Chau-Chyun Chen

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

127 papers	6,289 citations	36 h-index	78 g-index
136 ext. papers	6,945 ext. citations	3.5 avg, IF	6.04 L-index

#	Paper	IF	Citations
127	Thermodynamic analysis of hydrogel swelling in aqueous sodium chloride solutions. *Journal of Molecular Liquids*, **2022**, 348, 118421	6	0
126	Thermodynamic modeling of aqueous polyelectrolyte solutions with mixed-valent counterions. *Journal of Chemical Thermodynamics*, **2022**, 169, 106761	2.9	
125	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	5.3	0
124	Thermodynamic modeling of calcium carbonate scale precipitation: aqueous Na+-Ca2+-Cl−HCO3−CO32−CO2 system. *Fluid Phase Equilibria*, **2021**, 113263	2.5	0
123	Thermodynamic Modeling of Aqueous LiCl, LiBr, LiI, and LiNO3 Solutions. *Fluid Phase Equilibria*, **2021**, 531, 112914	2.5	3
122	A simple and practical process modeling methodology for pressure swing adsorption. *Computers and Chemical Engineering*, **2021**, 147, 107235	4	2
121	Modeling dissociation of ionic liquids with electrolyte NRTL model. *Journal of Molecular Liquids*, **2021**, 329, 115524	6	3
120	Modeling Ion Transport in Electrodialysis of Concentrated Solutions. *Materials and Energy*, **2021**, 193-226		
119	Modeling fluid phase equilibria of carbon dioxide-methanol binary system. *Fluid Phase Equilibria*, **2021**, 529, 112866	2.5	1
118	Nonrandom two-liquid activity coefficient model with association theory. *AICHE Journal*, **2021**, 67,	3.6	9
117	Mobile ion partitioning in ion exchange membranes immersed in saline solutions. *Journal of Membrane Science*, **2021**, 620, 118760	9.6	9
116	Modeling aqueous multivalent polyelectrolytes systems with polyelectrolyte NRTL model. *Journal of Molecular Liquids*, **2021**, 336, 116237	6	2
115	Modeling swelling behavior of hydrogels in aqueous organic solvents. *Chemical Engineering Science*, **2021**, 242, 116744	4.4	6
114	Extended thermodynamic model for high salinity produced waters. *Chemical Engineering Science*, **2021**, 243, 116754	4.4	1
113	Molecular thermodynamics for scaling prediction: Case of membrane distillation. *Separation and Purification Technology*, **2021**, 276, 119231	8.3	3
112	Isosteric heat of adsorption from thermodynamic Langmuir isotherm. *Adsorption*, **2021**, 27, 979-989	2.6	5
111	Collective nucleation dynamics in two-dimensional emulsions with hexagonal packing. *Physical Review E*, **2020**, 101, 030602	2.4	2

110	Aggregation thermodynamics of asphaltenes: Prediction of asphaltene precipitation in petroleum fluids with NRTL-SAC. *Fluid Phase Equilibria*, **2020**, 520, 112655	2.5	3
109	Catastrophic thermal destabilization of two-dimensional close-packed emulsions due to synchronous coalescence initiation. *Soft Matter*, **2020**, 16, 6032-6037	3.6	0
108	Prediction of mixed-gas adsorption equilibria from pure component adsorption isotherms. *AICHE Journal*, **2020**, 66, e16243	3.6	3
107	A comprehensive thermodynamic model for high salinity produced waters. *AICHE Journal*, **2020**, 66, e16818	3.6	10
106	Predicting wax appearance temperature and precipitation profile of normal alkane systems: An explicit co-crystal model. *Fluid Phase Equilibria*, **2020**, 509, 112466	2.5	2
105	An activity-based formulation for Langmuir adsorption isotherm. *Adsorption*, **2020**, 26, 375-386	2.6	9
104	Prediction of thermodynamic properties of organic mixtures: Combining molecular simulations with classical thermodynamics. *Fluid Phase Equilibria*, **2020**, 523, 112759	2.5	3
103	Performance of sweeping gas membrane distillation for treating produced water: Modeling and experiments. *Desalination*, **2020**, 492, 114597	10.3	9
102	A Novel Approach to Modeling Biomass Pyrolysis in a Fluidized Bed Reactor. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 14605-14615	8.3	5
101	Thermodynamic modeling of CO2 absorption in aqueous potassium carbonate solution with electrolyte NRTL model. *Fluid Phase Equilibria*, **2020**, 505, 112339	2.5	5
100	A rigorous process modeling methodology for biomass fast pyrolysis with an entrained-flow reactor. *Journal of Advanced Manufacturing and Processing*, **2020**, 2,	2.7	2
99	Nonrandom Two-Liquid Segment Activity Coefficient Model with Association Theory. *Industrial & Engineering Chemistry Research*, **2019**, 58, 12773-12786	3.9	11
98	Nonrandom two-liquid activity coefficient model for aqueous polyelectrolyte solutions. *Fluid Phase Equilibria*, **2019**, 497, 1-9	2.5	9
97	Local composition activity coefficient model for mixed-gas adsorption equilibria. *Adsorption*, **2019**, 25, 951-964	2.6	12
96	THERMODYNAMIC MODELING OF AQUEOUS AND MIXED SOLVENT ELECTROLYTE SYSTEMS **2019**, 493-504		
95	Molecular thermodynamic modeling of aqueous Na+-K+-Mg2+-Ca2+-SO42□quinary system. *Fluid Phase Equilibria*, **2019**, 491, 77-87	2.5	7
94	Development of a Thermophysical Properties Model for Flowsheet Simulation of Biomass Pyrolysis Processes. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 9017-9027	8.3	10
93	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	9.3	20

92	Bridging two-liquid theory with molecular simulations for electrolytes: An investigation of aqueous NaCl solution. *AICHE Journal*, **2019**, 65, 1315-1324	3.6	10
91	Predicting NRTL binary interaction parameters from molecular simulations. *AICHE Journal*, **2018**, 64, 2758-2769	3.6	19
90	Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production. *Fluid Phase Equilibria*, **2018**, 460, 175-188	2.5	9
89	Thermodynamic modeling of asphaltene precipitation in pure and mixed solvents with NRTL-SAC. *Fluid Phase Equilibria*, **2018**, 473, 255-261	2.5	8
88	Revisiting electrolyte thermodynamic models: Insights from molecular simulations. *AICHE Journal*, **2018**, 64, 3728-3734	3.6	13
87	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study of aqueous Sr2+-Na+-Cl−-SO42−quaternary system. *Fluid Phase Equilibria*, **2018**, 470, 221-231	2.5	12
86	Prediction of Parameter of Polymer Blends by Combining Molecular Simulations and Integral Equation Theory. *Journal of Physical Chemistry B*, **2018**, 122, 9022-9031	3.4	3
85	Thermodynamic modeling of HCl-H2O binary system with symmetric electrolyte NRTL model. *Journal of Chemical Thermodynamics*, **2018**, 125, 159-171	2.9	8
84	Thermodynamic model of aqueous Mg2+ -Na+ -K+ -Cl−quaternary system. *Fluid Phase Equilibria*, **2017**, 437, 56-68	2.5	16
83	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	2.8	9
82	Thermodynamic modeling of HNO3-H2SO4-H2O ternary system with symmetric electrolyte NRTL model. *AICHE Journal*, **2017**, 63, 3110-3117	3.6	8
81	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study on aqueous Ba 2+ -Na + -Cl −SO 4 2−quaternary system. *Fluid Phase Equilibria*, **2017**, 447, 29-38	2.5	15
80	Prediction of Asphaltene Precipitation in Organic Solvents via COSMO-SAC. *Energy & Fuels*, **2017**, 31, 8985-8996	4.1	6
79	Solubility Thermodynamics of Organic Energetic Materials **2017**, 43-62		1
78	Thermodynamic modeling of aqueous Ca2+-Na+ -K+ -Cl−quaternary system. *Fluid Phase Equilibria*, **2016**, 409, 193-206	2.5	24
77	Thermodynamic representation of aqueous sodium nitrate and nitric acid solution with electrolyte NRTL model. *Fluid Phase Equilibria*, **2016**, 407, 105-116	2.5	11
76	Aggregation thermodynamics for asphaltene precipitation. *AICHE Journal*, **2016**, 62, 1254-1264	3.6	11
75	Temperature dependence of interaction parameters in electrolyte NRTL model. *AICHE Journal*, **2016**, 62, 1244-1253	3.6	19

74	Correlations for Densities of Aqueous Electrolyte Solutions. *Journal of Chemical & Engineering Data*, **2016**, 61, 740-747	2.8	2
73	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	0.2	5
72	Environmental Impacts of Hydraulic Fracturing **2016**, 199-219		2
71	Thermodynamic modeling of aqueous Na+K+Mg2+SO42quaternary system. *Fluid Phase Equilibria*, **2015**, 404, 141-149	2.5	8
70	Thermodynamic modeling of aqueous Na+K+ClSO42quaternary system with electrolyte NRTL model. *Fluid Phase Equilibria*, **2015**, 403, 1-9	2.5	14
69	Thermodynamic modeling of KCl + H2O and KCl + NaCl + H2O systems using electrolyte NRTL model. *Fluid Phase Equilibria*, **2015**, 387, 169-177	2.5	26
68	COSMO-SAC Sigma Profile Generation with Conceptual Segment Concept. *Industrial & Engineering Chemistry Research*, **2015**, 54, 4441-4454	3.9	21
67	Modeling CO2 Absorption and Desorption by Aqueous Monoethanolamine Solution with Aspen Rate-based Model. *Energy Procedia*, **2013**, 37, 1584-1596	2.3	75
66	New mass-transfer correlations for packed towers. *AICHE Journal*, **2012**, 58, 132-152	3.6	88
65	Optimal Solvent Screening for the Crystallization of Pharmaceutical Compounds from Multisolvent Systems. *Industrial & Engineering Chemistry Research*, **2012**, 51, 13792-13802	3.9	21
64	Modeling Gas Solubilities in the Aqueous Solution of Methyldiethanolamine. *Industrial & Engineering Chemistry Research*, **2011**, 50, 6436-6446	3.9	19
63	Thermodynamic Modeling for CO2 Absorption in Aqueous MDEA Solution with Electrolyte NRTL Model. *Industrial & Engineering Chemistry Research*, **2011**, 50, 163-175	3.9	125
62	Extension of COSMO-SAC Solvation Model for Electrolytes. *Industrial & Engineering Chemistry Research*, **2011**, 50, 176-187	3.9	20
61	Industrial Applications of Plant-Wide Equation-Oriented Process Modeling2010. *Advances in Chemical Engineering*, **2011**, 40, 119-152	0.6	
60	Thermodynamic Modeling of the Sulfuric AcidWaterSulfur Trioxide System with the Symmetric Electrolyte NRTL Model. *Journal of Chemical & Engineering Data*, **2011**, 56, 963-977	2.8	43
59	Thermodynamic Modeling of the NH3CO2H2O System with Electrolyte NRTL Model. *Industrial & Engineering Chemistry Research*, **2011**, 50, 11406-11421	3.9	64
58	Thermodynamic modeling for CO2 absorption in aqueous MEA solution with electrolyte NRTL model. *Fluid Phase Equilibria*, **2011**, 311, 67-75	2.5	115
57	Thermodynamic representation of the NaCl+Na2SO4+H2O system with electrolyte NRTL model. *Fluid Phase Equilibria*, **2011**, 306, 149-161	2.5	36

56	Thermodynamic modeling of CO2 and H2S solubilities in aqueous DIPA solution, aqueous sulfolane–DIPA solution, and aqueous sulfolane–MDEA solution with electrolyte NRTL model. *Fluid Phase Equilibria*, **2011**, 306, 190-203	2.5	56
55	Predicting Thermophysical Properties of Mono- and Diglycerides with the Chemical Constituent Fragment Approach. *Industrial & Engineering Chemistry Research*, **2010**, 49, 5479-5484	3.9	22
54	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	3.9	42
53	Thermodynamic modeling of CO2 solubility in aqueous solutions of NaCl and Na2SO4. *Journal of Supercritical Fluids*, **2010**, 55, 623-634	4.2	47
52	Use of GAMESS/COSMO program in support of COSMO-SAC model applications in phase equilibrium prediction calculations. *Fluid Phase Equilibria*, **2009**, 276, 37-45	2.5	17
51	Symmetric Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. *Industrial & Engineering Chemistry Research*, **2009**, 48, 5522-5529	3.9	12
50	Symmetric Electrolyte Nonrandom Two-Liquid Activity Coefficient Model. *Industrial & Engineering Chemistry Research*, **2009**, 48, 7788-7797	3.9	147
49	Rate-Based Process Modeling Study of CO2 Capture with Aqueous Monoethanolamine Solution. *Industrial & Engineering Chemistry Research*, **2009**, 48, 9233-9246	3.9	205
48	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	3.9	36
47	Prediction of pharmaceutical solubility Via NRTL-SAC and COSMO-SAC. *Journal of Pharmaceutical Sciences*, **2008**, 97, 1813-20	3.9	72
46	Refined electrolyte-NRTL model: Activity coefficient expressions for application to multi-electrolyte systems. *AICHE Journal*, **2008**, 54, 1608-1624	3.6	61
45	Modeling Drug Molecule Solubility to Identify Optimal Solvent Systems for Crystallization. *Organic Process Research and Development*, **2008**, 12, 249-256	3.9	25
44	Refinement of COSMO-SAC and the Applications. *Industrial & Engineering Chemistry Research*, **2007**, 46, 7275-7288	3.9	148
43	Correlation and prediction of drug molecule solubility with the NRTL-SAC model. *Computer Aided Chemical Engineering*, **2006**, 859-864	0.6	5
42	Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods. *Industrial & Engineering Chemistry Research*, **2006**, 45, 4389-4415	3.9	238
41	Correlation and Prediction of Drug Molecule Solubility in Mixed Solvent Systems with the Nonrandom Two-Liquid Segment Activity Coefficient (NRTL-SAC) Model. *Industrial & Engineering Chemistry Research*, **2006**, 45, 4816-4824	3.9	129
40	Toward development of activity coefficient models for process and product design of complex chemical systems. *Fluid Phase Equilibria*, **2006**, 241, 103-112	2.5	31
39	Extension of Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. *Industrial & Engineering Chemistry Research*, **2005**, 44, 8909-8921	3.9	27

38	Steady-State and Dynamic Modeling of Gas-Phase Polypropylene Processes Using Stirred-Bed Reactors. *Industrial & Engineering Chemistry Research*, **2004**, 43, 884-900	3.9	60
37	Generalized electrolyte-NRTL model for mixed-solvent electrolyte systems. *AICHE Journal*, **2004**, 50, 1928-1941	3.6	185
36	New Mass-Transfer Model for Simulating Industrial Nylon-6 Production Trains. *Industrial & Engineering Chemistry Research*, **2004**, 43, 5063-5076	3.9	15
35	Segment-Based Eyring–NRTL Viscosity Model for Mixtures Containing Polymers. *Industrial & Engineering Chemistry Research*, **2004**, 43, 6231-6237	3.9	43
34	Solubility Modeling with a Nonrandom Two-Liquid Segment Activity Coefficient Model. *Industrial & Engineering Chemistry Research*, **2004**, 43, 8354-8362	3.9	165
33	Multicomponent flash algorithm for mixtures containing polydisperse polymers. *AICHE Journal*, **2003**, 49, 258-268	3.6	14
32	Liquid Viscosity Model for Polymer Solutions and Mixtures. *Industrial & Engineering Chemistry Research*, **2003**, 42, 2415-2422	3.9	44
31	A New Phase-Equilibrium Model for Simulating Industrial Nylon-6 Production Trains. *Industrial & Engineering Chemistry Research*, **2003**, 42, 3900-3913	3.9	24
30	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	3.9	36
29	Applied thermodynamics for process modeling. *AICHE Journal*, **2002**, 48, 194-200	3.6	125
28	Steady-State and Dynamic Modeling of Commercial Slurry High-Density Polyethylene (HDPE) Processes. *Industrial & Engineering Chemistry Research*, **2002**, 41, 5601-5618	3.9	68
27	Modeling Polyethylene Fractionation Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. *Industrial & Engineering Chemistry Research*, **2002**, 41, 968-988	3.9	33
26	Segment-based excess Gibbs energy model for aqueous organic electrolytes. *AICHE Journal*, **2001**, 47, 2593-2602	3.6	32
25	A segment contribution method for the vapor pressure of tall-oil chemicals. *Fluid Phase Equilibria*, **1999**, 155, 193-203	2.5	16
24	Use of hydration and dissociation chemistries with the electrolyte-NRTL model. *AICHE Journal*, **1999**, 45, 1576-1586	3.6	72
23	An extension of cubic equations of state to vapor-liquid equilibria in polymer-solvent mixtures. *Fluid Phase Equilibria*, **1998**, 145, 169-192	2.5	24
22	Polymer–Solvent Vapor–Liquid Equilibrium: Equations of State versus Activity Coefficient Models. *Industrial & Engineering Chemistry Research*, **1998**, 37, 1567-1573	3.9	26
21	Equation of State Modeling of Phase Equilibrium in the Low-Density Polyethylene Process: The Sanchez–Lacombe, Statistical Associating Fluid Theory, and Polymer-Soave–Redlich–Kwong Equations of State. *Industrial & Engineering Chemistry Research*, **1998**, 37, 4481-4491	3.9	43

20	Molecular thermodynamic model for gibbs energy of mixing of nonionic surfactant solutions. *AICHE Journal*, **1996**, 42, 3231-3240	3.6	26
19	A segment-based local composition model for the gibbs energy of polymer solutions. *Fluid Phase Equilibria*, **1993**, 83, 301-312	2.5	154
18	Molecular thermodynamic model to predict the alpha-helical secondary structure of polypeptide chains in solution. *Biochemistry*, **1992**, 31, 10591-601	3.2	5
17	Process simulation in polymer manufacturing. *Computers and Chemical Engineering*, **1992**, 16, S481-S490	4	2
16	A molecular thermodynamic approach to predict the secondary structure of homopolypeptides in aqueous systems. *Biopolymers*, **1992**, 32, 1375-92	2.2	17
15	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	3.9	249
14	Representation of phase equilibrium behavior of antibiotics. *Biotechnology Progress*, **1990**, 6, 266-72	2.8	15
13	Phase Partitioning of Biomolecules: Solubilities of Amino Acids. *Biotechnology Progress*, **1989**, 5, 111-118	2.8	100
12	The role of computerized modeling and simulation in the development of life support system technologies. *Advances in Space Research*, **1989**, 9, 121-31	2.4	2
11	Model of vapor-liquid equilibria for aqueous acid gas-alkanolamine systems using the electrolyte-NRTL equation. *Industrial & Engineering Chemistry Research*, **1989**, 28, 1060-1073	3.9	406
10	Some recent developments in process simulation for reactive chemical systems. *Pure and Applied Chemistry*, **1987**, 59, 1177-1188	2.1	7
9	A local composition model for the excess Gibbs energy of aqueous electrolyte systems. *AICHE Journal*, **1986**, 32, 444-454	3.6	704
8	Thermodynamic representation of phase equilibria of mixed-solvent electrolyte systems. *AICHE Journal*, **1986**, 32, 1655-1664	3.6	307
7	Representation of solid-liquid equilibrium of aqueous electrolyte systems with the electrolyte NRTL model. *Fluid Phase Equilibria*, **1986**, 27, 457-474	2.5	31
6	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	3.6	707
5	Extension and application of the pitzer equation for vapor-liquid equilibrium of aqueous electrolyte systems with molecular solutes. *AICHE Journal*, **1979**, 25, 820-831	3.6	133
4	From Langmuir isotherm to Brunauer–Emmett–Teller isotherm. *AICHE Journal*, e17523	3.6	0
3	Modeling Phase Equilibrium of Common Sugars Glucose, Fructose, and Sucrose in Mixed Solvents. *Journal of Chemical & Engineering Data*,	2.8	1

2	Association-based activity coefficient model for electrolyte solutions. *AICHE Journal*,e17422	3.6	4
1	Molecular Thermodynamics for Pharmaceutical Process Modeling and Simulation505-519		1