Ulrich K Deiters

List of Publications by Year
in descending order

123	2,733	159358	223531
papers	citations	30 h-index	46 g-index

129	129	129	1186
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Systematic investigation of the phase behavior in binary fluid mixtures. I. Calculations based on the Redlichâ€“Kwong equation of state. Journal of Chemical Physics, 1989, 90, 6632-6641.	1.2	149
2	A new semiempirical equation of state for fluidsâ€”I. Chemical Engineering Science, 1981, 36, 1139-1146.	1.9	98
3	Generalization of the Friction Theory for Viscosity Modeling. Journal of Physical Chemistry B, 2006, 110, 12820-12834.	1.2	96
4	Application of the Taylor dispersion method in supercritical fluids. International Journal of Thermophysics, 1993, 14, 893-922.	1.0	95
5	Excess enthalpies for (ethanol + water) at 298.15 K and pressures of 0.4, 5, 10, and 15 MPa. Journal of Chemical Thermodynamics, 1986, 18, 1-12.	1.0	92
6	Systematic investigation of the phase behavior in binary fluid mixtures. II. Calculations based on the Carnahanâ€“Starlingâ€“Redlichâ€“Kwong equation of state. Journal of Chemical Physics, 1992, 96, 539-547.	1.2	91
7	Prediction of the thermophysical properties of pure neon, pure argon, and the binary mixtures neon-argon and argon-krypton by Monte Carlo simulation usingab initiopotentials. Journal of Chemical Physics, 2004, 121, 6423-6434.	1.2	82
8	Novel classification of pure working fluids for Organic Rankine Cycle. Energy, 2018, 145, 288-300.	4.5	79
9	Evidence for Pericyclic and Stepwise Processes in the Cyclodimerization of Chloroprene and 1,3-Butadiene from Pressure Dependence and Stereochemistry. Experimental and Theoretical Volumes of Activation and Reaction. Journal of the American Chemical Society, 1994, 116, 7646-7657.	6.6	74
10	Closed-loop critical curves in simple hard-sphere van der Waals-fluid models consistent with the packing fraction limit. Journal of Chemical Physics, 1999, 110, 3079-3084.	1.2	60
11	High pressure phase equilibria: experimental methods. Fluid Phase Equilibria, 1986, 29, 145-160.	1.4	59
12	Magnetic particle nanorheology. Colloid and Polymer Science, 2014, 292, 2013-2023.	1.0	59
13	Guidelines for publication of equations of state I. Pure fluids (Technical Report). Pure and Applied Chemistry, 1997, 69, 1237-1250.	0.9	58
14	The pseudocritical regions for supercritical water. Nuclear Engineering and Design, 2012, 252, 179-183.	0.8	49
15	A new semiempirical equation of state for fluidsâ€”II. Chemical Engineering Science, 1981, 36, 1147-1151.	1.9	46
16	Prediction of thermodynamic properties of krypton by Monte Carlo simulation using ab initio interaction potentials. Journal of Chemical Physics, 2003, 119, 947-952.	1.2	44
17	Integrals over pair- and triplet-correlation functions for the Lennard-Jones (12â€“6)-fluid. Molecular Physics, 1986, 57, 241-253.	0.8	42
18	A new semiempirical equation of state for fluidsâ€”III Application to phase equilibria in binary mixtures. Chemical Engineering Science, 1982, 37, 855-861.	1.9	41

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19	Calculation of densities from cubic equations of state. AICHE Journal, 2002, 48, 882-886.	1.8	40
20	Density-dependent mixing rules for the calculation of fluid phased equilibria at high pressures. Fluid Phase Equilibria, 1987, 33, 267-293.	1.4	39
21	Soft Repulsion and the Behavior of Equations of State at High Pressures. International Journal of Thermophysics, 2010, 31, 227-252.	1.0	39
22	Guidelines for publication of equations of state. Fluid Phase Equilibria, 1999, 161, 205-219.	1.4	37
23	Two-body interatomic potentials for He, Ne, Ar, Kr, and Xe from ab initio data. Journal of Chemical Physics, 2019, 150, 134504.	1.2	36
24	High pressure molecular dynamics of the partially miscible fluid mixture neon/krypton. Molecular Physics, 1979, 37, 95-109.	0.8	35
25	A classification of phase diagrams of ternary fluid systems. Physical Chemistry Chemical Physics, 1999, 1, 4307-4313.	1.3	35
26	Correlation for the Viscosity of Sulfur Hexafluoride (SF6) from the Triple Point to 1000 K and Pressures to 50 MPa. Journal of Physical and Chemical Reference Data, 2012, 41, 023102-023102-11.	1.9	34
27	The extension of pure fluid thermodynamic properties to supercritical mixtures. Molecular Physics, 1983, 49, 159-170.	0.8	33
28	Global phase behavior based on the simplifiedâ€perturbed hardâ€chain equation of state. Journal of Chemical Physics, 1995, 102, 3361-3375.	1.2	33
29	Application of an EOS chain association theory to the calculation of thermodynamic properties of (alkane + 1-alkanol) mixtures. Fluid Phase Equilibria, 1993, 89, 229-242.	1.4	31
30	Monte Carlo simulations of nitrogen using anab initiopotential. Molecular Physics, 2002, 100, 2571-2585.	0.8	31
31	The equation of state for molecules with shifted Lennard-Jones pair potentials. Fluid Phase Equilibria, 1995, 103, 199-212.	1.4	28
32	On the construction of binary mixture pâ€x and Tâ€x diagrams from isochoric thermodynamics. AICHE Journal, 2018, 64, 2745-2757.	1.8	26
33	Thermodynamic Testing of Equations of State of Dense Simple Liquids. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 1179-1186.	0.9	24
34	A Modular Program System for the Calculation of Thermodynamic Properties of Fluids. Chemical Engineering and Technology, 2000, 23, 581-584.	0.9	24
35	Hydrophobic Interactions by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2006, 220, 349-369.	1.4	24
36	Coordination numbers for rigid spheres of different sizeâ€”estimating the number of next-neighbour interactions in a mixture. Fluid Phase Equilibria, 1982, 8, 123-129.	1.4	23

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37	Calculation and prediction of fluid phase equilibria from an equation of state. Fluid Phase Equilibria, 1983, 10, 173-182.	1.4	23
38	Hydrophobic Interactions of Xenon by Monte Carlo Simulations. Zeitschrift Fur Physikalische Chemie, 2007, 221, 785-799.	1.4	21
39	Computer Simulation of the Characteristic Curves of Pure Fluids. Journal of Chemical & Engineering Data, 2016, 61, 2720-2728.	1.0	21
40	Density-dependent mixing rules for the calculation of fluid phase equilibria at high pressures. Fluid Phase Equilibria, 1987, 34, 309-310.	1.4	20
41	Characteristic Curves of the Lennard-Jones Fluid. International Journal of Thermophysics, 2020, 41, 147.	1.0	20
42	Calculation of equilibria between fluid and solid phases in binary mixtures at high pressures from equations of state. Fluid Phase Equilibria, 1985, 20, 275-282.	1.4	19
43	Guidelines for publication of equations of stateâ€”I. Pure fluids. Chemical Engineering Journal, 1998, 69, 69-81.	6.6	19
44	Calculation of Densities from Cubic Equations of State: Revisited. Industrial & Engineering Chemistry Research, 2014, 53, 2529-2536.	1.8	19
45	An efficient algorithm for the calculation of phase envelopes of fluid mixtures. Fluid Phase Equilibria, 2012, 329, 22-31.	1.4	18
46	Fully a priori prediction of the vapor-liquid equilibria of Ar, Kr, and Xe from ab initio two-body plus three-body interatomic potentials. Journal of Chemical Physics, 2019, 151, 034509.	1.2	18
47	Monte Carlo simulations of neon and argon using ab initio potentials. Molecular Physics, 2000, 98, 1603-1616.	0.8	18
48	Implementing an Equation of State without Derivatives: teqp. Industrial & Engineering Chemistry Research, 2022, 61, 6010-6027.	1.8	18
49	Monte Carlo study of the thermodynamic properties and the static dielectric constant of liquid trifluoromethane. Fluid Phase Equilibria, 1998, 149, 41-56.	1.4	17
50	A new generalized corresponding-states equation of state for the extension of the Leeâ€“Kesler equation to fluids consisting of polar and larger nonpolar molecules. Chemical Engineering Science, 2008, 63, 1490-1496.	1.9	17
51	Calculation of intermolecular potentials for H 2 H 2 and H 2 O 2 dimers ab initio and prediction of second virial coefficients. Chemical Physics, 2015, 457, 171-179.	0.9	16
52	A modification of Newton-Raphson algorithm for phase equilibria calculations using numerical differentiation of the gibbs energy. Fluid Phase Equilibria, 1985, 19, 287-293.	1.4	15
53	Extended 1-fluid theory for mixtures containing non-spherical molecules. Fluid Phase Equilibria, 1989, 48, 185-195.	1.4	15
54	Fast Coding of the Minimum Image Convention. Molecular Simulation, 1998, 20, 239-244.	0.9	15

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55	Estimation of the Thermodynamic Limit of Overheating for Bulk Water from Interfacial Properties. International Journal of Thermophysics, 2013, 34, 2053-2064.	1.0	15
56	Differential equations for the calculation of isopleths of multicomponent fluid mixtures. Fluid Phase Equilibria, 2017, 447, 72-83.	1.4	15
57	Unphysical Critical Curves of Binary Mixtures Predicted with GERG Models. International Journal of Thermophysics, 2020, 41, 1.	1.0	15
58	The evolution of multicomponent systems at high pressures. Part IV. The genesis of optical activity in high-density, abiotic fluids. Physical Chemistry Chemical Physics, 2000, 2, 3163-3174.	1.3	14
59	Modeling of the N2O4â€“NO2 reacting system. Physical Chemistry Chemical Physics, 2000, 2, 5606-5613.	1.3	14
60	A combined determination of phase diagrams of asymmetric binary mixtures by equations of state and transitiometry. Fluid Phase Equilibria, 2007, 260, 87-97.	1.4	14
61	Non-Newtonian Viscosity Modeling of Crude Oilsâ€”Comparison Among Models. International Journal of Thermophysics, 2009, 30, 1089-1105.	1.0	14
62	Calculation of Critical Curves of Fluid Mixtures through Solution of Differential Equations. Industrial & Engineering Chemistry Research, 2020, 59, 19062-19076.	1.8	14
63	Ab Initio Interatomic Potentials and the Classical Molecular Simulation Prediction of the Thermophysical Properties of Helium. Journal of Physical Chemistry B, 2020, 124, 2268-2276.	1.2	14
64	Interatomic Interactions Responsible for the Solidâ€“Liquid and Vaporâ€“Liquid Phase Equilibria of Neon. Journal of Physical Chemistry B, 2021, 125, 8522-8531.	1.2	14
65	An equation of state for pure fluids describing the critical region. International Journal of Thermophysics, 1994, 15, 261-281.	1.0	13
66	Friction Theory Modeling of the Non-Newtonian Viscosity of Crude Oils. Energy & Fuels, 2008, 22, 799-804.	2.5	13
67	Adiabatic Processes in the Liquidâ€“Vapor Two-Phase Region. 1. Pure Fluids. Industrial & Engineering Chemistry Research, 2014, 53, 13529-13542.	1.8	13
68	Special aspects of the calculation of phase equilibria in cryogenic mixtures at very high pressures. Fluid Phase Equilibria, 1983, 13, 109-120.	1.4	12
69	Calculation of phase envelopes of fluid mixtures through parametric marching. AICHE Journal, 2019, 65, e16730.	1.8	12
70	Liquidâ€“vapour equilibrium in the krypton + methane system. Journal of the Chemical Society Faraday Transactions I, 1981, 77, 2503.	1.0	11
71	Liquid mixtures involving cyclic molecules: (vapour + liquid) equilibria of (xenon + ethylene oxide). Journal of Chemical Thermodynamics, 1996, 28, 201-207.	1.0	11
72	The isothermal vanâ€™t Hoff equation for phase equilibriaâ€”A forgotten relation?. Fluid Phase Equilibria, 2012, 336, 22-27.	1.4	11

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73	Comments on the modeling of hydrogen and hydrogen-containing mixtures with cubic equations of state. Fluid Phase Equilibria, 2013, 352, 93-96.	1.4	11
74	Differential equations for the calculation of fluid phase equilibria. Fluid Phase Equilibria, 2016, 428, 164-173.	1.4	11
75	Estimation of the entropy of fluids with Monte Carlo computer simulation. Molecular Physics, 2017, 115, 1074-1085.	0.8	11
76	First-principles determination of the solid-liquid-vapor triple point: The noble gases. Physical Review E, 2022, 105, .	0.8	11
77	PVT measurements of hydrogen/methane mixtures at high pressures. Journal of Chemical & Engineering Data, 1988, 33, 148-152.	1.0	10
78	Prediction of the Thermodynamic Properties of Hydrogenâ€Oxygen Mixtures from 80 to 373 K and to 100 MPa. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1993, 97, 649-657.	0.9	10
79	Efficient Coding of the Minimum Image Convention. Zeitschrift Fur Physikalische Chemie, 2013, 227, 345-352.	1.4	10
80	Structure and Contact Angle in Sessile Droplets of Binary Mixtures of Lennard-Jones Chains: A Molecular Dynamics Study. Langmuir, 2021, 37, 10945-10957.	1.6	10
81	Algorithm to Identify Vaporâ€“Liquidâ€“Liquid Equilibria of Binary Mixtures from Vaporâ€“Liquid Equilibria. Industrial & Engineering Chemistry Research, 2022, 61, 2592-2599.	1.8	10
82	â€œCoordination numbers for rigid spheres of different sizesâ€”estimating the number of next-neighbour interactions in a mixtureâ€•by G.H. Eduljee. Fluid Phase Equilibria, 1983, 12, 193-197.	1.4	9
83	Calculation of Fluid-Fluid and Solid-Fluid Equilibria in Cryogenic Mixtures at High Pressures. ACS Symposium Series, 1986, , 371-388.	0.5	9
84	Some comments on the double retrograde vaporization. Journal of Chemical Thermodynamics, 2003, 35, 583-589.	1.0	9
85	New Model for the Correlation of the Surface Tension Based on Friction Theory. Journal of Physical Chemistry B, 2009, 113, 3504-3511.	1.2	9
86	Calculation of second virial coefficients using ab initio intermolecular pair potentials for F2-F2 and H2-F2 dimers. Chemical Physics, 2017, 485-486, 67-80.	0.9	9
87	Theoretical methods for the prediction of phase equilibria in hydrogen-containing mixtures. Chemical Engineering Science, 1985, 40, 1831-1841.	1.9	8
88	Some remarks on the nomenclature of refrigerants. Fluid Phase Equilibria, 1997, 132, 265-270.	1.4	8
89	Monte Carlo simulations of acetonitrile with an anisotropic polarizable molecular model. Molecular Physics, 1997, 90, 593-598.	0.8	7
90	Shape effects on the thermodynamic properties of dense fluid mixtures of enantiomers. Fluid Phase Equilibria, 2001, 182, 17-26.	1.4	7

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91	Calculating Thermodynamic Properties of an Ionic Liquid with Monte Carlo Simulations with an Orthorhombic and a Cubic Simulation Box. Journal of Physical Chemistry B, 2010, 114, 8954-8960.	1.2	7
92	Adiabatic Processes in the Vaporâ€“Liquid Two-Phase Region. 2. Binary Mixtures. Industrial & Engineering Chemistry Research, 2015, 54, 6559-6568.	1.8	7
93	Chemical potentials and phase equilibria of Lennard-Jones chain fluids. Molecular Physics, 2015, 113, 28-35.	0.8	7
94	Superancillary Equations for Cubic Equations of State. Industrial & Engineering Chemistry Research, 2021, 60, 9983-9991.	1.8	7
95	The equation of state of soft repulsive spherical molecules. Molecular Physics, 1991, 74, 153-160.	0.8	6
96	The limiting behaviour of the simplified-perturbed-hard-chain theory at high temperatures. Fluid Phase Equilibria, 1993, 90, 45-56.	1.4	6
97	Liquid mixtures involving triangular molecules: (vapour + liquid) equilibria of (xenon +) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 5	1.0	6
98	Correlation of binary diffusion coefficients of organic substances in supercritical carbon dioxide based on equations of state. Journal of Supercritical Fluids, 2007, 42, 212-218.	1.6	6
99	The influence of the simulation box geometry in solid-state molecular simulations: phase behaviour of lithium iodide in a dynamic Monte Carlo simulation. Molecular Simulation, 2010, 36, 364-372.	0.9	5
100	The Characteristic Curves of Water. International Journal of Thermophysics, 2016, 37, 1.	1.0	5
101	Determination of the Residual Entropy of Simple Mixtures by Monte Carlo Simulation. Langmuir, 2017, 33, 11603-11610.	1.6	5
102	Interfacial properties of binary mixtures of Lennard-Jones chains in planar interfaces by molecular dynamics simulation. Journal of Chemical Physics, 2021, 154, 084704.	1.2	4
103	Precise Numerical Differentiation of Thermodynamic Functions with Multicomplex Variables. Journal of Research of the National Institute of Standards and Technology, 2021, 126, .	0.4	4
104	Minimum Image Convention Coding of Microcomputers. Molecular Simulation, 1989, 3, 343-344.	0.9	3
105	Calculation of the apparent heat capacity in scanning calorimetry experiments on fluid phase equilibria. Journal of Supercritical Fluids, 2012, 66, 66-72.	1.6	3
106	Calculation of cross second virial coefficients using ab initio intermolecular potential energy surfaces for dimer H2-N2. Chemical Physics, 2019, 517, 208-221.	0.9	3
107	On the VDW1 mixing rules applied to conformal binary mixtures at infinite dilution. Molecular Physics, 1992, 77, 1071-1083.	0.8	2
108	The free volume as a unified basis for comparison of pressure- and composition programming in Supercritical Fluid Chromatography (SFC). Fresenius' Journal of Analytical Chemistry, 1992, 344, 463-466.	1.5	2

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109	Application of a generalized van der Waals equation of state to several nonpolar mixtures. Fluid Phase Equilibria, 1996, 118, 153-174.	1.4	2
110	Non-ideality of the system NH3â€“H2â€“N2. Comparison of equation of state and simulation predictions with experimental data. Physical Chemistry Chemical Physics, 1999, 1, 4069-4074.	1.3	2
111	Title is missing!. International Journal of Thermophysics, 2001, 22, 1869-1870.	1.0	2
112	The pressure-dependence of the dimerization of 1,3-butadiene: Experimental and theoretical volumes of activation and reaction. High Pressure Research, 1994, 13, 1-5.	0.4	1
113	Gerhard M. Schneider â€“ celebrating his 70th birthday. Journal of Chemical Thermodynamics, 2003, 35, 569-572.	1.0	1
114	Comments on a publication by J. GarcÄ±Ìa-GonzÃ¡lez, M.J. Molina, F. Rodriguez, F. Mirada, â€œSolubilities of hydroquinone and p-quinone in supercritical carbon dioxideâ€•[Fluid Phase Equilib. 200 (2002) 31â€“39]. Fluid Phase Equilibria, 2003, 207, 319-321.	1.4	1
115	Stability and Equilibrium. Supercritical Fluid Science and Technology, 2012, 2, 99-155.	0.5	1
116	Comments on the Heidaryanâ€“Jarrahian variant of the Redlichâ€“Kwong equation of state. Journal of Supercritical Fluids, 2016, 117, 13-17.	1.6	1
117	Thermodynamic Properties of Vapor-Liquid Equilibria from Monte-Carlo Simulation using ab initio Intermolecular Potentials of Systems H₂-H₂ and F₂-F₂. Zeitschrift Fur Physikalische Chemie, 2019, 233, 493-525.	1.4	1
118	Application of a generalized van der Waals equation of state to several nonpolar mixtures at high pressures. Process Technol, 1996, , 405-410.	0.1	0
119	Calculation of high-pressure phase equilibria involving light gases. Process Technol, 1996, 12, 451-456.	0.1	0
120	Preface to the Gerhard M. Schneider Festschrift. Journal of Chemical & Engineering Data, 2009, 54, 1415-1416.	1.0	0
121	Modelling Supercritical Phase Equilibria: Problems and Pitfalls. Periodica Polytechnica: Chemical Engineering, 2019, 63, 261-269.	0.5	0
122	Professor Dr. rer. nat. Gerhard Manfred Schneider (May 7, 1932 â€“ October 16, 2020). Journal of Supercritical Fluids, 2021, 174, 105219.	1.6	0
123	Preface. Prof. Dr. Andreas Heintz. Zeitschrift Fur Physikalische Chemie, 2013, 227, 153-156.	1.4	0