Jadran Vrabec

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6198629/publications.pdf

Version: 2024-02-01

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	Vapour liquid equilibria of the Lennard-Jones fluid from theNpTplus test particle method. Molecular Physics, 1992, 76, 1319-1333.	0.8	420
2	A Set of Molecular Models for Symmetric Quadrupolar Fluids. Journal of Physical Chemistry B, 2001, 105, 12126-12133.	1.2	346
3	An equation-of-state contribution for polar components: Dipolar molecules. AICHE Journal, 2006, 52, 1194-1204.	1.8	321
4	Comprehensive study of the vapourâ€“liquid coexistence of the truncated and shifted Lennardâ€“Jones fluid including planar and spherical interface properties. Molecular Physics, 2006, 104, 1509-1527.	0.8	189
5	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
6	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
7	Equation of State for the Lennard-Jones Fluid. Journal of Physical and Chemical Reference Data, 2016, 45, .	1.9	133
8	Grand Equilibrium: vapour-liquid equilibria by a new molecular simulation method. Molecular Physics, 2002, 100, 3375-3383.	0.8	124
9	A molecular simulation study of shear and bulk viscosity and thermal conductivity of simple real fluids. Fluid Phase Equilibria, 2004, 221, 157-163.	1.4	108
10	ls1 mardyn: The Massively Parallel Molecular Dynamics Code for Large Systems. Journal of Chemical Theory and Computation, 2014, 10, 4455-4464.	2.3	108
11	Prediction of Transport Properties by Molecular Simulation: Methanol and Ethanol and Their Mixture. Journal of Physical Chemistry B, 2008, 112, 16664-16674.	1.2	106
12	An accurate Van der Waals-type equation of state for the Lennard-Jones fluid. International Journal of Thermophysics, 1996, 17, 391-404.	1.0	102
13	ms2: A molecular simulation tool for thermodynamic properties. Computer Physics Communications, 2011, 182, 2350-2367.	3.0	102
14	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. Journal of Chemical Information and Modeling, 2019, 59, 4248-4265.	2.5	101
15	Hydrogen Bonding of Methanol in Supercritical CO₂:â€‰ Comparison between ¹H NMR Spectroscopic Data and Molecular Simulation Results. Journal of Physical Chemistry B, 2007, 111, 9871-9878.	1.2	100
16	Unlike Lennardâ€“Jones parameters for vaporâ€“liquid equilibria. Journal of Molecular Liquids, 2007, 135, 170-178.	2.3	100
17	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
18	Henryâ€™s law constants of methane, nitrogen, oxygen and carbon dioxide in ethanol from 273 to 498â€‰K: Prediction from molecular simulation. Fluid Phase Equilibria, 2005, 233, 134-143.	1.4	91

#	Article	IF	Citations
19	Vaporâ^'Liquid Equilibria Simulation and an Equation of State Contribution for Dipoleâ^'Quadrupole Interactions. Journal of Physical Chemistry B, 2008, 112, 51-60.	1.2	91
20	Vaporâ€"liquid equilibria of mixtures containing nitrogen, oxygen, carbon dioxide, and ethane. AICHE Journal, 2003, 49, 2187-2198.	1.8	88
21	A set of molecular models for carbon monoxide and halogenated hydrocarbons. Journal of Chemical Physics, 2003, 119, 11396-11407.	1.2	88
22	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
23	Mutual diffusion in the ternary mixture of water + methanol + ethanol and its binary subsystems. Physical Chemistry Chemical Physics, 2013, 15, 3985.	1.3	76
24	A Benchmark Open-Source Implementation of COSMO-SAC. Journal of Chemical Theory and Computation, 2020, 16, 2635-2646.	2.3	74
25	Comprehensive study of the vapourâ€"liquid equilibria of the pure two-centre Lennardâ€"Jones plus pointquadrupole fluid. Fluid Phase Equilibria, 2001, 179, 339-362.	1.4	73
26	Modification of the classical nucleation theory based on molecular simulation data for surface tension, critical nucleus size, and nucleation rate. Physical Review E, 2008, 78, 011603.	0.8	73
27	Molecular model for carbon dioxide optimized to vapor-liquid equilibria. Journal of Chemical Physics, 2010, 132, 234512.	1.2	71
28	<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
29	<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
30	Vapour liquid equilibria of mixtures from theNpTplus test particle method. Molecular Physics, 1995, 85, 781-792.	0.8	66
31	MolMod â€" an open access database of force fields for molecular simulations of fluids. Molecular Simulation, 2019, 45, 806-814.	0.9	65
32	A set of molecular models for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2012, 136, 084501.	1.2	62
33	How well does the Lennard-Jones potential represent the thermodynamic properties of noble gases?. Molecular Physics, 2017, 115, 1104-1121.	0.8	59
34	On the application of force fields for predicting a wide variety of properties: Ethylene oxide as an example. Fluid Phase Equilibria, 2008, 274, 16-26.	1.4	56
35	Comprehensive Assessment of COSMO-SAC Models for Predictions of Fluid-Phase Equilibria. Industrial & Engineering Chemistry Research, 2017, 56, 9868-9884.	1.8	56
36	Molecular models for 267 binary mixtures validated by vaporâ€"liquid equilibria: A systematic approach. Fluid Phase Equilibria, 2009, 279, 120-135.	1.4	54

#	Article	IF	Citations
37	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
38	Equation of State for the Lennard-Jones Truncated and Shifted Model Fluid. International Journal of Thermophysics, 2015, 36, 25-43.	1.0	53
39	Self Diffusion and Binary Maxwellâ€“Stefan Diffusion in Simple Fluids with the Greenâ€“Kubo Method. International Journal of Thermophysics, 2004, 25, 175-186.	1.0	52
40	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
41	Set of Molecular Models Based on Quantum Mechanical Ab Initio Calculations and Thermodynamic Data. Journal of Physical Chemistry B, 2008, 112, 12710-12721.	1.2	51
42	Comprehensive study of the vapourâ€“liquid equilibria of the pure two-centre Lennardâ€–Jones plus pointdipole fluid. Fluid Phase Equilibria, 2003, 209, 29-53.	1.4	50
43	Chemical potential of quadrupolar two-centre Lennard-Jones fluids by gradual insertion. Chemical Physics Letters, 2002, 356, 431-436.	1.2	49
44	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
45	Prediction of Jouleâ€“Thomson inversion curves for pure fluids and one mixture by molecular simulation. Cryogenics, 2005, 45, 253-258.	0.9	47
46	Molecular models of unlike interactions in fluid mixtures. Molecular Simulation, 2005, 31, 215-221.	0.9	47
47	An optimised molecular model for ammonia. Molecular Physics, 2008, 106, 1039-1046.	0.8	47
48	Evaporation from a free liquid surface. International Journal of Heat and Mass Transfer, 2014, 73, 303-317.	2.5	47
49	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
50	Fundamental equation of state correlation for hexamethyldisiloxane based on experimental and molecular simulation data. Fluid Phase Equilibria, 2016, 418, 133-151.	1.4	46
51	GROW: A gradient-based optimization workflow for the automated development of molecular models. Computer Physics Communications, 2010, 181, 499-513.	3.0	44
52	Excess equimolar radius of liquid drops. Physical Review E, 2012, 85, 031605.	0.8	44
53	TweTriS: Twenty trillion-atom simulation. International Journal of High Performance Computing Applications, 2019, 33, 838-854.	2.4	43
54	Vaporâ€“liquid equilibria of the ternary mixture CH4+ C2H6+ CO2 from molecular simulation. AIChE Journal, 1997, 43, 212-217.	1.8	42

#	Article	IF	Citations
55	Phase equilibria of methane clathrate hydrates from Grand Canonical Monte Carlo simulations. Fluid Phase Equilibria, 2014, 369, 47-54.	1.4	41
56	Self-Diffusion and Binary Maxwellâ€“Stefan Diffusion Coefficients of Quadrupolar Real Fluids from Molecular Simulation. International Journal of Thermophysics, 2005, 26, 1389-1407.	1.0	40
57	Vapor-liquid equilibria of binary mixtures containing methane, ethane, and carbon dioxide from molecular simulation. International Journal of Thermophysics, 1996, 17, 889-908.	1.0	39
58	Jouleâ€“Thomson inversion curves of mixtures by molecular simulation in comparison to advanced equations of state: Natural gas as an example. Fluid Phase Equilibria, 2007, 258, 34-40.	1.4	37
59	Molecular dispersion energy parameters for alkali and halide ions in aqueous solution. Journal of Chemical Physics, 2014, 140, 044504.	1.2	36
60	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
61	591 TFLOPS Multi-trillion Particles Simulation on SuperMUC. Lecture Notes in Computer Science, 2013, , 1-12.	1.0	34
62	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
63	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
64	Vapour liquid equilibria of Lennard-Jones model mixtures from the NpT plus test particle method. Fluid Phase Equilibria, 1995, 112, 173-197.	1.4	32
65	Comparative study of the GrÃ¼neisen parameter for 28 pure fluids. Journal of Chemical Physics, 2016, 144, 244505.	1.2	32
66	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
67	Molecular Models for the Hydrogen Age: Hydrogen, Nitrogen, Oxygen, Argon, and Water. Journal of Chemical & Engineering Data, 2018, 63, 305-320.	1.0	32
68	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. Computer Physics Communications, 2021, 262, 107860.	3.0	31
69	Homogeneous nucleation in supersaturated vapors of methane, ethane, and carbon dioxide predicted by brute force molecular dynamics. Journal of Chemical Physics, 2008, 128, 164510.	1.2	30
70	Description of HFO-1234yf with BACKONE equation of state. Fluid Phase Equilibria, 2011, 305, 204-211.	1.4	30
71	Diffusion of methane in supercritical carbon dioxide across the Widom line. Scientific Reports, 2019, 9, 8466.	1.6	30
72	Thermal properties of the metastable supersaturated vapor of the Lennard-Jones fluid. Journal of Chemical Physics, 2005, 122, 144506.	1.2	29

#	Article	IF	Citations
73	A Set of Molecular Models for Alkaline-Earth Cations in Aqueous Solution. Journal of Physical Chemistry B, 2012, 116, 5448-5457.	1.2	29
74	Fundamental equation of state for ethylene oxide based on a hybrid dataset. Chemical Engineering Science, 2015, 121, 87-99.	1.9	29
75	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
76	Engineering Molecular Models: Efficient Parameterization Procedure and Cyclohexanol as Case Study. Soft Materials, 2012, 10, 3-25.	0.8	28
77	Orthobaric Densities from Simulations of the Liquid Vapour Interface. Molecular Simulation, 1990, 5, 233-243.	0.9	27
78	Long-range correction for multi-site Lennard-Jones models and planar interfaces. Molecular Physics, 2014, 112, 2227-2234.	0.8	27
79	Assessment of numerical optimization algorithms for the development of molecular models. Computer Physics Communications, 2010, 181, 887-905.	3.0	26
80	Communication: Fundamental equation of state correlation with hybrid data sets. Journal of Chemical Physics, 2013, 139, 041102.	1.2	26
81	Visual Verification and Analysis of Cluster Detection for Molecular Dynamics. IEEE Transactions on Visualization and Computer Graphics, 2007, 13, 1624-1631.	2.9	25
82	Molecular simulation study of hydrogen bonding mixtures and new molecular models for mono- and dimethylamine. Fluid Phase Equilibria, 2008, 263, 144-159.	1.4	25
83	Contact Angle Dependence on the Fluidâ^'Wall Dispersive Energy. Langmuir, 2010, 26, 10913-10917.	1.6	25
84	Lennard-Jones force field parameters for cyclic alkanes from cyclopropane to cyclohexane. Fluid Phase Equilibria, 2015, 404, 150-160.	1.4	25
85	Thermodynamic Properties of Octamethylcyclotetrasiloxane. Journal of Chemical & Engineering Data, 2016, 61, 2580-2595.	1.0	25
86	Molecular Insight into the Liquid Propan-2-ol + Water Mixture. Journal of Physical Chemistry B, 2018, 122, 8718-8729.	1.2	25
87	Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields. Topics in Current Chemistry, 2011, 307, 201-249.	4.0	24
88	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
89	Diffusion in Multicomponent Liquids: From Microscopic to Macroscopic Scales. Journal of Physical Chemistry B, 2016, 120, 12193-12210.	1.2	24
90	Evaporation sampled by stationary molecular dynamics simulation. Journal of Chemical Physics, 2019, 151, 044704.	1.2	24

#	Article	IF	Citations
91	An equation of state for dipolar two-center Lennardâ€“Jones molecules and its application to refrigerants. Fluid Phase Equilibria, 1998, 142, 15-32.	1.4	23
92	Shear viscosity and thermal conductivity of quadrupolar real fluids from molecular simulation. Molecular Simulation, 2005, 31, 787-793.	0.9	23
93	Software design for a highly parallel molecular dynamics simulation framework in chemical engineering. Journal of Computational Science, 2011, 2, 124-129.	1.5	23
94	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
95	Vaporâ€“liquid equilibrium measurements of the binary mixtures CO2+acetone and CO2+pentanones. Journal of Supercritical Fluids, 2015, 100, 160-166.	1.6	23
96	Diffusion Coefficients of a Highly Nonideal Ternary Liquid Mixture: Cyclohexaneâ€“Tolueneâ€“Methanol. Industrial & Engineering Chemistry Research, 2018, 57, 16508-16517.	1.8	23
97	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
98	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
99	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
100	Semantic Interoperability and Characterization of Data Provenance in Computational Molecular Engineering. Journal of Chemical & Engineering Data, 2020, 65, 1313-1329.	1.0	21
101	Molecular model for formic acid adjusted to vaporâ€“liquid equilibria. Chemical Physics Letters, 2007, 435, 268-272.	1.2	20
102	Prediction of ternary vaporâ€“liquid equilibria for 33 systems by molecular simulation. Fluid Phase Equilibria, 2009, 287, 62-69.	1.4	20
103	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
104	Do ternary liquid mixtures exhibit negative main Fick diffusion coefficients?. Physical Chemistry Chemical Physics, 2019, 21, 2140-2152.	1.3	20
105	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
106	Thermodynamic models for vaporâ€“liquid equilibria of nitrogen+oxygen+carbon dioxide at low temperatures. Cryogenics, 2009, 49, 72-79.	0.9	19
107	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
108	Kirkwood-Buff integration: A promising route to entropic properties?. Fluid Phase Equilibria, 2019, 485, 270-281.	1.4	18

#	Article	IF	Citations
109	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
110	Diffusion of the carbon dioxideâ€“ethanol mixture in the extended critical region. Physical Chemistry Chemical Physics, 2021, 23, 3106-3115.	1.3	18
111	Experimental study of two cascaded organic Rankine cycles with varying working fluids. Energy Conversion and Management, 2021, 230, 113818.	4.4	18
112	Vapor pressure of R227eaâ€‰+â€‰ethanol at 343.13â€‰K by molecular simulation. Fluid Phase Equilibria, 2007, 260, 177-182.	1.4	17
113	Grand canonical steady-state simulation of nucleation. Journal of Chemical Physics, 2009, 131, 184104.	1.2	17
114	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
115	Influence of unlike dispersion interactions in modeling methane clathrate hydrates. Fluid Phase Equilibria, 2014, 381, 108-115.	1.4	17
116	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
117	Thermodynamic Properties of Dodecamethylpentasiloxane, Tetradecamethylhexasiloxane, and Decamethylcyclopentasiloxane. Industrial & Engineering Chemistry Research, 2019, 58, 9617-9635.	1.8	17
118	Droplet coalescence by molecular dynamics and phase-field modeling. Physics of Fluids, 2022, 34, .	1.6	17
119	Shear viscosity and thermal conductivity of dipolar real fluids from equilibrium molecular dynamics simulation. Cryogenics, 2006, 46, 711-717.	0.9	16
120	Comment on â€œAn optimized potential for carbon dioxideâ€•[J. Chem. Phys. 122, 214507 (2005)]. Journal of Chemical Physics, 2008, 129, 087101.	1.2	16
121	Henryâ€™s Law Constant from Molecular Simulation: A Systematic Study of 95 Systems. International Journal of Thermophysics, 2009, 30, 1791-1810.	1.0	16
122	Molecular simulation study on the solubility of carbon dioxide in mixtures of cyclohexane+cyclohexanone. Fluid Phase Equilibria, 2012, 315, 77-83.	1.4	16
123	Fick Diffusion Coefficient Matrix of a Quaternary Liquid Mixture by Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 4527-4535.	1.2	16
124	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
125	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
126	Experimental setup of a cascaded two-stage organic Rankine cycle. Applied Thermal Engineering, 2018, 131, 958-964.	3.0	15

#	Article	IF	Citations
127	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
128	Flexible or rigid molecular models? A study on vapourâ€“liquid equilibrium properties of ammonia. Molecular Physics, 2011, 109, 619-624.	0.8	14
129	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
130	Liquid state isomorphism, Rosenfeld-Tarazona temperature scaling, and Riemannian thermodynamic geometry. Physical Review E, 2018, 97, 052149.	0.8	14
131	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
132	Digitalization in Thermodynamics. Chemie-Ingenieur-Technik, 2019, 91, 201-214.	0.4	14
133	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
134	Evaporation driven by conductive heat transport. Molecular Physics, 2021, 119, .	0.8	14
135	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
136	Equation of state for 1,2-dichloroethane based on a hybrid data set. Molecular Physics, 2017, 115, 1166-1185.	0.8	13
137	Thermodynamic factor of quaternary mixtures from Kirkwoodâ€“Buff integration. Molecular Physics, 2020, 118, .	0.8	13
138	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
139	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
140	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
141	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
142	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
143	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
144	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

#	Article	IF	Citations
145	Empirical Fundamental Equation of State for Phosgene Based on Molecular Simulation Data. Journal of Chemical & Engineering Data, 2015, 60, 2895-2905.	1.0	11
146	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
147	Interplay of structure and diffusion in ternary liquid mixtures of benzene + acetone + varying alcohols. Journal of Chemical Physics, 2018, 149, 064504.	1.2	11
148	Diffusion limited evaporation of a binary liquid film. International Journal of Heat and Mass Transfer, 2019, 132, 1296-1305.	2.5	11
149	Thermodynamic Speed of Sound Data for Liquid and Supercritical Alcohols. Journal of Chemical & Engineering Data, 2019, 64, 1035-1044.	1.0	11
150	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
151	Liquidâ€“liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics. Fluid Phase Equilibria, 2011, 310, 25-31.	1.4	10
152	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
153	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
154	Bulk viscosity of liquid noble gases. Journal of Chemical Physics, 2020, 152, 094503.	1.2	10
155	Investigating the real life energy consumption of refrigeration appliances in Germany: Are present policies sufficient?. Energy Policy, 2021, 155, 112275.	4.2	10
156	Recent vapour pressure equations for the Lennard-Jones fluid based on molecular simulations. Fluid Phase Equilibria, 1993, 89, 383-385.	1.4	9
157	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
158	Thermodynamic correlation of molecular simulation data. Molecular Physics, 2015, 113, 910-931.	0.8	9
159	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
160	Structure and dynamics of the Lennard-Jones fcc-solid focusing on melting precursors. Journal of Chemical Physics, 2020, 153, 104506.	1.2	9
161	The air pressure effect on the homogeneous nucleation of carbon dioxide by molecular simulation. Atmospheric Research, 2011, 101, 519-526.	1.8	8
162	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

#	Article	IF	Citations
163	Steady-state molecular dynamics simulation of vapour to liquid nucleation with McDonald's dÃ¦mon. Journal of Physical Studies, 2009, 13, .	0.2	8
164	Molekulare Modellierung und Simulation fÃ¼r das Prozessdesign. Chemie-Ingenieur-Technik, 2008, 80, 25-33.	0.4	7
165	Automatized determination of fundamental equations of state based on molecular simulations in the cloud. Fluid Phase Equilibria, 2016, 425, 84-92.	1.4	7
166	SkaSim â€“ Scalable HPC Software for Molecular Simulation in the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 295-306.	0.4	7
167	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
168	Assessment of thermodynamic models via Jouleâ€“Thomson inversion. Fluid Phase Equilibria, 2022, 556, 113401.	1.4	7
169	On the Treatment of Electrostatic Interactions of Non-spherical Molecules in Equation of State Models. Soft Materials, 2012, 10, 81-105.	0.8	6
170	On the application of binary correction factors in lattice distortion calculations for methane clathrate hydrates. Philosophical Magazine, 2014, 94, 974-990.	0.7	6
171	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
172	AutoPas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. Journal of Computational Science, 2021, 50, 101296.	1.5	6
173	Impact of aging on the energy efficiency of household refrigerating appliances. Applied Thermal Engineering, 2022, 205, 117992.	3.0	6
174	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
175	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
176	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
177	Thermodynamic speed of sound of xenon. Journal of Chemical Thermodynamics, 2020, 141, 105933.	1.0	5
178	Density and Thermodynamic Speed of Sound of Liquid Vinyl Chloride. Journal of Chemical & Engineering Data, 2020, 65, 2495-2504.	1.0	5
179	Computational Molecular Engineering as an Emerging Technology in Process Engineering. IT - Information Technology, 2013, 55, 97-101.	0.6	5
180	Transport properties of anisotropic polar fluids. Fluid Phase Equilibria, 2006, 249, 131-139.	1.4	4

#	Article	IF	Citations
181	Transport properties of anisotropic polar fluids. Fluid Phase Equilibria, 2006, 249, 120-130.	1.4	4
182	Molecular simulation of the vaporâ€“liquid phase behavior of cyanides and their binary mixtures. Fluid Phase Equilibria, 2013, 354, 286-297.	1.4	4
183	Diffusion in multicomponent aqueous alcoholic mixtures. Scientific Reports, 2021, 11, 12319.	1.6	4
184	Molecular Simulation of Fluids with Short Range Potentials. , 2006, , 187-195.		4
185	Development of Models for Large Molecules and Electrolytes in Solution for Process Engineering. , 2010, , 165-176.		4
186	Thermodynamic Properties of Methyl Diethanolamine. International Journal of Thermophysics, 2022, 43, 1.	1.0	4
187	Erratum to â€œHenry's law constants of methane, nitrogen, oxygen and carbon dioxide in ethanol from 273 to 498 K: Prediction from molecular simulationâ€•[Fluid Phase Equilib. 233 (2005) 134â€“143]. Fluid Phase Equilibria, 2005, 236, 272.	1.4	3
188	Thermophysical Properties of Dry and Humid Air by Molecular Simulation Including Dew Point Calculations with the Mollier Ensemble. Industrial & Engineering Chemistry Research, 2009, 48, 10110-10119.	1.8	3
189	Communication: Molecular simulation study of kaolinite intercalation with realistic layer size. Journal of Chemical Physics, 2014, 141, 091102.	1.2	3
190	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
191	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
192	Molecular simulation study of the curling behavior of the finite free-standing kaolinte layer. Computational Materials Science, 2021, 186, 110037.	1.4	3
193	Determining the heat flow through the cabinet walls of household refrigerating appliances. International Journal of Refrigeration, 2021, 121, 235-242.	1.8	3
194	Molecular Models for Cyclic Alkanes and Ethyl Acetate As Well As Surface Tension Data from Molecular Simulation. , 2015, , 645-659.		3
195	Atomistic Simulations of Electrolyte Solutions and Hydrogels with Explicit Solvent Models. , 2012, , 185-199.		3
196	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
197	Connecting entropy scaling and density scaling. Journal of Chemical Physics, 2022, 157, .	1.2	3
198	ms2: A Molecular Simulation Tool for Thermodynamic Properties. Chemie-Ingenieur-Technik, 2012, 84, 114-120.	0.4	2

#	Article	IF	Citations
199	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
200	Measurement procedure for acoustic absorption and bulk viscosity of liquids. Measurement: Journal of the International Measurement Confederation, 2021, 184, 109919.	2.5	2
201	Understanding the Scalability of Molecular Simulation Using Empirical Performance Modeling. Lecture Notes in Computer Science, 2019, , 125-143.	1.0	2
202	Surface Tension, Large Scale Thermodynamic Data Generation and Vapor-Liquid Equilibria of Real Compounds. , 2013, , 635-646.		2
203	Molecular Modelling and Simulation of Electrolyte Solutions, Biomolecules, and Wetting of Component Surfaces. , 2013, , 647-661.		2
204	Molecular Simulation Study of Transport Properties for 20 Binary Liquid Mixtures and New Force Fields for Benzene, Toluene and CCl4. , 2016, , 613-634.		2
205	Vaporâ€“Liquidâ€“Liquid Equilibria of Nitrogen + Ethane by Molecular Simulation. Industrial & Engineering Chemistry Research, 2022, 61, 3104-3112.	1.8	2
206	How well does the Tang-Toennies potential represent the thermodynamic properties of argon?. Molecular Physics, 2022, 120, .	0.8	2
207	Berechnung von Dampf/FlÃ¼ssigkeits-Phasengleichgewichten mittels molekularer Simulationen. Chemie-Ingenieur-Technik, 1997, 69, 1126-1129.	0.4	1
208	Molecular Modeling of Hydrogen Bonding Fluids: Vapor-Liquid Coexistence and Interfacial Properties. , 2010, , 471-483.		1
209	Dynamic simulation of particle-filled hollow spheres. Proceedings in Applied Mathematics and Mechanics, 2011, 11, 881-882.	0.2	1
210	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
211	Molecular Modeling and Simulation: Force Field Development, Evaporation Processes and Thermophysical Properties of Mixtures. , 2019, , 457-474.		1
212	Special Issue Honoring Hans Hasse. Journal of Chemical & Engineering Data, 2020, 65, 941-942.	1.0	1
213	PetaFLOP Molecular Dynamics for Engineering Applications. , 2019, , 397-407.		1
214	Molecular Modeling and Simulation of Thermophysical Properties: Application to Pure Substances and Mixtures. , 2009, , 119-133.		1
215	Molecular Modeling of Hydrogen Bonding Fluids: New Cyclohexanol Model and Transport Properties of Short Monohydric Alcohols. , 2009, , 529-541.		1
216	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

#	Article	IF	Citations
217	56. Berechnung von Dampf/FlÃ¼ssigkeits-Phasengleichgewichten mittels molekularer Simulationen. Chemie-Ingenieur-Technik, 1996, 68, 1101-1102.	0.4	0
218	Anwendung molekularer Methoden zur Vorhersage thermophysikalischer Stoffdaten am Beispiel Ethylenoxid. Chemie-Ingenieur-Technik, 2008, 80, 1297-1298.	0.4	0
219	Transportkoeffizienten von Alkoholen und Wasser: Molekulare Simulation und Messungen mit der Taylorâ€Dispersions Methode. Chemie-Ingenieur-Technik, 2009, 81, 1069-1069.	0.4	0
220	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
221	Empirical Fundamental Equations of State Correlations Based on Hybrid Datasets. Chemie-Ingenieur-Technik, 2015, 87, 1091-1091.	0.4	0
222	Insight into the Nature of Evaporation Processes Enabled by Massively Parallel Molecular Dynamics Simulations. , 2016, , .		0
223	Molecular Dynamics Simulation of Nucleation in CO₂. Chemie-Ingenieur-Technik, 2016, 88, 1286-1286.	0.4	0
224	Empirische Fundamentalgleichungen auf der Basis von molekularen Simulationen - Ein Ãœberblick. Chemie-Ingenieur-Technik, 2016, 88, 1285-1285.	0.4	0
225	Special Issue of Molecular Physics in Honour of Professor Johann Fischer. Molecular Physics, 2017, 115, 1015-1016.	0.8	0
226	Atomistic Simulations: The Driving Force Behind Modern Thermodynamic Research. , 2021, , 569-581.		0
227	Long range corrections for inhomogeneous fluids containing a droplet or a bubble. Molecular Simulation, 2022, 48, 73-86.	0.9	0
228	Molecular Modeling of Hydrogen Bonding Fluids: Transport Properties and Vapor-Liquid Coexistence. , 2011, , 543-551.		0
229	Molecular Modeling of Hydrogen Bonding Fluids: Phase Behavior of Industrial Fluids. , 2012, , 567-579.		0
230	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
231	10.1063/1.5111759.1. , 2019, , .		0
232	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