Christoph Held

List of Publications by Year
in descending order

113	4,070	101543	133252
papers	citations	36 h-index	59 g-index

114	114	114	2937
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tunable Hydrophobic Eutectic Solvents Based on Terpenes and Monocarboxylic Acids. ACS Sustainable Chemistry and Engineering, 2018, 6, 8836-8846.	6.7	207
2	Modeling aqueous electrolyte solutions. Fluid Phase Equilibria, 2008, 270, 87-96.	2.5	173
3	ePC-SAFT revised. Chemical Engineering Research and Design, 2014, 92, 2884-2897.	5.6	158
4	Measuring and Modeling Activity Coefficients in Aqueous Amino-Acid Solutions. Industrial & Engineering Chemistry Research, 2011, 50, 131-141.	3.7	129
5	Modeling imidazolium-based ionic liquids with ePC-SAFT. Fluid Phase Equilibria, 2012, 335, 64-73.	2.5	128
6	Cryptic speciation in the giant Antarctic isopod <i>Glyptonotus antarcticus</i> (Isopoda,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	6.6	121
7	PC-SAFT Modeling of CO₂ Solubilities in Deep Eutectic Solvents. Journal of Physical Chemistry B, 2016, 120, 2300-2310.	2.6	110
8	Measuring and modeling aqueous electrolyte/amino-acid solutions with ePC-SAFT. Journal of Chemical Thermodynamics, 2014, 68, 1-12.	2.0	97
9	Separation Performance of BioRenewable Deep Eutectic Solvents. Industrial & Engineering Chemistry Research, 2015, 54, 3498-3504.	3.7	97
10	Modeling aqueous electrolyte solutions. Part 2. Weak electrolytes. Fluid Phase Equilibria, 2009, 279, 141-148.	2.5	90
11	Compatible solutes: Thermodynamic properties and biological impact of ectoines and prolines. Biophysical Chemistry, 2010, 152, 28-39.	2.8	90
12	Liquidâ€“Liquid Equilibria of 1-Butanol/Water/IL Systems. Industrial & Engineering Chemistry Research, 2013, 52, 18472-18481.	3.7	90
13	Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids. Fluid Phase Equilibria, 2017, 448, 69-80.	2.5	88
14	Vaporâ€“Liquid Equilibria of Water + Alkylimidazolium-Based Ionic Liquids: Measurements and Perturbed-Chain Statistical Associating Fluid Theory Modeling. Industrial & Engineering Chemistry Research, 2014, 53, 3737-3748.	3.7	82
15	Crowders and Cosolventsâ€”Major Contributors to the Cellular Milieu and Efficient Means to Counteract Environmental Stresses. ChemPhysChem, 2017, 18, 2951-2972.	2.1	82
16	Long-distance island hopping without dispersal stages: transportation across major zoogeographic barriers in a Southern Ocean isopod. Die Naturwissenschaften, 2010, 97, 583-594.	1.6	80
17	Measurement and Modeling Solubility of Aqueous Multisolute Amino-Acid Solutions. Industrial & Engineering Chemistry Research, 2010, 49, 1395-1401.	3.7	69
18	Determination of the Total Vapor Pressure of Hydrophobic Deep Eutectic Solvents: Experiments and Perturbed-Chain Statistical Associating Fluid Theory Modeling. ACS Sustainable Chemistry and Engineering, 2019, 7, 4047-4057.	6.7	69

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19	Solubility of Sugars and Sugar Alcohols in Ionic Liquids: Measurement and PC-SAFT Modeling. Journal of Physical Chemistry B, 2013, 117, 9980-9995.	2.6	67
20	Modeling imidazolium-based ionic liquids with ePC-SAFT. Part II. Application to H2S and synthesis-gas components. Fluid Phase Equilibria, 2014, 363, 59-65.	2.5	65
21	Measuring and modeling alcohol/salt systems. Chemical Engineering Science, 2012, 68, 328-339.	3.8	64
22	Modeling thermodynamic properties of aqueous singleâ€solute and multiâ€solute sugar solutions with PCâ€SAFT. AICHE Journal, 2013, 59, 4794-4805.	3.6	57
23	Influence of Salts on the Partitioning of 5-Hydroxymethylfurfural in Water/MIBK. Journal of Physical Chemistry B, 2016, 120, 3797-3808.	2.6	57
24	Benchmark Thermochemistry for Biologically Relevant Adenine and Cytosine. A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2015, 119, 9680-9691.	2.5	56
25	Incorporating a concentration-dependent dielectric constant into ePC-SAFT. An application to binary mixtures containing ionic liquids. Fluid Phase Equilibria, 2019, 492, 26-33.	2.5	48
26	The Role of Polyfunctionality in the Formation of [Ch]Cl-Carboxylic Acid-Based Deep Eutectic Solvents. Industrial & Engineering Chemistry Research, 2018, 57, 11195-11209.	3.7	46
27	Modeling pH and Solubilities in Aqueous Multisolute Amino Acid Solutions. Industrial & Engineering Chemistry Research, 2011, 50, 3503-3509.	3.7	45
28	Catalytic Low-Temperature Dehydration of Fructose to 5-Hydroxymethylfurfural Using Acidic Deep Eutectic Solvents and Polyoxometalate Catalysts. Frontiers in Chemistry, 2019, 7, 661.	3.6	44
29	Modeling thermodynamic derivative properties of ionic liquids with ePC-SAFT. Fluid Phase Equilibria, 2015, 405, 73-82.	2.5	43
30	Predicting CO2 solubility in aqueous N-methyldiethanolamine solutions with ePC-SAFT. Fluid Phase Equilibria, 2015, 393, 91-100.	2.5	42
31	Thermodynamics of Bioreactions. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 395-414.	6.8	42
32	Compatible solutes: Thermodynamic properties relevant for effective protection against osmotic stress. Fluid Phase Equilibria, 2016, 407, 224-235.	2.5	42
33	110th Anniversary: Distribution Coefficients of Furfural and 5-Hydroxymethylfurfural in Hydrophobic Deep Eutectic Solvent + Water Systems: Experiments and Perturbed-Chain Statistical Associating Fluid Theory Predictions. Industrial & Engineering Chemistry Research, 2019, 58, 4240-4247.	3.7	42
34	Encounter of lithodid crab Paralomis birsteini on the continental slope off Antarctica, sampled by ROV. Polar Biology, 2008, 31, 1143-1148.	1.2	41
35	Molecular Interactions in 1-Butanol + IL Solutions by Measuring and Modeling Activity Coefficients. Journal of Physical Chemistry B, 2013, 117, 3173-3185.	2.6	41
36	Modeling the density of ionic liquids with ePC-SAFT. Fluid Phase Equilibria, 2016, 410, 9-22.	2.5	39

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37	Toward Thermodynamic Predictions of Aqueous Vitamin Solubility: An Activity Coefficient-Based Approach. Industrial & Engineering Chemistry Research, 2019, 58, 7362-7369.	3.7	39
38	Thermophysical properties of glycelineâ€“water mixtures investigated by molecular modelling. Physical Chemistry Chemical Physics, 2019, 21, 6467-6476.	2.8	38
39	Density of Mixtures Containing Sugars and Ionic Liquids: Experimental Data and PC-SAFT Modeling. Journal of Chemical & Engineering Data, 2014, 59, 2942-2954.	1.9	36
40	Benzoic Acid and Chlorobenzoic Acids: Thermodynamic Study of the Pure Compounds and Binary Mixtures With Water. Journal of Pharmaceutical Sciences, 2016, 105, 1050-1058.	3.3	35
41	Perspective: Increasing blue carbon around Antarctica is an ecosystem service of considerable societal and economic value worth protecting. Global Change Biology, 2021, 27, 5-12.	9.5	35
42	Thermodynamic properties of aqueous salt containing urea solutions. Fluid Phase Equilibria, 2012, 325, 71-79.	2.5	34
43	Modeling Thermodynamic Derivative Properties and Gas Solubility of Ionic Liquids with ePC-SAFT. Industrial & Engineering Chemistry Research, 2019, 58, 8401-8417.	3.7	33
44	Modeling the CO₂ Solubility in Aqueous Electrolyte Solutions Using ePC-SAFT. Journal of Chemical & Engineering Data, 2020, 65, 5768-5777.	1.9	33
45	Thermodynamics of the alanine aminotransferase reaction. Fluid Phase Equilibria, 2016, 422, 87-98.	2.5	32
46	Standard Gibbs energy of metabolic reactions: II. Glucose-6-phosphatase reaction and ATP hydrolysis. Biophysical Chemistry, 2017, 223, 30-38.	2.8	32
47	The role of activity coefficients in bioreaction equilibria: Thermodynamics of methyl ferulate hydrolysis. Biophysical Chemistry, 2013, 173-174, 21-30.	2.8	29
48	Telomere-independent ageing in the longest-lived non-colonial animal, Arctica islandica. Experimental Gerontology, 2014, 51, 38-45.	2.8	29
49	A thermodynamic investigation of the glucose-6-phosphate isomerization. Biophysical Chemistry, 2014, 195, 22-31.	2.8	29
50	Thermodynamics of enzyme-catalyzed esterifications: II. Levulinic acid esterification with short-chain alcohols. Applied Microbiology and Biotechnology, 2017, 101, 7509-7521.	3.6	27
51	Aggregation control of Ru and Ir nanoparticles by tunable aryl alkyl imidazolium ionic liquids. Nanoscale, 2019, 11, 4073-4082.	5.6	26
52	Measurement and PC-SAFT modelling of three-phase behaviour. Physical Chemistry Chemical Physics, 2015, 17, 1800-1810.	2.8	25
53	Inducing the Alternative Oxidase Forms Part of the Molecular Strategy of Anoxic Survival in Freshwater Bivalves. Frontiers in Physiology, 2018, 9, 100.	2.8	25
54	Standard Gibbs Energy of Metabolic Reactions: I. Hexokinase Reaction. Biochemistry, 2016, 55, 5665-5674.	2.5	23

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55	Effect of salts on the solubility of ionic liquids in water: experimental and electrolyte Perturbed-Chain Statistical Associating Fluid Theory. Physical Chemistry Chemical Physics, 2015, 17, 32044-32052.	2.8	22
56	Combined co-solvent and pressure effect on kinetics of a peptide hydrolysis: an activity-based approach. Physical Chemistry Chemical Physics, 2019, 21, 22224-22229.	2.8	22
57	Thermodynamics of a model biological reaction: A comprehensive combined experimental and theoretical study. Fluid Phase Equilibria, 2016, 422, 99-110.	2.5	21
58	Thermodynamic g^E Models and Equations of State for Electrolytes in a Water-Poor Medium: A Review. Journal of Chemical & Engineering Data, 2020, 65, 5073-5082.	1.9	21
59	A Distinct Mitochondrial Genome with DUI-Like Inheritance in the Ocean QuahogArctica islandica. Molecular Biology and Evolution, 2016, 33, 375-383.	8.9	20
60	Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling. Fluid Phase Equilibria, 2016, 409, 399-407.	2.5	20
61	Effect of different organic salts on amino acids partition behaviour in PEG-salt ATPS. Fluid Phase Equilibria, 2018, 456, 84-91.	2.5	20
62	Liquidâ€“Liquid Equilibria for Separation of Alcohols from Esters Using Deep Eutectic Solvents Based on Choline Chloride: Experimental Study and Thermodynamic Modeling. Journal of Chemical & Engineering Data, 2019, 64, 6049-6059.	1.9	20
63	Predicting the high concentration co-solvent influence on the reaction equilibria of the ADH-catalyzed reduction of acetophenone. Journal of Chemical Thermodynamics, 2019, 128, 275-282.	2.0	20
64	Unravelling the nature of citric acid:<scp>l</scp>-arginine:water mixtures: the bifunctional role of water. Physical Chemistry Chemical Physics, 2021, 23, 1706-1717.	2.8	20
65	Prediction and Experimental Validation of Coâ€Solvent Influence on Michaelis Constants: A Thermodynamic Activityâ€Based Approach. Chemistry - A European Journal, 2018, 24, 16418-16425.	3.3	19
66	Prediction of saltingâ€out in liquidâ€liquid twoâ€phase systems with ePCâ€SAFT: Effect of the Born term and of a concentrationâ€dependent dielectric constant. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 1305-1314.	1.2	19
67	Solubility of Electrolytes in Organic Solvents: Solvent-Specific Effects and Ion-Specific Effects. Journal of Chemical & Engineering Data, 2022, 67, 2706-2718.	1.9	19
68	Measurement and PC-SAFT Modeling of the Solubility of Gallic Acid in Aqueous Mixtures of Deep Eutectic Solvents. Journal of Chemical & Engineering Data, 2021, 66, 958-967.	1.9	17
69	Boosting the kinetic efficiency of formate dehydrogenase by combining the effects of temperature, high pressure and co-solvent mixtures. Colloids and Surfaces B: Biointerfaces, 2021, 208, 112127.	5.0	17
70	Thermodynamics of enzyme-catalyzed esterifications: I. Succinic acid esterification with ethanol. Applied Microbiology and Biotechnology, 2017, 101, 5973-5984.	3.6	16
71	Standard Gibbs Energy of Metabolic Reactions: III The 3-Phosphoglycerate Kinase Reaction. ACS Omega, 2018, 3, 1783-1790.	3.5	16
72	Promising Thiolanium Ionic Liquid for Extraction of Aromatics from Aliphatics: Experiments and Modeling. Industrial & Engineering Chemistry Research, 2020, 59, 15707-15717.	3.7	16

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73	Modelling interfacial properties of ionic liquids with ePC-SAFT combined with density gradient theory. Molecular Physics, 2016, 114, 2492-2499.	1.7	14
74	Protecting Antarctic blue carbon: as marine ice retreats can the law fill the gap?. Climate Policy, 2020, 20, 149-162.	5.1	14
75	Predicting Vaporâ€“Liquid Equilibria for Sour-Gas Absorption in Aqueous Mixtures of Chemical and Physical Solvents or Ionic Liquids with ePC-SAFT. Industrial & Engineering Chemistry Research, 2021, 60, 6327-6336.	3.7	14
76	Ancient globetrottersâ€”connectivity and putative native ranges of two cosmopolitan biofouling amphipods. PeerJ, 2020, 8, e9613.	2.0	14
77	Melting Properties of Peptides and Their Solubility in Water. Part 2: Di- and Tripeptides Based on Glycine, Alanine, Leucine, Proline, and Serine. Industrial & Engineering Chemistry Research, 2021, 60, 4693-4704.	3.7	13
78	Thermodynamic Properties of Aqueous Glucoseâ€“Ureaâ€“Salt Systems. Journal of Solution Chemistry, 2014, 43, 1110-1131.	1.2	12
79	Activity coefficients at infinite dilution for different alcohols and ketones in [EMpy][ESO4]: Experimental data and modeling with PC-SAFT. Fluid Phase Equilibria, 2016, 424, 32-40.	2.5	12
80	Measuring and Predicting the Extraction Behavior of Biogenic Formic Acid in Biphasic Aqueous/Organic Reaction Mixtures. ACS Omega, 2017, 2, 8982-8989.	3.5	12
81	Mutual Influence of Furfural and Furancarboxylic Acids on Their Solubility in Aqueous Solutions: Experiments and Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) Predictions. Journal of Chemical & Engineering Data, 2018, 63, 1460-1470.	1.9	12
82	Solubility Enhancement of Vitamins in Water in the Presence of Covitamins: Measurements and ePC-SAFT Predictions. Industrial & Engineering Chemistry Research, 2019, 58, 21761-21771.	3.7	12
83	Vapor Pressure Assessment of Sulfolane-Based Eutectic Solvents: Experimental, PC-SAFT, and Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10386-10397.	2.6	12
84	Cation Effect on the Water Activity of Ternary (S)-Aminobutanedioic Acid Magnesium Salt Solutions at 298.15 and 310.15 K. Journal of Chemical & Engineering Data, 2016, 61, 3190-3199.	1.9	10
85	Phase Behavior of Binary Mixtures Containing Succinic Acid or Its Esters. Journal of Chemical & Engineering Data, 2017, 62, 1983-1993.	1.9	10
86	Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description. Biophysical Chemistry, 2019, 254, 106260.	2.8	10
87	Cosolvent and pressure effects on enzyme-catalysed hydrolysis reactions. Biophysical Chemistry, 2019, 252, 106209.	2.8	10
88	Standard Gibbs energy of metabolic reactions: IV. Triosephosphate isomerase reaction. Biophysical Chemistry, 2020, 258, 106330.	2.8	10
89	Standard Gibbs energy of metabolic reactions: V. Enolase reaction. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140365.	2.3	10
90	Calculation of Multiphase Equilibria Containing Mixed Solvents and Mixed Electrolytes: General Formulation and Case Studies. Journal of Chemical & Engineering Data, 2022, 67, 1972-1984.	1.9	10

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91	Thermodynamic Properties of Systems Comprising Esters: Experimental Data and Modeling with PC-SAFT and SAFT-Î³ Mie. Industrial & Engineering Chemistry Research, 2019, 58, 6841-6849.	3.7	9
92	Partitioning of waterâ€soluble vitamins in biodegradable aqueous twoâ€phase systems: Electrolyte perturbedâ€chain statistical associating fluid theory predictions and experimental validation. AIChE Journal, 2020, 66, e16984.	3.6	9
93	Prediction of pH in multiphase multicomponent systems with ePC-SAFT advanced. Chemical Communications, 2022, 58, 8436-8439.	4.1	9
94	Density variations of TMAO solutions in the kilobar range: Experiments, PC-SAFT predictions, and molecular dynamics simulations. Biophysical Chemistry, 2019, 253, 106222.	2.8	8
95	5-Hydroxymethylfurfural Synthesis in Nonaqueous Two-Phase Systems (NTPS)â€“PC-SAFT Predictions and Validation. Organic Process Research and Development, 2020, 24, 1052-1062.	2.7	8
96	Tetrahydrothiopheneâ€Based Ionic Liquids: Synthesis and Thermodynamic Characterizations. ChemistryOpen, 2021, 10, 153-163.	1.9	8
97	Thermodynamic properties of aqueous osmolyte solutions at high-pressure conditions. Biophysical Chemistry, 2019, 253, 106211.	2.8	7
98	Simultaneous Prediction of Cosolvent Influence on Reaction Equilibrium and Michaelis Constants of Enzyme-Catalyzed Ketone Reductions. ACS Omega, 2019, 4, 6264-6272.	3.5	7
99	Extremely Low Vaporâ€Pressure Data as Access to PCâ€SAFT Parameter Estimation for Ionic Liquids and Modeling of Precursor Solubility in Ionic Liquids. ChemistryOpen, 2021, 10, 216-226.	1.9	7
100	Interfacial Properties of Deep Eutectic Solvents by Density Gradient Theory. Industrial & Engineering Chemistry Research, 2022, 61, 2580-2591.	3.7	6
101	Influence of cytosolic conditions on the reaction equilibrium and the reaction enthalpy of the enolase reaction accessed by calorimetry and van â€˜t HOFF. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129675.	2.4	5
102	Thermodynamics and Kinetics of Glycolytic Reactions. Part I: Kinetic Modeling Based on Irreversible Thermodynamics and Validation by Calorimetry. International Journal of Molecular Sciences, 2020, 21, 8341.	4.1	4
103	Thermodynamics and Kinetics of Glycolytic Reactions. Part II: Influence of Cytosolic Conditions on Thermodynamic State Variables and Kinetic Parameters. International Journal of Molecular Sciences, 2020, 21, 7921.	4.1	4
104	Highâ€Pressureâ€Mediated Thioureaâ€Organocatalyzed Asymmetric Michael Addition to (Hetero)aromatic Nitroolefins: Prediction of Reaction Parameters by PCPâ€SAFT Modelling. ChemPlusChem, 2020, 85, 1292-1296.	2.8	4
105	New thermodynamic activity-based approach allows predicting the feasibility of glycolysis. Scientific Reports, 2021, 11, 6125.	3.3	4
106	Phylogenetic relationship within Cumacea (Crustacea: Peracarida) and genetic variability of two Antarctic species of the family Leuconidae. Scientia Marina, 2020, 84, 385-392.	0.6	3
107	Solvent Selection for the Extraction of 2-Phenylethanol from Aqueous Phases: Density and Viscosity Studies. Journal of Chemical & Engineering Data, 2022, 67, 1893-1904.	1.9	3
108	The melting properties of D-Î±-glucose, D-Î²-fructose, D-sucrose, D-Î±-galactose, and D-Î±-xylose and their solubility in water: A revision. Food Biophysics, 2022, 17, 181-197.	3.0	3

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109	Guanidinium Cation Effect on the Water Activity of Ternary (S)Aminopentanedioic Acid Sodium Salt Solutions at 298.15 and 310.15 K. Journal of Chemical & Engineering Data, 2019, 64, 1256-1264.	1.9	2
110	Isolation and characterization of 11 microsatellite markers from the squat lobster Munida gregaria (Decapoda: Galatheidae) around the Falkland Islands/Islas Malvinas. Conservation Genetics Resources, 2015, 7, 147-149.	0.8	1
111	Molecular aspects of lipid metabolism in the midgut gland of the brown shrimp Crangon crangon. Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 2020, 248-249, 110465.	1.6	1
112	Modelling Specific Ion Effects in Engineering Science. , 2009, , 85-115.		0
113	Isolation and characterization of 10 polymorphic loci for the giant Antarctic isopod, Glyptonotus antarcticus. Conservation Genetics Resources, 2013, 5, 963-965.	0.8	0