Jadran Vrabec

List of Publications by Year
in descending order

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232 papers	7,385 citations	50170 46 h-index	74018 75 g-index
249 all docs	249 docs citations	249 times ranked	3682 citing authors

#	Article	IF	Citations
1	Long range corrections for inhomogeneous fluids containing a droplet or a bubble. Molecular Simulation, 2022, 48, 73-86.	0.9	0
2	Thermodynamic Properties of Methyl Diethanolamine. International Journal of Thermophysics, 2022, 43, 1.	1.0	4
3	Impact of aging on the energy efficiency of household refrigerating appliances. Applied Thermal Engineering, 2022, 205, 117992.	3.0	6
4	Assessment of thermodynamic models via Jouleâ€“Thomson inversion. Fluid Phase Equilibria, 2022, 556, 113401.	1.4	7
5	Vaporâ€“Liquidâ€“Liquid Equilibria of Nitrogen + Ethane by Molecular Simulation. Industrial & Engineering Chemistry Research, 2022, 61, 3104-3112.	1.8	2
6	Droplet coalescence by molecular dynamics and phase-field modeling. Physics of Fluids, 2022, 34, .	1.6	17
7	Apparatus for the measurement of the thermodynamic speed of sound of diethylene glycol and triethylene glycol. Journal of Chemical Thermodynamics, 2022, 170, 106766.	1.0	0
8	How well does the Tang-Toennies potential represent the thermodynamic properties of argon?. Molecular Physics, 2022, 120, .	0.8	2
9	Experimental investigation of organic Rankine cycle performance using alkanes or hexamethyldisiloxane as a working fluid. Energy Conversion and Management: X, 2022, 15, 100244.	0.9	3
10	Connecting entropy scaling and density scaling. Journal of Chemical Physics, 2022, 157, .	1.2	3
11	Evaporation driven by conductive heat transport. Molecular Physics, 2021, 119, .	0.8	14
12	Molecular simulation study of the curling behavior of the finite free-standing kaolinte layer. Computational Materials Science, 2021, 186, 110037.	1.4	3
13	Determining the heat flow through the cabinet walls of household refrigerating appliances. International Journal of Refrigeration, 2021, 121, 235-242.	1.8	3
14	Atomistic Simulations: The Driving Force Behind Modern Thermodynamic Research. , 2021, , 569-581.		0
15	Diffusion of the carbon dioxideâ€“ethanol mixture in the extended critical region. Physical Chemistry Chemical Physics, 2021, 23, 3106-3115.	1.3	18
16	Experimental study of two cascaded organic Rankine cycles with varying working fluids. Energy Conversion and Management, 2021, 230, 113818.	4.4	18
17	AutoPas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. Journal of Computational Science, 2021, 50, 101296.	1.5	6
18	Comparison of macro- and microscopic solutions of the Riemann problem II. Two-phase shock tube. Journal of Computational Physics, 2021, 429, 110027.	1.9	13

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19	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. Computer Physics Communications, 2021, 262, 107860.	3.0	31
20	Diffusion in multicomponent aqueous alcoholic mixtures. Scientific Reports, 2021, 11, 12319.	1.6	4
21	Density and Partial Molar Volumes of the Liquid Mixture Water + Methanol + Ethanol + 2-Propanol at 298.15 K and 0.1 MPa. Journal of Chemical & Engineering Data, 2021, 66, 2425-2435.	1.0	7
22	Investigating the real life energy consumption of refrigeration appliances in Germany: Are present policies sufficient?. Energy Policy, 2021, 155, 112275.	4.2	10
23	Measurement procedure for acoustic absorption and bulk viscosity of liquids. Measurement: Journal of the International Measurement Confederation, 2021, 184, 109919.	2.5	2
24	Cascaded dual-loop organic Rankine cycle with alkanes and low global warming potential refrigerants as working fluids. Energy Conversion and Management, 2021, 249, 114843.	4.4	15
25	Thermodynamic speed of sound of xenon. Journal of Chemical Thermodynamics, 2020, 141, 105933.	1.0	5
26	Henryâ€™s Law Constant of Noble Gases in Water, Methanol, Ethanol, and Isopropanol by Experiment and Molecular Simulation. Journal of Chemical & Engineering Data, 2020, 65, 1180-1188.	1.0	6
27	Thermodynamic factor of quaternary mixtures from Kirkwoodâ€“Buff integration. Molecular Physics, 2020, 118, .	0.8	13
28	Henryâ€™s Law Constant of Nitrogen, Oxygen, and Argon in Ternary Aqueous Alcoholic Solvent Mixtures. Journal of Chemical & Engineering Data, 2020, 65, 1189-1196.	1.0	10
29	Comparison of macro- and microscopic solutions of the Riemann problem I. Supercritical shock tube and expansion into vacuum. Journal of Computational Physics, 2020, 402, 109077.	1.9	14
30	Semantic Interoperability and Characterization of Data Provenance in Computational Molecular Engineering. Journal of Chemical & Engineering Data, 2020, 65, 1313-1329.	1.0	21
31	Structure and dynamics of the Lennard-Jones fcc-solid focusing on melting precursors. Journal of Chemical Physics, 2020, 153, 104506.	1.2	9
32	Improving the performance of household refrigerating appliances through the integration of phase change materials in the context of the new global refrigerator standard IECÂ62552:2015. International Journal of Refrigeration, 2020, 119, 448-456.	1.8	18
33	Age-related efficiency loss of household refrigeration appliances: Development of an approach to measure the degradation of insulation properties. Applied Thermal Engineering, 2020, 173, 115113.	3.0	11
34	Bulk viscosity of liquid noble gases. Journal of Chemical Physics, 2020, 152, 094503.	1.2	10
35	Special Issue Honoring Hans Hasse. Journal of Chemical & Engineering Data, 2020, 65, 941-942.	1.0	1
36	Fick Diffusion Coefficient Matrix of a Quaternary Liquid Mixture by Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 4527-4535.	1.2	16

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37	A Benchmark Open-Source Implementation of COSMO-SAC. Journal of Chemical Theory and Computation, 2020, 16, 2635-2646.	2.3	74
38	Experimental investigation of a cascaded organic Rankine cycle plant for the utilization of waste heat at high and low temperature levels. Energy Conversion and Management, 2020, 205, 112381.	4.4	20
39	Density and Thermodynamic Speed of Sound of Liquid Vinyl Chloride. Journal of Chemical & Engineering Data, 2020, 65, 2495-2504.	1.0	5
40	Dielectric constant and density of aqueous alkali halide solutions by molecular dynamics: A force field assessment. Journal of Chemical Physics, 2020, 152, 164502.	1.2	23
41	Design and test of a multi-coil helical evaporator for a high temperature organic Rankine cycle plant driven by biogas waste heat. Energy Conversion and Management, 2019, 195, 1402-1414.	4.4	14
42	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. Journal of Chemical Information and Modeling, 2019, 59, 4248-4265.	2.5	101
43	Acoustic absorption measurement for the determination of the volume viscosity of pure fluids / Messverfahren fÃ¼r die akustischen Absorption zur Bestimmung der VolumenviskositÃt reiner Fluide. TM Technisches Messen, 2019, 86, 2-6.	0.3	10
44	Evaporation sampled by stationary molecular dynamics simulation. Journal of Chemical Physics, 2019, 151, 044704.	1.2	24
45	TweTriS: Twenty trillion-atom simulation. International Journal of High Performance Computing Applications, 2019, 33, 838-854.	2.4	43
46	Do ternary liquid mixtures exhibit negative main Fick diffusion coefficients?. Physical Chemistry Chemical Physics, 2019, 21, 2140-2152.	1.3	20
47	Molecular Modeling and Simulation: Force Field Development, Evaporation Processes and Thermophysical Properties of Mixtures. , 2019, , 457-474.		1
48	Diffusion of methane in supercritical carbon dioxide across the Widom line. Scientific Reports, 2019, 9, 8466.	1.6	30
49	Thermodynamic Properties of Dodecamethylpentasiloxane, Tetradecamethylhexasiloxane, and Decamethylcyclopentasiloxane. Industrial & Engineering Chemistry Research, 2019, 58, 9617-9635.	1.8	17
50	MolMod â€“ an open access database of force fields for molecular simulations of fluids. Molecular Simulation, 2019, 45, 806-814.	0.9	65
51	Digitalization in Thermodynamics. Chemie-Ingenieur-Technik, 2019, 91, 201-214.	0.4	14
52	Diffusion limited evaporation of a binary liquid film. International Journal of Heat and Mass Transfer, 2019, 132, 1296-1305.	2.5	11
53	Thermodynamic Speed of Sound Data for Liquid and Supercritical Alcohols. Journal of Chemical & Engineering Data, 2019, 64, 1035-1044.	1.0	11
54	Kirkwood-Buff integration: A promising route to entropic properties?. Fluid Phase Equilibria, 2019, 485, 270-281.	1.4	18

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55	PetaFLOP Molecular Dynamics for Engineering Applications. , 2019, , 397-407.		1
56	Understanding the Scalability of Molecular Simulation Using Empirical Performance Modeling. Lecture Notes in Computer Science, 2019, , 125-143.	1.0	2
57	10.1063/1.5111759.1. , 2019, , .		0
58	Speed of Sound Measurements and a Fundamental Equation of State for Hydrogen Chloride. Journal of Chemical & Engineering Data, 2018, 63, 2533-2547.	1.0	15
59	Molecular Models for the Hydrogen Age: Hydrogen, Nitrogen, Oxygen, Argon, and Water. Journal of Chemical & Engineering Data, 2018, 63, 305-320.	1.0	32
60	SkaSim â€“ Scalable HPC Software for Molecular Simulation in the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 295-306.	0.4	7
61	Experimental setup of a cascaded two-stage organic Rankine cycle. Applied Thermal Engineering, 2018, 131, 958-964.	3.0	15
62	Composition dependent transport diffusion in non-ideal mixtures from spatially resolved nuclear magnetic resonance spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 28185-28192.	1.3	5
63	The effect of alcohols as the third component on diffusion in mixtures of aromatics and ketones. RSC Advances, 2018, 8, 10017-10022.	1.7	9
64	Diffusion Coefficients of a Highly Nonideal Ternary Liquid Mixture: Cyclohexaneâ€“Tolueneâ€“Methanol. Industrial & Engineering Chemistry Research, 2018, 57, 16508-16517.	1.8	23
65	Molecular Insight into the Liquid Propan-2-ol + Water Mixture. Journal of Physical Chemistry B, 2018, 122, 8718-8729.	1.2	25
66	Interplay of structure and diffusion in ternary liquid mixtures of benzene + acetone + varying alcohols. Journal of Chemical Physics, 2018, 149, 064504.	1.2	11
67	Liquid state isomorphism, Rosenfeld-Tarazona temperature scaling, and Riemannian thermodynamic geometry. Physical Review E, 2018, 97, 052149.	0.8	14
68	Experimental and Computational Study on the Solubility of Argon in Propan-2-ol at High Temperatures. Chemistry Letters, 2017, 46, 990-991.	0.7	1
69	Understanding the Differing Fluid Phase Behavior of Cyclohexane + Benzene and Their Hydroxylated or Aminated Forms. Journal of Physical Chemistry B, 2017, 121, 5374-5384.	1.2	5
70	Special Issue of Molecular Physics in Honour of Professor Johann Fischer. Molecular Physics, 2017, 115, 1015-1016.	0.8	0
71	Vaporâ€“Liquid Equilibria of Nitrogen + Diethyl Ether and Nitrogen + 1,1,1,2,2,4,5,5,5-Nonafluoro-4-(trifluoromethyl)-3-pentanone by Experiment, Pengâ€“Robinson and PC-SAFT Equations of State. Journal of Chemical & Engineering Data, 2017, 62, 2110-2114.	1.0	3
72	Premelting, solid-fluid equilibria, and thermodynamic properties in the high density region based on the Lennard-Jones potential. Journal of Chemical Physics, 2017, 147, 144502.	1.2	13

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73	Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. Journal of Chemical Theory and Computation, 2017, 13, 4270-4280.	2.3	48
74	Speed of Sound Measurements and Fundamental Equations of State for Octamethyltrisiloxane and Decamethyltetrasiloxane. Journal of Chemical & Engineering Data, 2017, 62, 2633-2648.	1.0	33
75	Comprehensive Assessment of COSMO-SAC Models for Predictions of Fluid-Phase Equilibria. Industrial & Engineering Chemistry Research, 2017, 56, 9868-9884.	1.8	56
76	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml56" display="inline" overflow="scroll" altimg="si19.gif"><mml:mi>m</mml:mi><mml:mi>s</mml:mi><mml:mn>2</mml:mn></mml:math>: A molecular simulation tool for thermodynamic properties, release 3.0. Computer Physics Communications, 2017, 221, 343-351.	3.0	70
77	Equation of state for 1,2-dichloroethane based on a hybrid data set. Molecular Physics, 2017, 115, 1166-1185.	0.8	13
78	Mutual diffusion governed by kinetics and thermodynamics in the partially miscible mixture methanol + cyclohexane. Physical Chemistry Chemical Physics, 2017, 19, 31856-31873.	1.3	32
79	How well does the Lennard-Jones potential represent the thermodynamic properties of noble gases?. Molecular Physics, 2017, 115, 1104-1121.	0.8	59
80	The Experimental Study of Solubility of Helium in Propan-2-ol at Temperatures 360, 420 and 480 Đš. Izvestiya of Saratov University New Series Series: Chemistry Biology Ecology, 2017, 17, 155-162.	0.0	1
81	Assessing the accuracy of improved forceâ€matched water models derived from Ab initio molecular dynamics simulations. Journal of Computational Chemistry, 2016, 37, 1828-1838.	1.5	11
82	Communication: Evaporation: Influence of heat transport in the liquid on the interface temperature and the particle flux. Journal of Chemical Physics, 2016, 145, 081101.	1.2	29
83	Insight into the Nature of Evaporation Processes Enabled by Massively Parallel Molecular Dynamics Simulations. , 2016, , .		0
84	Comparative study of the GrÃ¼neisen parameter for 28 pure fluids. Journal of Chemical Physics, 2016, 144, 244505.	1.2	32
85	Equation of State for the Lennard-Jones Fluid. Journal of Physical and Chemical Reference Data, 2016, 45, .	1.9	133
86	Mutual diffusion of binary liquid mixtures containing methanol, ethanol, acetone, benzene, cyclohexane, toluene, and carbon tetrachloride. Journal of Chemical Physics, 2016, 144, 124501.	1.2	79
87	Experimental study of phase change materials for photovoltaic modules: Energy performance and economic yield for the EPEX spot market. Solar Energy, 2016, 140, 51-59.	2.9	46
88	Diffusion in Multicomponent Liquids: From Microscopic to Macroscopic Scales. Journal of Physical Chemistry B, 2016, 120, 12193-12210.	1.2	24
89	Molecular Dynamics Simulation of Nucleation in CO₂. Chemie-Ingenieur-Technik, 2016, 88, 1286-1286.	0.4	0
90	Empirische Fundamentalgleichungen auf der Basis von molekularen Simulationen - Ein Ãœberblick. Chemie-Ingenieur-Technik, 2016, 88, 1285-1285.	0.4	0

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91	Automatized determination of fundamental equations of state based on molecular simulations in the cloud. Fluid Phase Equilibria, 2016, 425, 84-92.	1.4	7
92	Thermodynamic Properties of Octamethylcyclotetrasiloxane. Journal of Chemical & Engineering Data, 2016, 61, 2580-2595.	1.0	25
93	Speed of Sound of Oxygen in Supercritical States up to 500 K and 100 MPa. Journal of Chemical & Engineering Data, 2016, 61, 1632-1636.	1.0	3
94	Fundamental equation of state correlation for hexamethyldisiloxane based on experimental and molecular simulation data. Fluid Phase Equilibria, 2016, 418, 133-151.	1.4	46
95	Molecular Simulation Study of Transport Properties for 20 Binary Liquid Mixtures and New Force Fields for Benzene, Toluene and CCl4. , 2016, , 613-634.		2
96	Comment on â€œThe gas-liquid surface tension of argon: A reconciliation between experiment and simulationâ€•[J. Chem. Phys. 140, 244710 (2014)]. Journal of Chemical Physics, 2015, 142, 107101.	1.2	12
97	Mutual Diffusion of Binary and Ternary Liquid Mixtures Containing Acetone, Benzene, Cyclohexane, Methanol, Tetrachloromethane, and Toluene by Molecular Simulation. Chemie-Ingenieur-Technik, 2015, 87, 1091-1092.	0.4	0
98	Empirical Fundamental Equations of State Correlations Based on Hybrid Datasets. Chemie-Ingenieur-Technik, 2015, 87, 1091-1091.	0.4	0
99	Thermodynamic correlation of molecular simulation data. Molecular Physics, 2015, 113, 910-931.	0.8	9
100	Vaporâ€“liquid equilibrium measurements of the binary mixtures CO2+acetone and CO2+pentanones. Journal of Supercritical Fluids, 2015, 100, 160-166.	1.6	23
101	Reducing the power consumption of household refrigerators through the integration of latent heat storage elements in wire-and-tube condensers. International Journal of Refrigeration, 2015, 51, 154-160.	1.8	52
102	Lennard-Jones force field parameters for cyclic alkanes from cyclopropane to cyclohexane. Fluid Phase Equilibria, 2015, 404, 150-160.	1.4	25
103	Vapor-phase chemical equilibrium and combined chemical and vaporâ€“liquid equilibrium for the ternary system ethylene+water+ethanol from reaction-ensemble and reactive Gibbs-ensemble molecular simulations. Fluid Phase Equilibria, 2015, 403, 104-113.	1.4	2
104	Burst design and signal processing for the speed of sound measurement of fluids with the pulse-echo technique. Review of Scientific Instruments, 2015, 86, 054903.	0.6	18
105	Excess properties of non-ideal binary mixtures containing water, methanol and ethanol by molecular simulation. Journal of Molecular Liquids, 2015, 212, 90-95.	2.3	17
106	Fluid phase interface properties of acetone, oxygen, nitrogen and their binary mixtures by molecular simulation. Physical Chemistry Chemical Physics, 2015, 17, 27195-27203.	1.3	24
107	Copolymer-bound phase change materials for household refrigerating appliances: experimental investigation of power consumption, temperature distribution and demand side management potential. International Journal of Refrigeration, 2015, 60, 166-173.	1.8	21
108	Empirical Fundamental Equation of State for Phosgene Based on Molecular Simulation Data. Journal of Chemical & Engineering Data, 2015, 60, 2895-2905.	1.0	11

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109	Equation of State for the Lennard-Jones Truncated and Shifted Model Fluid. International Journal of Thermophysics, 2015, 36, 25-43.	1.0	53
110	Fundamental equation of state for ethylene oxide based on a hybrid dataset. Chemical Engineering Science, 2015, 121, 87-99.	1.9	29
111	Molecular Models for Cyclic Alkanes and Ethyl Acetate As Well As Surface Tension Data from Molecular Simulation. , 2015, , 645-659.		3
112	Performance Predictions of Axial Turbines for Organic Rankine Cycle (ORC) Applications Based on Measurements of the Flow Through Two-Dimensional Cascades of Blades. , 2014, , .		5
113	Molecular dispersion energy parameters for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2014, 140, 044504.	1.2	36
114	Communication: Molecular simulation study of kaolinite intercalation with realistic layer size. Journal of Chemical Physics, 2014, 141, 091102.	1.2	3
115	Phase equilibria of methane clathrate hydrates from Grand Canonical Monte Carlo simulations. Fluid Phase Equilibria, 2014, 369, 47-54.	1.4	41
116	Fluid Phase Behavior of Nitrogen + Acetone and Oxygen + Acetone by Molecular Simulation, Experiment and the Pengâ€“Robinson Equation of State. Journal of Chemical & Engineering Data, 2014, 59, 28-38.	1.0	22
117	Long-range correction for multi-site Lennard-Jones models and planar interfaces. Molecular Physics, 2014, 112, 2227-2234.	0.8	27
118	On the application of binary correction factors in lattice distortion calculations for methane clathrate hydrates. Philosophical Magazine, 2014, 94, 974-990.	0.7	6
119	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mi>m</mml:mi><mml:mi>s</mml:mi><mml:mn>2</mml:mn></mml:math>: A molecular simulation tool for thermodynamic properties, new version release. Computer Physics Communications, 2014, 185, 3302-3306.	3.0	67
120	Apparatus for the measurement of the speed of sound of ammonia up to high temperatures and pressures. Review of Scientific Instruments, 2014, 85, 084901.	0.6	14
121	ls1 mardyn: The Massively Parallel Molecular Dynamics Code for Large Systems. Journal of Chemical Theory and Computation, 2014, 10, 4455-4464.	2.3	108
122	Influence of unlike dispersion interactions in modeling methane clathrate hydrates. Fluid Phase Equilibria, 2014, 381, 108-115.	1.4	17
123	Considering the dispersive interactions in the COSMO-SAC model for more accurate predictions of fluid phase behavior. Fluid Phase Equilibria, 2014, 367, 109-116.	1.4	54
124	Evaporation from a free liquid surface. International Journal of Heat and Mass Transfer, 2014, 73, 303-317.	2.5	47
125	Molecular simulation of the vaporâ€“liquid phase behavior of cyanides and their binary mixtures. Fluid Phase Equilibria, 2013, 354, 286-297.	1.4	4
126	Vaporâ€“Liquid Equilibria of CO₂ + C1â€“C5 Alcohols from the Experiment and the COSMO-SAC Model. Journal of Chemical & Engineering Data, 2013, 58, 3420-3429.	1.0	20

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127	591 TFLOPS Multi-trillion Particles Simulation on SuperMUC. Lecture Notes in Computer Science, 2013, , 1-12.	1.0	34
128	Fluidâ€phase coexistence for the oxidation of <scp>CO</scp>₂ expanded cyclohexane: Experiment, molecular simulation, and <scp>COSMO</scp>â€<scp>SAC</scp>. AICHE Journal, 2013, 59, 2236-2250.	1.8	9
129	Communication: Fundamental equation of state correlation with hybrid data sets. Journal of Chemical Physics, 2013, 139, 041102.	1.2	26
130	Automated development of force fields for the calculation of thermodynamic properties: acetonitrile as a case study. Molecular Simulation, 2013, 39, 109-118.	0.9	17
131	Mutual diffusion in the ternary mixture of water + methanol + ethanol and its binary subsystems. Physical Chemistry Chemical Physics, 2013, 15, 3985.	1.3	76
132	Surface Tension, Large Scale Thermodynamic Data Generation and Vapor-Liquid Equilibria of Real Compounds. , 2013, , 635-646.		2
133	Molecular Modelling and Simulation of Electrolyte Solutions, Biomolecules, and Wetting of Component Surfaces. , 2013, , 647-661.		2
134	Computational Molecular Engineering as an Emerging Technology in Process Engineering. IT - Information Technology, 2013, 55, 97-101.	0.6	5
135	Simulation of Liquid-Liquid Equilibria with Molecular Models Optimized to Vapor-Liquid Equilibria and Model Development for Hydrazine and Two of Its Derivatives. , 2013, , 451-460.		0
136	Engineering Molecular Models: Efficient Parameterization Procedure and Cyclohexanol as Case Study. Soft Materials, 2012, 10, 3-25.	0.8	28
137	A set of molecular models for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2012, 136, 084501.	1.2	62
138	Vaporâ€“liquid equilibria of ethylene (C2H4)+decafluorobutane (C4F10) at 268â€“298K from experiment, molecular simulation and the Pengâ€–Robinson equation of state. Fluid Phase Equilibria, 2012, 336, 104-112.	1.4	11
139	Molecular Dynamics and Experimental Study of Conformation Change of Poly(N-isopropylacrylamide) Hydrogels in Mixtures of Water and Methanol. Journal of Physical Chemistry B, 2012, 116, 5251-5259.	1.2	145
140	A Set of Molecular Models for Alkaline-Earth Cations in Aqueous Solution. Journal of Physical Chemistry B, 2012, 116, 5448-5457.	1.2	29
141	Vaporâ€“Liquid Equilibrium Measurements of the Binary Mixtures Nitrogen + Acetone and Oxygen + Acetone. Journal of Chemical & Engineering Data, 2012, 57, 1672-1677.	1.0	15
142	Molecular Modeling and Simulation of Vaporâ€“Liquid Equilibria of Ethylene Oxide, Ethylene Glycol, and Water as Well as their Binary Mixtures. Industrial & Engineering Chemistry Research, 2012, 51, 7428-7440.	1.8	33
143	On the Treatment of Electrostatic Interactions of Non-spherical Molecules in Equation of State Models. Soft Materials, 2012, 10, 81-105.	0.8	6
144	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	0.8	44

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145	Prediction of Transport Properties of Liquid Ammonia and Its Binary Mixture with Methanol by Molecular Simulation. International Journal of Thermophysics, 2012, 33, 449-468.	1.0	23
146	Molecular simulation study on the solubility of carbon dioxide in mixtures of cyclohexane+cyclohexanone. Fluid Phase Equilibria, 2012, 315, 77-83.	1.4	16
147	On the prediction of transport properties of monomethylamine, dimethylamine, dimethylether and hydrogen chloride by molecular simulation. Fluid Phase Equilibria, 2012, 316, 46-54.	1.4	11
148	Fluid phase behavior from molecular simulation: Hydrazine, Monomethylhydrazine, Dimethylhydrazine and binary mixtures containing these compounds. Fluid Phase Equilibria, 2012, 322-323, 79-91.	1.4	11
149	Gas solubility of carbon dioxide and of oxygen in cyclohexanol by experiment and molecular simulation. Journal of Chemical Thermodynamics, 2012, 49, 114-118.	1.0	8
150	ms2: A Molecular Simulation Tool for Thermodynamic Properties. Chemie-Ingenieur-Technik, 2012, 84, 114-120.	0.4	2
151	Atomistic Simulations of Electrolyte Solutions and Hydrogels with Explicit Solvent Models. , 2012, , 185-199.		3
152	Molecular Modeling of Hydrogen Bonding Fluids: Phase Behavior of Industrial Fluids. , 2012, , 567-579.		0
153	On the difference between a point multipole and an equivalent linear arrangement of point charges in force field models for vapourâ€“liquid equilibria; partial charge based models for 59 real fluids. Molecular Physics, 2011, 109, 1975-1982.	0.8	12
154	Prediction of self-diffusion coefficient and shear viscosity of water and its binary mixtures with methanol and ethanol by molecular simulation. Journal of Chemical Physics, 2011, 134, 074508.	1.2	182
155	Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields. Topics in Current Chemistry, 2011, 307, 201-249.	4.0	24
156	Flexible or rigid molecular models? A study on vapourâ€“liquid equilibrium properties of ammonia. Molecular Physics, 2011, 109, 619-624.	0.8	14
157	The air pressure effect on the homogeneous nucleation of carbon dioxide by molecular simulation. Atmospheric Research, 2011, 101, 519-526.	1.8	8
158	ms2: A molecular simulation tool for thermodynamic properties. Computer Physics Communications, 2011, 182, 2350-2367.	3.0	102
159	Liquidâ€“liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics. Fluid Phase Equilibria, 2011, 310, 25-31.	1.4	10
160	Dynamic simulation of particle-filled hollow spheres. Proceedings in Applied Mathematics and Mechanics, 2011, 11, 881-882.	0.2	1
161	Vaporâ€“liquid equilibria of hydrogen chloride, phosgene, benzene, chlorobenzene, orthoâ€dichlorobenzene, and toluene by molecular simulation. AICHE Journal, 2011, 57, 1043-1060.	1.8	35
162	Description of HFO-1234yf with BACKONE equation of state. Fluid Phase Equilibria, 2011, 305, 204-211.	1.4	30

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163	Software design for a highly parallel molecular dynamics simulation framework in chemical engineering. Journal of Computational Science, 2011, 2, 124-129.	1.5	23
164	Molecular Modeling of Hydrogen Bonding Fluids: Transport Properties and Vapor-Liquid Coexistence. , 2011, , 543-551.		0
165	GROW: A gradient-based optimization workflow for the automated development of molecular models. Computer Physics Communications, 2010, 181, 499-513.	3.0	44
166	Assessment of numerical optimization algorithms for the development of molecular models. Computer Physics Communications, 2010, 181, 887-905.	3.0	26
167	Molecular dynamics and experimental study of conformation change of poly(N-isopropylacrylamide) hydrogels in water. Fluid Phase Equilibria, 2010, 296, 164-172.	1.4	98
168	Molecular model for carbon dioxide optimized to vapor-liquid equilibria. Journal of Chemical Physics, 2010, 132, 234512.	1.2	71
169	Molecular Modeling of Hydrogen Bonding Fluids: Vapor-Liquid Coexistence and Interfacial Properties. , 2010, , 471-483.		1
170	Contact Angle Dependence on the Fluidâ^'Wall Dispersive Energy. Langmuir, 2010, 26, 10913-10917.	1.6	25
171	Development of Models for Large Molecules and Electrolytes in Solution for Process Engineering. , 2010, , 165-176.		4
172	Molecular Dynamics Based Analysis of Nucleation and Surface Energy of Droplets in Supersaturated Vapors of Methane and Ethane. Journal of Heat Transfer, 2009, 131, .	1.2	11
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