-22.	1.4	13
117	Behavior of ethylene and ethane within single-walled carbon nanotubes. 1-Adsorption and equilibrium properties. Adsorption, 2009, 15, 1-12.	1.4	25
118	Interfacial properties of selected binary mixtures containing n-alkanes. Fluid Phase Equilibria, 2009, 282, 68-81.	1.4	98
119	Determination of the surface area and porosity of carbon nanotube bundles from a Langmuirian analysis of sub- and supercritical adsorption data. Carbon, 2009, 47, 948-956.	5.4	42
120	Molecular dynamics simulation of the mesophase behaviour of a model bolaamphiphilic liquid crystal with a lateral flexible chain. Soft Matter, 2008, 4, 1820.	1.2	65
121	Staggered Alignment of Quadrupolar Molecules Inside Carbon Nanotubes. Journal of Physical Chemistry B, 2008, 112, 8999-9005.	1.2	18
122	Observation of Surface Nematization at the Solidâ^'Liquid Crystal Interface via Molecular Simulation. Journal of Physical Chemistry C, 2007, 111, 15998-16005.	1.5	10
123	Shape factors in equations of state : Part II. Repulsion phenomena in multicomponent chain fluids. Physical Chemistry Chemical Physics, 2006, 8, 2619-2623.	1.3	4
124	Mesoscopic Simulation of Aggregation of Asphaltene and Resin Molecules in Crude Oils. Energy & Fuels, 2006, 20, 327-338.	2.5	81
125	Intensification of turbulent free heat transport in various configurations with adequate binary gas mixtures. International Communications in Heat and Mass Transfer, 2005, 32, 1298-1306.	2.9	2
126	Temperature-quench Molecular Dynamics Simulations for Fluid Phase Equilibria. Molecular Simulation, 2005, 31, 33-43.	0.9	29

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127	Adsorption of Super Greenhouse Gases on Microporous Carbons. Environmental Science & Technology, 2005, 39, 8736-8741.	4.6	35
128	Modelling of Ethane/Ethylene Separation Using Microporous. Adsorption Science and Technology, 2005, 23, 855-865.	1.5	13
129	Molecular Modeling of Fluid-Phase Equilibria Using an Isotropic Multipolar Potential. Industrial & Engineering Chemistry Research, 2003, 42, 4123-4131.	1.8	31
130	On the Calculation of Supercritical Fluidâ^'Solid Equilibria by Molecular Simulation. Journal of Physical Chemistry B, 2003, 107, 1672-1678.	1.2	23
131	Wetting of Planar Surfaces by a Gay-Berne Liquid Crystal. Molecular Simulation, 2003, 29, 385-391.	0.9	10
132	Dense packing of binary and polydisperse hard spheres. Molecular Physics, 2002, 100, 2461-2469.	0.8	71
133	Location of phase equilibria by temperature-quench molecular dynamics simulations. Fluid Phase Equilibria, 2002, 203, 1-14.	1.4	40
134	Molecular-Based Equations of State for Associating Fluids: A Review of SAFT and Related Approaches. Industrial & Engineering Chemistry Research, 2001, 40, 2193-2211.	1.8	600
135	Adsorption of Water Vaporâ^'Methane Mixtures on Activated Carbons. Langmuir, 2000, 16, 5418-5424.	1.6	124
136	12 Associating fluids and fluid mixtures. Experimental Thermodynamics, 2000, , 435-477.	0.1	28
137	Molecular simulation of the Jouleâ€“Thomson inversion curve of carbon dioxide. Fluid Phase Equilibria, 1999, 165, 147-155.	1.4	45
138	Molecular Simulation of Jouleâ€“Thomson Inversion Curves. International Journal of Thermophysics, 1999, 20, 229-235.	1.0	37
139	Simplified equation of state for non-spherical hard particles: an optimized shape factor approach. Physical Chemistry Chemical Physics, 1999, 1, 4919-4924.	1.3	24
140	Shape factors and interaction parameters in equations of state Part I. Repulsion phenomena in rigid particle systems. Physical Chemistry Chemical Physics, 1999, 1, 4259-4266.	1.3	9
141	A Molecular Model for Adsorption of Water on Activated Carbon:Â Comparison of Simulation and Experiment. Langmuir, 1999, 15, 533-544.	1.6	287
142	Molecular simulation study of hydrophilic and hydrophobic behavior of activated carbon surfaces. Carbon, 1998, 36, 1433-1438.	5.4	180
143	Correlations for Direct Calculation of Vapor Pressures from Cubic Equations of State. Industrial & Engineering Chemistry Research, 1998, 37, 1673-1678.	1.8	2
144	Joule-Thomson Inversion Curves by Molecular Simulation. Molecular Simulation, 1997, 19, 237-246.	0.9	25

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145	Adsorption of Water on Activated Carbons:Â A Molecular Simulation Study. The Journal of Physical Chemistry, 1996, 100, 1189-1196.	2.9	353
146	Effect of surface active sites on adsorption of associating chain molecules in pores: A Monte Carlo study. Adsorption, 1996, 2, 59-68.	1.4	11
147	Adsorption Isotherms of Associating Fluids in Slit-Like Pores. A Monte Carlo Simulation Study. Kluwer International Series in Engineering and Computer Science, 1996, , 993-1000.	0.2	1
148	Molecular simulation and theory of associating chain molecules. International Journal of Thermophysics, 1995, 16, 705-713.	1.0	20
149	Mixtures of Associating and Non-associating Chains on Activated Surfaces: A Monte Carlo Approach. Molecular Simulation, 1995, 15, 141-154.	0.9	9
150	Adsorption isotherms of associating chain molecules from Monte Carlo simulations. Molecular Physics, 1995, 85, 9-21.	0.8	24
151	Comment on the accuracy of Wertheimâ€™s theory of associating fluids. Journal of Chemical Physics, 1995, 103, 3868-3869.	1.2	19
152	An Equation of State for Water from a Simplified Intermolecular Potential. Industrial & Engineering Chemistry Research, 1995, 34, 3662-3673.	1.8	127
153	Spectroscopic Data on the Kinetics of Hydrate Formation and Decomposition. Annals of the New York Academy of Sciences, 1994, 715, 561-563.	1.8	3
154	Theory and simulation of associating fluids: Lennard-Jones chains with association sites. Molecular Physics, 1994, 83, 1209-1222.	0.8	40
155	Triplet correlation function for hard sphere systems. Molecular Physics, 1993, 80, 91-101.	0.8	39
156	Simulation of hard triatomic and tetratomic molecules. Molecular Physics, 1993, 80, 957-976.	0.8	75
157	Densities and excess volumes in aqueous poly(ethylene glycol) solutions. Journal of Chemical & Engineering Data, 1991, 36, 214-217.	1.0	126
158	Mixing expansivities and Grashof numbers in supercritical fluids using cubic equations-of-state. Journal of Supercritical Fluids, 1990, 3, 136-142.	1.6	18
159	IMPROVING FLOW PATTERNS IN A DISTILLATION TRAY BY MODIFYING DOWNCOMER APRON SHAPE. Chemical Engineering Communications, 1988, 74, 195-208.	1.5	6