Chau-Chyun Chen

List of Publications by Year
in descending order

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129	7,732	87843 38	53190 85
papers	citations	h-index	g-index

136	136	136	3355
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Local composition model for excess Gibbs energy of electrolyte systems. Part I: Single solvent, single completely dissociated electrolyte systems. AICHE Journal, 1982, 28, 588-596.	1.8	816
2	A local composition model for the excess Gibbs energy of aqueous electrolyte systems. AICHE Journal, 1986, 32, 444-454.	1.8	803
3	Model of vapor-liquid equilibria for aqueous acid gas-alkanolamine systems using the electrolyte-NRTL equation. Industrial & Engineering Chemistry Research, 1989, 28, 1060-1073.	1.8	455
4	Thermodynamic representation of phase equilibria of mixed-solvent electrolyte systems. AICHE Journal, 1986, 32, 1655-1664.	1.8	345
5	Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods. Industrial & Engineering Chemistry Research, 2006, 45, 4389-4415.	1.8	324
6	Model of vapor-liquid equilibria for aqueous acid gas-alkanolamine systems. 2. Representation of hydrogen sulfide and carbon dioxide solubility in aqueous MDEA and carbon dioxide solubility in aqueous mixtures of MDEA with MEA or DEA. Industrial & Engineering Chemistry Research, 1991, 30, 543-555.	1.8	276
7	Rate-Based Process Modeling Study of CO₂ Capture with Aqueous Monoethanolamine Solution. Industrial & Engineering Chemistry Research, 2009, 48, 9233-9246.	1.8	249
8	Generalized electrolyte-NRTL model for mixed-solvent electrolyte systems. AICHE Journal, 2004, 50, 1928-1941.	1.8	225
9	Solubility Modeling with a Nonrandom Two-Liquid Segment Activity Coefficient Model. Industrial & Engineering Chemistry Research, 2004, 43, 8354-8362.	1.8	196
10	Refinement of COSMOâ˜SAC and the Applications. Industrial & Engineering Chemistry Research, 2007, 46, 7275-7288.	1.8	180
11	Symmetric Electrolyte Nonrandom Two-Liquid Activity Coefficient Model. Industrial & Engineering Chemistry Research, 2009, 48, 7788-7797.	1.8	177
12	A segment-based local composition model for the gibbs energy of polymer solutions. Fluid Phase Equilibria, 1993, 83, 301-312.	1.4	170
13	Applied thermodynamics for process modeling. AICHE Journal, 2002, 48, 194-200.	1.8	150
14	Thermodynamic Modeling for CO₂ Absorption in Aqueous MDEA Solution with Electrolyte NRTL Model. Industrial & Engineering Chemistry Research, 2011, 50, 163-175.	1.8	148
15	Extension and application of the pitzer equation for vapor-liquid equilibrium of aqueous electrolyte systems with molecular solutes. AICHE Journal, 1979, 25, 820-831.	1.8	147
16	Thermodynamic modeling for CO2 absorption in aqueous MEA solution with electrolyte NRTL model. Fluid Phase Equilibria, 2011, 311, 67-75.	1.4	144
17	Correlation and Prediction of Drug Molecule Solubility in Mixed Solvent Systems with the Nonrandom Two-Liquid Segment Activity Coefficient (NRTLâ˜SAC) Model. Industrial & Engineering Chemistry Research, 2006, 45, 4816-4824.	1.8	142
18	Phase Partitioning of Biomolecules: Solubilities of Amino Acids. Biotechnology Progress, 1989, 5, 111-118.	1.3	116

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19	New massâ€transfer correlations for packed towers. AICHE Journal, 2012, 58, 132-152.	1.8	115
20	Modeling CO2 Absorption and Desorption by Aqueous Monoethanolamine Solution with Aspen Rate-based Model. Energy Procedia, 2013, 37, 1584-1596.	1.8	98
21	Steady-State and Dynamic Modeling of Commercial Slurry High-Density Polyethylene (HDPE) Processes. Industrial & Engineering Chemistry Research, 2002, 41, 5601-5618.	1.8	85
22	Use of hydration and dissociation chemistries with the electrolyteâ€“NRTL model. AICHE Journal, 1999, 45, 1576-1586.	1.8	80
23	Steady-State and Dynamic Modeling of Gas-Phase Polypropylene Processes Using Stirred-Bed Reactors. Industrial & Engineering Chemistry Research, 2004, 43, 884-900.	1.8	79
24	Prediction of Pharmaceutical Solubility Via NRTL-SAC and COSMO-SAC. Journal of Pharmaceutical Sciences, 2008, 97, 1813-1820.	1.6	79
25	Refined electrolyteâ€NRTL model: Activity coefficient expressions for application to multiâ€electrolyte systems. AICHE Journal, 2008, 54, 1608-1624.	1.8	75
26	Thermodynamic Modeling of the NH₃â€“CO₂â€“H₂O System with Electrolyte NRTL Model. Industrial & Engineering Chemistry Research, 2011, 50, 11406-11421.	1.8	73
27	Thermodynamic modeling of CO2 and H2S solubilities in aqueous DIPA solution, aqueous sulfolaneâ€“DIPA solution, and aqueous sulfolaneâ€“MDEA solution with electrolyte NRTL model. Fluid Phase Equilibria, 2011, 306, 190-203.	1.4	68
28	Thermodynamic modeling of CO2 solubility in aqueous solutions of NaCl and Na2SO4. Journal of Supercritical Fluids, 2010, 55, 623-634.	1.6	60
29	Liquid Viscosity Model for Polymer Solutions and Mixtures. Industrial & Engineering Chemistry Research, 2003, 42, 2415-2422.	1.8	52
30	Segment-Based Eyringâ^'NRTL Viscosity Model for Mixtures Containing Polymers. Industrial & Engineering Chemistry Research, 2004, 43, 6231-6237.	1.8	50
31	Thermodynamic representation of the NaCl+Na2SO4+H2O system with electrolyte NRTL model. Fluid Phase Equilibria, 2011, 306, 149-161.	1.4	50
32	Quantifying Relationships among the Molecular Weight Distribution, Non-Newtonian Shear Viscosity, and Melt Index for Linear Polymers. Industrial & Engineering Chemistry Research, 2003, 42, 5354-5362.	1.8	48
33	Equation of State Modeling of Phase Equilibrium in the Low-Density Polyethylene Process:Â The Sanchezâ^'Lacombe, Statistical Associating Fluid Theory, and Polymer-Soaveâ^'Redlichâ^'Kwong Equations of State. Industrial & Engineering Chemistry Research, 1998, 37, 4481-4491.	1.8	47
34	Thermodynamic Modeling of the Sulfuric Acidâ^'Waterâ^'Sulfur Trioxide System with the Symmetric Electrolyte NRTL Model. Journal of Chemical & Engineering Data, 2011, 56, 963-977.	1.0	47
35	Fragment-Based Approach for Estimating Thermophysical Properties of Fats and Vegetable Oils for Modeling Biodiesel Production Processes. Industrial & Engineering Chemistry Research, 2010, 49, 876-886.	1.8	46
36	Segment-based excess Gibbs energy model for aqueous organic electrolytes. AICHE Journal, 2001, 47, 2593-2602.	1.8	41

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37	Modeling Polyethylene Fractionation Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. Industrial & Engineering Chemistry Research, 2002, 41, 968-988.	1.8	41
38	Correlation and Prediction of Phase Behavior of Organic Compounds in Ionic Liquids Using the Nonrandom Two-Liquid Segment Activity Coefficient Model. Industrial & Engineering Chemistry Research, 2008, 47, 7081-7093.	1.8	39
39	Representation of solid-liquid equilibrium of aqueous electrolyte systems with the electrolyte NRTL model. Fluid Phase Equilibria, 1986, 27, 457-474.	1.4	37
40	Isosteric heat of adsorption from thermodynamic Langmuir isotherm. Adsorption, 2021, 27, 979-989.	1.4	37
41	Toward development of activity coefficient models for process and product design of complex chemical systems. Fluid Phase Equilibria, 2006, 241, 103-112.	1.4	36
42	Thermodynamic modeling of KCl + H2O and KCl + NaCl + H2O systems using electrolyte NRTL model. Fluid Phase Equilibria, 2015, 387, 169-177.	1.4	33
43	Development of a Thermophysical Properties Model for Flowsheet Simulation of Biomass Pyrolysis Processes. ACS Sustainable Chemistry and Engineering, 2019, 7, 9017-9027.	3.2	33
44	Molecular thermodynamic model for gibbs energy of mixing of nonionic surfactant solutions. AICHE Journal, 1996, 42, 3231-3240.	1.8	32
45	Performance of sweeping gas membrane distillation for treating produced water: Modeling and experiments. Desalination, 2020, 492, 114597.	4.0	32
46	Extension of Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. Industrial & Engineering Chemistry Research, 2005, 44, 8909-8921.	1.8	31
47	Thermodynamic modeling of aqueous Ca 2+ â€“ Na + â€“ K + â€“ Cl â^' quaternary system. Fluid Phase Equilibria, 2016, 409, 193-206.	1.4	31
48	Polymerâ^'Solvent Vaporâ^'Liquid Equilibrium:Â Equations of State versus Activity Coefficient Models. Industrial & Engineering Chemistry Research, 1998, 37, 1567-1573.	1.8	30
49	COSMO-SAC Sigma Profile Generation with Conceptual Segment Concept. Industrial & Engineering Chemistry Research, 2015, 54, 4441-4454.	1.8	30
50	Predicting Thermophysical Properties of Mono- and Diglycerides with the Chemical Constituent Fragment Approach. Industrial & Engineering Chemistry Research, 2010, 49, 5479-5484.	1.8	29
51	An extension of cubic equations of state to vapor-liquid equilibria in polymer-solvent mixtures. Fluid Phase Equilibria, 1998, 145, 169-192.	1.4	28
52	Optimal Solvent Screening for the Crystallization of Pharmaceutical Compounds from Multisolvent Systems. Industrial & Engineering Chemistry Research, 2012, 51, 13792-13802.	1.8	28
53	Microfluidic production of size-tunable hexadecane-in-water emulsions: Effect of droplet size on destabilization of two-dimensional emulsions due to partial coalescence. Journal of Colloid and Interface Science, 2019, 533, 59-70.	5.0	28
54	An activity-based formulation for Langmuir adsorption isotherm. Adsorption, 2020, 26, 375-386.	1.4	27

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55	A New Phase-Equilibrium Model for Simulating Industrial Nylon-6 Production Trains. Industrial & Engineering Chemistry Research, 2003, 42, 3900-3913.	1.8	25
56	Modeling Drug Molecule Solubility to Identify Optimal Solvent Systems for Crystallization. Organic Process Research and Development, 2008, 12, 249-256.	1.3	25
57	Temperature dependence of interaction parameters in electrolyte <scp>NRTL</scp> model. AICHE Journal, 2016, 62, 1244-1253.	1.8	25
58	A molecular thermodynamic approach to predict the secondary structure of homopolypeptides in aqueous systems. Biopolymers, 1992, 32, 1375-1392.	1.2	24
59	Predicting NRTL binary interaction parameters from molecular simulations. AICHE Journal, 2018, 64, 2758-2769.	1.8	23
60	Modeling Gas Solubilities in the Aqueous Solution of Methyldiethanolamine. Industrial & Engineering Chemistry Research, 2011, 50, 6436-6446.	1.8	22
61	Extension of COSMO-SAC Solvation Model for Electrolytes. Industrial & Engineering Chemistry Research, 2011, 50, 176-187.	1.8	22
62	Thermodynamic model of aqueous Mg2+ â€“ Na+ â€“ K+ â€“ Clâ^' quaternary system. Fluid Phase Equilibria, 2017, 437, 56-68.	1.4	22
63	Local composition activity coefficient model for mixed-gas adsorption equilibria. Adsorption, 2019, 25, 951-964.	1.4	22
64	Use of GAMESS/COSMO program in support of COSMO-SAC model applications in phase equilibrium prediction calculations. Fluid Phase Equilibria, 2009, 276, 37-45.	1.4	20
65	Mobile ion partitioning in ion exchange membranes immersed in saline solutions. Journal of Membrane Science, 2021, 620, 118760.	4.1	20
66	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study on aqueous Ba 2+ -Na + -Cl â^' -SO 4 2â^' quaternary system. Fluid Phase Equilibria, 2017, 447, 29-38.	1.4	19
67	Revisiting electrolyte thermodynamic models: Insights from molecular simulations. AICHE Journal, 2018, 64, 3728-3734.	1.8	19
68	Nonrandom Two-Liquid Segment Activity Coefficient Model with Association Theory. Industrial & Engineering Chemistry Research, 2019, 58, 12773-12786.	1.8	19
69	Nonrandom twoâ€liquid activity coefficient model with association theory. AICHE Journal, 2021, 67, .	1.8	19
70	Representation of phase equilibrium behavior of antibiotics. Biotechnology Progress, 1990, 6, 266-272.	1.3	18
71	Multicomponent flash algorithm for mixtures containing polydisperse polymers. AICHE Journal, 2003, 49, 258-268.	1.8	18
72	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study of aqueous Sr2+-Na+-Clâ^'-SO42â^' quaternary system. Fluid Phase Equilibria, 2018, 470, 221-231.	1.4	18

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73	A comprehensive thermodynamic model for high salinity produced waters. AICHE Journal, 2020, 66, e16818.	1.8	18
74	Modeling swelling behavior of hydrogels in aqueous organic solvents. Chemical Engineering Science, 2021, 242, 116744.	1.9	18
75	Thermodynamic modeling of aqueous Na + â€“K + â€“Cl â^' â€“SO 4 2â^' quaternary system with electrolyte NRTL model. Fluid Phase Equilibria, 2015, 403, 1-9.	1.4	17
76	Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX. Journal of Chemical & Engineering Data, 2017, 62, 967-972.	1.0	17
77	A segment contribution method for the vapor pressure of tall-oil chemicals. Fluid Phase Equilibria, 1999, 155, 193-203.	1.4	16
78	Bridging twoâ€liquid theory with molecular simulations for electrolytes: An investigation of aqueous NaCl solution. AICHE Journal, 2019, 65, 1315-1324.	1.8	16
79	Molecular thermodynamics for scaling prediction: Case of membrane distillation. Separation and Purification Technology, 2021, 276, 119231.	3.9	16
80	New Mass-Transfer Model for Simulating Industrial Nylon-6 Production Trains. Industrial & Engineering Chemistry Research, 2004, 43, 5063-5076.	1.8	15
81	Aggregation thermodynamics for asphaltene precipitation. AICHE Journal, 2016, 62, 1254-1264.	1.8	15
82	Associationâ€based activity coefficient model for electrolyte solutions. AICHE Journal, 2022, 68, e17422.	1.8	15
83	Symmetric Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. Industrial & Engineering Chemistry Research, 2009, 48, 5522-5529.	1.8	14
84	Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production. Fluid Phase Equilibria, 2018, 460, 175-188.	1.4	14
85	Molecular thermodynamic modeling of aqueous Na+-K+-Mg2+-Ca2+-SO42â^' quinary system. Fluid Phase Equilibria, 2019, 491, 77-87.	1.4	14
86	Thermodynamic representation of aqueous sodium nitrate and nitric acid solution with electrolyte NRTL model. Fluid Phase Equilibria, 2016, 407, 105-116.	1.4	13
87	Thermodynamic modeling of HCl-H2O binary system with symmetric electrolyte NRTL model. Journal of Chemical Thermodynamics, 2018, 125, 159-171.	1.0	13
88	Some recent developments in process simulation for reactive chemical systems. Pure and Applied Chemistry, 1987, 59, 1177-1188.	0.9	12
89	Thermodynamic modeling of asphaltene precipitation in pure and mixed solvents with NRTL-SAC. Fluid Phase Equilibria, 2018, 473, 255-261.	1.4	12
90	Nonrandom two-liquid activity coefficient model for aqueous polyelectrolyte solutions. Fluid Phase Equilibria, 2019, 497, 1-9.	1.4	12

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91	Thermodynamic modeling of CO2 absorption in aqueous potassium carbonate solution with electrolyte NRTL model. Fluid Phase Equilibria, 2020, 505, 112339.	1.4	12
92	Modeling dissociation of ionic liquids with electrolyte NRTL model. Journal of Molecular Liquids, 2021, 329, 115524.	2.3	12
93	Thermodynamic modeling of calcium carbonate scale precipitation: aqueous Na+-Ca2+-Clâ€“-HCO3â€“-CO32â€“-CO2 system. Fluid Phase Equilibria, 2022, 552, 113263.	1.4	11
94	Thermodynamic modeling of aqueous Na+â€“K+â€“Mg2+â€“SO42â˜ quaternary system. Fluid Phase Equilibria, 2015, 404, 141-149.	1.4	10
95	A rigorous process modeling methodology for biomass fast pyrolysis with an entrainedâ€flow reactor. Journal of Advanced Manufacturing and Processing, 2020, 2, .	1.4	10
96	Generalization of thermodynamic Langmuir isotherm for mixedâ€gas adsorption equilibria. AICHE Journal, 2022, 68, .	1.8	10
97	Thermodynamic modeling of HNO₃â€H₂SO₄â€H₂O ternary system with symmetric electrolyte NRTL model. AICHE Journal, 2017, 63, 3110-3117.	1.8	9
98	Prediction of Asphaltene Precipitation in Organic Solvents via COSMO-SAC. Energy & Fuels, 2017, 31, 8985-8996.	2.5	9
99	Prediction of <scp>mixedâ€gas</scp> adsorption equilibria from pure component adsorption isotherms. AICHE Journal, 2020, 66, e16243.	1.8	9
100	From Langmuir isotherm to Brunauerâ€“Emmettâ€“Teller isotherm. AICHE Journal, 2022, 68, e17523.	1.8	9
101	Molecular thermodynamic model to predict the .alpha.-helical secondary structure of polypeptide chains in solution. Biochemistry, 1992, 31, 10591-10601.	1.2	8
102	Correlation and prediction of drug molecule solubility with the NRTL-SAC model. Computer Aided Chemical Engineering, 2006, , 859-864.	0.3	7
103	Predicting wax appearance temperature and precipitation profile of normal alkane systems: An explicit co-crystal model. Fluid Phase Equilibria, 2020, 509, 112466.	1.4	7
104	Prediction of thermodynamic properties of organic mixtures: Combining molecular simulations with classical thermodynamics. Fluid Phase Equilibria, 2020, 523, 112759.	1.4	7
105	A Novel Approach to Modeling Biomass Pyrolysis in a Fluidized Bed Reactor. ACS Sustainable Chemistry and Engineering, 2020, 8, 14605-14615.	3.2	7
106	Modeling fluid phase equilibria of carbon dioxide-methanol binary system. Fluid Phase Equilibria, 2021, 529, 112866.	1.4	7
107	Thermodynamic Modeling of Aqueous LiCl, LiBr, LiI, and LiNO3 Solutions. Fluid Phase Equilibria, 2021, 531, 112914.	1.4	7
108	Solubility of Nutraceutical Compounds in Generally Recognized as Safe Solvents at 298 K. International Journal of Chemical Engineering and Applications (IJCEA), 2016, 7, 289-294.	0.3	7

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109	Aggregation thermodynamics of asphaltenes: Prediction of asphaltene precipitation in petroleum fluids with NRTL-SAC. Fluid Phase Equilibria, 2020, 520, 112655.	1.4	6
110	A simple and practical process modeling methodology for pressure swing adsorption. Computers and Chemical Engineering, 2021, 147, 107235.	2.0	6
111	Prediction of Ï‡ Parameter of Polymer Blends by Combining Molecular Simulations and Integral Equation Theory. Journal of Physical Chemistry B, 2018, 122, 9022-9031.	1.2	5
112	Environmental Impacts of Hydraulic Fracturing. , 2016, , 199-219.		5
113	Correlations for Densities of Aqueous Electrolyte Solutions. Journal of Chemical & Engineering Data, 2016, 61, 740-747.	1.0	4
114	Modeling aqueous multivalent polyelectrolytes systems with polyelectrolyte NRTL model. Journal of Molecular Liquids, 2021, 336, 116237.	2.3	4
115	Process Modeling of CO₂ Absorption with Monoethanolamine Aqueous Solutions Using Rotating Packed Beds. Industrial & Engineering Chemistry Research, 2022, 61, 12142-12152.	1.8	4
116	Estimating CO₂ Solubility in Aqueous Na⁺â€“K⁺â€“Mg²⁺â€“Ca²⁺â€“Cl^{â€“}â€“SO₄<sup>2â€“ Solutions with Electrolyte NRTLâ€“PC-SAFT Model. Journal of Chemical & Engineering Data, 2022, 67, 1932-1950.	1.0	4
117	Deep learning neural network potential for simulating gaseous adsorption in metalâ€“organic frameworks. Materials Advances, 2022, 3, 5299-5303.	2.6	4
118	Batch-screening guided continuous flow synthesis of the metal-organic framework HKUST-1 in a millifluidic droplet reactor. Microporous and Mesoporous Materials, 2022, 339, 112005.	2.2	4
119	The role of computerized modeling and simulation in the development of life support system technologies. Advances in Space Research, 1989, 9, 121-131.	1.2	3
120	Process simulation in polymer manufacturing. Computers and Chemical Engineering, 1992, 16, S481-S490.	2.0	2
121	Industrial Applications of Plant-Wide Equation-Oriented Process Modelingâ€”2010. Advances in Chemical Engineering, 2011, 40, 119-152.	0.5	2
122	Collective nucleation dynamics in two-dimensional emulsions with hexagonal packing. Physical Review E, 2020, 101, 030602.	0.8	2
123	Modeling Phase Equilibrium of Common Sugars Glucose, Fructose, and Sucrose in Mixed Solvents. Journal of Chemical & Engineering Data, 2021, 66, 4193-4205.	1.0	2
124	Extended thermodynamic model for high salinity produced waters. Chemical Engineering Science, 2021, 243, 116754.	1.9	2
125	Thermodynamic analysis of hydrogel swelling in aqueous sodium chloride solutions. Journal of Molecular Liquids, 2022, 348, 118421.	2.3	2
126	Catastrophic thermal destabilization of two-dimensional close-packed emulsions due to synchronous coalescence initiation. Soft Matter, 2020, 16, 6032-6037.	1.2	1

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127	Solubility Thermodynamics of Organic Energetic Materials. , 2017, , 43-62.		1
128	Modeling Ion Transport in Electrodialysis of Concentrated Solutions. Materials and Energy, 2021, , 193-226.	2.5	0
129	Thermodynamic modeling of aqueous polyelectrolyte solutions with mixed-valent counterions. Journal of Chemical Thermodynamics, 2022, 169, 106761.	1.0	0