Ioannis Economou

List of Publications by Citations

234 papers	6,949 citations	44 h-index	70 g-index
252 ext. papers	7,786 ext. citations	3.8 avg, IF	6.26 L-index

#	Paper	IF	Citations
234	Statistical Associating Fluid Theory: A Successful Model for the Calculation of Thermodynamic and Phase Equilibrium Properties of Complex Fluid Mixtures. *Industrial & Engineering Chemistry Research*, **2002**, 41, 953-962	3.9	290
233	Industrial Requirements for Thermodynamics and Transport Properties. *Industrial & Engineering Chemistry Research*, **2010**, 49, 11131-11141	3.9	186
232	Modeling of the carbon dioxide solubility in imidazolium-based ionic liquids with the tPC-PSAFT equation of state. *Journal of Physical Chemistry B*, **2006**, 110, 9262-9	3.4	153
231	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. *Journal of Physical Chemistry B*, **1998**, 102, 1029-1035	3.4	148
230	Associating models and mixing rules in equations of state for water/hydrocarbon mixtures. *Chemical Engineering Science*, **1997**, 52, 511-525	4.4	122
229	Chemical, quasi-chemical and perturbation theories for associating fluids. *AICHE Journal*, **1991**, 37, 1875-1894	3.8	118
228	Molecular Simulation of Phase Equilibria for Water□Methane and Water□Ethane Mixtures. *Journal of Physical Chemistry B*, **1998**, 102, 8865-8873	3.4	108
227	Water/Hydrocarbon Phase Equilibria Using the Thermodynamic Perturbation Theory. *Industrial & Engineering Chemistry Research*, **2000**, 39, 797-804	3.9	107
226	Adsorption of N2, CH4, CO and CO2 gases in single walled carbon nanotubes: A combined experimental and Monte Carlo molecular simulation study. *Journal of Supercritical Fluids*, **2010**, 55, 510-523	4.2	106
225	Extended statistical associating fluid theory (SAFT) equations of state for dipolar fluids. *AICHE Journal*, **2005**, 51, 2328-2342	3.6	106
224	Perturbed chain-statistical associating fluid theory extended to dipolar and quadrupolar molecular fluids. *Journal of Physical Chemistry B*, **2006**, 110, 9252-61	3.4	101
223	1-Octanol/Water Partition Coefficients of n-Alkanes from Molecular Simulations of Absolute Solvation Free Energies. *Journal of Chemical Theory and Computation*, **2009**, 5, 2436-46	6.4	96
222	Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 1. Pure Fluids. *Industrial & Engineering Chemistry Research*, **2004**, 43, 6592-6606	3.9	91
221	Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 2. Multicomponent Mixtures. *Industrial & Engineering Chemistry Research*, **2007**, 46, 2628-2636	3.9	89
220	tPC-PSAFT Modeling of Gas Solubility in Imidazolium-Based Ionic Liquids□ *Journal of Physical Chemistry C*, **2007**, 111, 15487-15492	3.8	88
219	ZIF-67 Framework: A Promising New Candidate for Propylene/Propane Separation. Experimental Data and Molecular Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 8116-8124	3.8	86
218	Molecular modeling of imidazolium-based [Tf2N-] ionic liquids: microscopic structure, thermodynamic and dynamic properties, and segmental dynamics. *Journal of Physical Chemistry B*, **2009**, 113, 7211-24	3.4	85

217	Mutual solubilities of hydrocarbons and water: III. 1-hexene; 1-octene; C10?C12 hydrocarbons. *AICHE Journal*, **1997**, 43, 535-546	3.6	82
216	Prediction of the phase equilibria of methane hydrates using the direct phase coexistence methodology. *Journal of Chemical Physics*, **2015**, 142, 044501	3.9	81
215	Evaluation of Statistical Associating Fluid Theory (SAFT) and Perturbed Chain-SAFT Equations of State for the Calculation of Thermodynamic Derivative Properties of Fluids Related to Carbon Capture and Sequestration. *Energy & Fuels*, **2011**, 25, 3334-3343	4.1	80
214	Transferable potentials for phase equilibria-united atom description of five- and six-membered cyclic alkanes and ethers. *Journal of Physical Chemistry B*, **2012**, 116, 11234-46	3.4	79
213	Evaluation of Cubic, SAFT, and PC-SAFT Equations of State for the Vapor□liquid Equilibrium Modeling of CO2 Mixtures with Other Gases. *Industrial & Engineering Chemistry Research*, **2013**, 52, 3933-3942	3.9	78
212	Molecular Simulation Studies of the Diffusion of Methane, Ethane, Propane, and Propylene in ZIF-8. *Journal of Physical Chemistry C*, **2015**, 119, 27028-27037	3.8	74
211	Molecular Dynamics Simulation of n-Alkanes and CO2 Confined by Calcite Nanopores. *Energy & Fuels*, **2018**, 32, 1934-1941	4.1	73
210	Effect of the Integration Method on the Accuracy and Computational Efficiency of Free Energy Calculations Using Thermodynamic Integration. *Journal of Chemical Theory and Computation*, **2010**, 6, 1018-1027	6.4	71
209	Density-tuned polyolefin phase equilibria. 2. Multicomponent solutions of alternating poly(ethylene-propylene) in subcritical and supercritical olefins. Experiment and SAFT model. *Macromolecules*, **1992**, 25, 4987-4995	5.5	71
208	Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies. *Molecular Simulation*, **2019**, 45, 425-453	2	69
207	Equation of state with multiple associating sites for water and water-hydrocarbon mixtures. *Industrial & Engineering Chemistry Research*, **1992**, 31, 2388-2394	3.9	68
206	Evaluation of the Truncated Perturbed Chain-Polar Statistical Associating Fluid Theory for Complex Mixture Fluid Phase Equilibria. *Industrial & Engineering Chemistry Research*, **2006**, 45, 6063-6074	3.9	64
205	Atomistic molecular dynamics simulations of CO□diffusivity in H□O for a wide range of temperatures and pressures. *Journal of Physical Chemistry B*, **2014**, 118, 5532-41	3.4	63
204	Viscosity, Interfacial Tension, Self-Diffusion Coefficient, Density, and Refractive Index of the Ionic Liquid 1-Ethyl-3-methylimidazolium Tetracyanoborate as a Function of Temperature at Atmospheric Pressure. *Journal of Chemical & Engineering Data*, **2012**, 57, 828-835	2.8	63
203	Morphology and Organization of Poly(propylene imine) Dendrimers in the Melt from Molecular Dynamics Simulation. *Macromolecules*, **2002**, 35, 1814-1821	5.5	60
202	System-size corrections for self-diffusion coefficients calculated from molecular dynamics simulations: The case of CO2, n-alkanes, and poly(ethylene glycol) dimethyl ethers. *Journal of Chemical Physics*, **2016**, 145, 074109	3.9	60
201	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain Statistical Associating Fluid Theory (sPC-SAFT). 1. Vapor□liquid Equilibria. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5636-5650	3.9	59
200	Molecular simulation of diffusion of hydrogen, carbon monoxide, and water in heavy n-alkanes. *Journal of Physical Chemistry B*, **2011**, 115, 1429-39	3.4	57

199	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain Statistical Associating Fluid Theory (sPC-SAFT). 2. Liquid Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5651-5659	3.9	57
198	On the calculation of the chemical potential using the particle deletion scheme. *Molecular Physics*, **1999**, 96, 905-913	1.7	56
197	Computational Study of ZIF-8 and ZIF-67 Performance for Separation of Gas Mixtures. *Journal of Physical Chemistry C*, **2017**, 121, 17999-18011	3.8	50
196	Thermodynamic and Transport Properties of H2O + NaCl from Polarizable Force Fields. *Journal of Chemical Theory and Computation*, **2015**, 11, 3802-10	6.4	49
195	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. *Journal of Chemical Physics*, **2014**, 141, 234507	3.9	49
194	Use of monomer fraction data in the parametrization of association theories. *Fluid Phase Equilibria*, **2010**, 296, 219-229	2.5	49
193	Molecular Dynamics Simulations of Electric Field Poled Nonlinear Optical Chromophores Incorporated in a Polymer Matrix. *Journal of Physical Chemistry B*, **2004**, 108, 588-596	3.4	49
192	Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. *Physical Review Letters*, **1998**, 80, 4466-4469	7.4	49
191	A transient outflow model for pipeline puncture. *Chemical Engineering Science*, **2003**, 58, 4591-4604	4.4	45
190	Molecular Dynamics Simulation of Structure and Thermodynamic Properties of Poly(dimethylsilamethylene) and Hydrocarbon Solubility Therein: Toward the Development of Novel Membrane Materials for Hydrocarbon Separation. *Macromolecules*, **2004**, 37, 1102-1112	5.5	44
189	Molecular Simulation of Phase Equilibria for Water-Butane and Water-Hexane Mixtures. *Journal of Physical Chemistry B*, **2000**, 104, 4958-4963	3.4	44
188	Modeling the phase behavior in mixtures of pharmaceuticals with liquid or supercritical solvents. *Journal of Physical Chemistry B*, **2009**, 113, 6446-58	3.4	43
187	Thermodynamics of pharmaceuticals: Prediction of solubility in pure and mixed solvents with PC-SAFT. *Fluid Phase Equilibria*, **2011**, 302, 331-337	2.5	42
186	The role of intermolecular interactions in the prediction of the phase equilibria of carbon dioxide hydrates. *Journal of Chemical Physics*, **2015**, 143, 094506	3.9	41
185	Equations of state: From the ideas of van der Waals to association theories. *Journal of Supercritical Fluids*, **2010**, 55, 421-437	4.2	41
184	Thermodynamics of Chain Fluids from Atomistic Simulation: A Test of the Chain Increment Method for Chemical Potential. *Macromolecules*, **1997**, 30, 4744-4755	5.5	41
183	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. *Journal of Chemical Physics*, **2001**, 115, 8231-8237	3.9	41
182	Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study. *Journal of Chemical Physics*, **2016**, 145, 084702	3.9	40

181	Equation of state modeling of the phase equilibria of ionic liquid mixtures at low and high pressure. *Physical Chemistry Chemical Physics*, **2008**, 10, 6160-8	3.6	39
180	Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane, and Squalane. *Journal of Physical Chemistry B*, **2016**, 120, 12890-12900	3.4	39
179	Prediction of the n-hexane/water and 1-octanol/water partition coefficients for environmentally relevant compounds using molecular simulation. *AICHE Journal*, **2012**, 58, 1929-1938	3.6	38
178	Equations of state for hydrogen bonding systems. *Fluid Phase Equilibria*, **1996**, 116, 518-529	2.5	37
177	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. *Molecular Simulation*, **2013**, 39, 1135-1142	2	36
176	Modeling the phase equilibria of a H2O□CO2 mixture with PC-SAFT and tPC-PSAFT equations of state. *Molecular Physics*, **2012**, 110, 1205-1212	1.7	36
175	Fast numerical simulation for full bore rupture of pressurized pipelines. *AICHE Journal*, **1999**, 45, 1191-1201	3.6	36
174	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. *Energy & Fuels*, **2017**, 31, 6004-6018	4.1	35
173	Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves. *Macromolecules*, **2005**, 38, 386-397	5.5	35
172	Simultaneous determination of thermal and mutual diffusivity of binary mixtures of n-octacosane with carbon monoxide, hydrogen, and water by dynamic light scattering. *Journal of Physical Chemistry B*, **2014**, 118, 3981-90	3.4	34
171	Phase equilibrium calculations for multi-component polar fluid mixtures with tPC-PSAFT. *Fluid Phase Equilibria*, **2007**, 261, 265-271	2.5	34
170	Tailoring the gas separation efficiency of metal organic framework ZIF-8 through metal substitution: a computational study. *Physical Chemistry Chemical Physics*, **2018**, 20, 4879-4892	3.6	33
169	Transport Properties of Shale Gas in Relation to Kerogen Porosity. *Journal of Physical Chemistry C*, **2018**, 122, 6166-6177	3.8	32
168	Thermophysical properties of the ionic liquids [EMIM][B(CN)4] and [HMIM][B(CN)4]. *Journal of Physical Chemistry B*, **2013**, 117, 8512-23	3.4	32
167	An integrated, multi-scale modelling approach for the simulation of multiphase dispersion from accidental CO2 pipeline releases in realistic terrain. *International Journal of Greenhouse Gas Control*, **2014**, 27, 221-238	4.2	31
166	Henry's Constant Analysis for Water and Nonpolar Solvents from Experimental Data, Macroscopic Models, and Molecular Simulation. *Journal of Physical Chemistry B*, **2001**, 105, 7792-7798	3.4	31
165	Self-diffusion coefficients of the binary (H 2 O + CO 2) mixture at high temperatures and pressures. *Journal of Chemical Thermodynamics*, **2016**, 93, 424-429	2.9	30
164	Methane solubility in aqueous solutions under two-phase (H□w) hydrate equilibrium conditions. *Fluid Phase Equilibria*, **2014**, 371, 106-120	2.5	30

163	Influence of combining rules on the cavity occupancy of clathrate hydrates by Monte Carlo simulations. *Molecular Physics*, **2014**, 112, 2258-2274	1.7	30
162	Using molecular simulation to predict solute solvation and partition coefficients in solvents of different polarity. *Physical Chemistry Chemical Physics*, **2011**, 13, 9155-64	3.6	30
161	Atomistic Simulation of Poly(dimethylsiloxane): Force Field Development, Structure, and Thermodynamic Properties of Polymer Melt and Solubility of n-Alkanes, n-Perfluoroalkanes, and Noble and Light Gases. *Macromolecules*, **2007**, 40, 1720-1729	5.5	30
160	Equation of State Description of Thermodynamic Properties of Near-Critical and Supercritical Water. *The Journal of Physical Chemistry*, **1994**, 98, 12080-12085		30
159	Industrial Requirements for Thermodynamic and Transport Properties: 2020. *Industrial & Engineering Chemistry Research*, **2021**, 60, 4987-5013	3.9	30
158	Molecular Dynamics Simulation of Pure -Alkanes and Their Mixtures at Elevated Temperatures Using Atomistic and Coarse-Grained Force Fields. *Journal of Physical Chemistry B*, **2019**, 123, 6229-6243	3.4	29
157	Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon. *Molecular Physics*, **2012**, 110, 1153-1160	1.7	29
156	Molecular dynamics simulations of the diffusion coefficients of light n-alkanes in water over a wide range of temperature and pressure. *Fluid Phase Equilibria*, **2016**, 407, 236-242	2.5	28
155	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370	3.4	28
154	Thermodynamic and transport property models for carbon capture and sequestration (CCS) processes with emphasis on CO2 transport. *Chemical Engineering Research and Design*, **2013**, 91, 1793-1806	5.5	28
153	Modeling the solid□liquid equilibrium in pharmaceutical-solvent mixtures: Systems with complex hydrogen bonding behavior. *AICHE Journal*, **2009**, 55, 756-770	3.6	28
152	Atomistic molecular dynamics simulations of H2O diffusivity in liquid and supercritical CO2. *Molecular Physics*, **2015**, 113, 2805-2814	1.7	27
151	Molecular Dynamics Simulation of Highly Confined Glassy Ionic Liquids. *Journal of Physical Chemistry C*, **2016**, 120, 1013-1024	3.8	27
150	Optimization of intermolecular potential parameters for the CO2/H2O mixture. *Journal of Physical Chemistry B*, **2014**, 118, 11504-11	3.4	27
149	Modeling fluid phase transition effects on dynamic behavior of ESDV. *AICHE Journal*, **2000**, 46, 997-1006	3.6	27
148	Development of a united-atom force field for 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid. *Molecular Physics*, **2012**, 110, 1115-1126	1.7	26
147	Modeling of fluid phase equilibria with two thermodynamic theories: Non-random hydrogen bonding (NRHB) and statistical associating fluid theory (SAFT). *Fluid Phase Equilibria*, **2007**, 253, 19-28	2.5	26
146	Molecular Simulation of □Olefins Using a New United-Atom Potential Model: Vapor□liquid Equilibria of Pure Compounds and Mixtures. *Journal of the American Chemical Society*, **1999**, 121, 3407-3413	16.4	26

145	Phase behavior of LCST and UCST solutions of branchy copolymers: experiment and SAFT modelling. *Fluid Phase Equilibria*, **1993**, 83, 391-398	2.5	26
144	Mutual and Self-Diffusivities in Binary Mixtures of [EMIM][B(CN)4] with Dissolved Gases by Using Dynamic Light Scattering and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 8583-92	3.4	25
143	A thermodynamic model for strong aqueous electrolytes based on the eSAFT-VR Mie equation of state. *Fluid Phase Equilibria*, **2018**, 464, 47-63	2.5	25
142	Gaussian-Charge Polarizable and Nonpolarizable Models for CO2. *Journal of Physical Chemistry B*, **2016**, 120, 984-94	3.4	25
141	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. *Langmuir* , **2017**, 33, 11291-11298	4	25
140	CO2PipeHaz: Quantitative Hazard Assessment for Next Generation CO2 Pipelines. *Energy Procedia*, **2014**, 63, 2510-2529	2.3	25
139	Equations of state and activity coefficient models for vapor-liquid equilibria of polymer solutions. *AICHE Journal*, **1994**, 40, 1711-1727	3.6	25
138	Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 23121-38	3.6	25
137	On the Efficient Separation of Gas Mixtures with the Mixed-Linker Zeolitic-Imidazolate Framework-7-8. *ACS Applied Materials & Interfaces*, **2018**, 10, 39631-39644	9.5	25
136	Characterization of Long Linear and Branched Alkanes and Alcohols for Temperatures up to 573.15 K by Surface Light Scattering and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 4146-4163	3.4	24
135	Diffusivities of Ternary Mixtures of n-Alkanes with Dissolved Gases by Dynamic Light Scattering. *Journal of Physical Chemistry B*, **2016**, 120, 10808-10823	3.4	24
134	Diffusion in Homogeneous and in Inhomogeneous Media: A New Unified Approach. *Journal of Chemical Theory and Computation*, **2016**, 12, 5247-5255	6.4	24
133	Direct phase coexistence molecular dynamics study of the phase equilibria of the ternary methane-carbon dioxide-water hydrate system. *Physical Chemistry Chemical Physics*, **2016**, 18, 23538-48	3.6	24
132	Predictions of water/oil interfacial tension at elevated temperatures and pressures: A molecular dynamics simulation study with biomolecular force fields. *Fluid Phase Equilibria*, **2018**, 476, 30-38	2.5	23
131	Structure, thermodynamic and transport properties of imidazolium-based bis(trifluoromethylsulfonyl)imide ionic liquids from molecular dynamics simulations. *Molecular Physics*, **2012**, 110, 1139-1152	1.7	23
130	Transport properties of silmethylene homo-polymers and random copolymers: experimental measurements and molecular simulation. *Polymer*, **2004**, 45, 6933-6944	3.9	23
129	Water-Salt Phase Equilibria at Elevated Temperatures and Pressures: Model Development and Mixture Predictions. *The Journal of Physical Chemistry*, **1995**, 99, 6182-6193		23
128	Solubilities of solid polynuclear aromatics (PNA's) in supercritical ethylene and ethane from statistical associating fluid theory (SAFT): toward separating PNA's by size and structure. *Industrial & Engineering Chemistry Research*, **1992**, 31, 2620-2624	3.9	22

127	Techno-economic assessment of CO2 quality effect on its storage and transport: CO2QUEST: An overview of aims, objectives and main findings. *International Journal of Greenhouse Gas Control*, **2016**, 54, 662-681	4.2	22
126	Phase Equilibria of Water/CO and Water/n-Alkane Mixtures from Polarizable Models. *Journal of Physical Chemistry B*, **2017**, 121, 1386-1395	3.4	21
125	Hydrate Fluid phase equilibria modeling using PC-SAFT and Peng Robinson equations of state. *Fluid Phase Equilibria*, **2016**, 413, 209-219	2.5	21
124	Thermodynamics of Lewis acid-base mixtures. *AICHE Journal*, **1990**, 36, 1851-1864	3.6	21
123	Viscosity of heavy n -alkanes and diffusion of gases therein based on molecular dynamics simulations and empirical correlations. *Journal of Chemical Thermodynamics*, **2015**, 91, 101-107	2.9	20
122	Storage of Methane in Clathrate Hydrates: Monte Carlo Simulations of sI Hydrates and Comparison with Experimental Measurements. *Journal of Chemical & Engineering Data*, **2016**, 61, 2886-2896	2.8	20
121	Enthalpy of dissociation of methane hydrates at a wide pressure and temperature range. *Fluid Phase Equilibria*, **2019**, 489, 30-40	2.5	19
120	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. *Journal of Physical Chemistry C*, **2018**, 122, 17170-17183	3.8	19
119	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
118	Predicting hydration Gibbs energies of alkyl-aromatics using molecular simulation: a comparison of current force fields and the development of a new parameter set for accurate solvation data. *Physical Chemistry Chemical Physics*, **2011**, 13, 17384-94	3.6	19
117	Multi-scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-based Ionic Liquids: Ab initio DFT Calculations, Molecular Simulation and Equation of State Predictions. *Oil and Gas Science and Technology*, **2008**, 63, 283-293	1.9	19
116	Evaluation of SAFT and PC-SAFT models for the description of homo- and co-polymer solution phase equilibria. *Polymer*, **2005**, 46, 10772-10781	3.9	19
115	Monte Carlo simulation studies of clathrate hydrates: A review. *Journal of Supercritical Fluids*, **2018**, 134, 51-60	4.2	19
114	Molecular dynamics simulation of structure, thermodynamic, and dynamic properties of poly(dimethylsilamethylene), poly(dimethylsilatrimethylene) and their alternating copolymer. *Journal of Physical Chemistry B*, **2006**, 110, 16047-58	3.4	18
113	Mean field calculations of thermodynamic properties of supercritical fluids. *AICHE Journal*, **1990**, 36, 1920-1925	3.6	18
112	Molecular dynamics simulations of pure methane and carbon dioxide hydrates: lattice constants and derivative properties. *Molecular Physics*, **2016**, 114, 2672-2687	1.7	17
111	Atomistic Simulation of Poly(dimethylsiloxane) Permeability Properties to Gases and n-Alkanes. *Macromolecules*, **2008**, 41, 5899-5907	5.5	17
110	Modeling of multicomponent vapor liquid equilibria for polymer solvent systems. *Fluid Phase Equilibria*, **2004**, 220, 11-20	2.5	17

109	Monte Carlo simulation of phase equilibria of aqueous systems. *Fluid Phase Equilibria*, **2001**, 183-184, 259-269	2.5	17
108	Benchmark Database Containing Binary-System-High-Quality-Certified Data for Cross-Comparing Thermodynamic Models and Assessing Their Accuracy. *Industrial & Engineering Chemistry Research*, **2020**, 59, 14981-15027	3.9	17
107	Molecular Modeling of Thermodynamic and Transport Properties for CO and Aqueous Brines. *Accounts of Chemical Research*, **2017**, 50, 751-758	24.3	16
106	Molecular simulation of structure, thermodynamic and transport properties of polyacrylonitrile, polystyrene and their alternating copolymers in high temperatures. *European Polymer Journal*, **2011**, 47, 735-745	5.2	16
105	Molecular simulation of absolute hydration Gibbs energies of polar compounds. *Fluid Phase Equilibria*, **2010**, 296, 110-115	2.5	16
104	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. *Macromolecules*, **2008**, 41, 6228-6238	5.5	16
103	Monte Carlo Simulation of the Phase Behavior of Model Dendrimers. *Macromolecules*, **2006**, 39, 6298-6305	5.5	16
102	Thermophysical Properties of Homologous Tetracyanoborate-Based Ionic Liquids Using Experiments and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 4145-4157	3.4	15
101	Modeling of physical properties and vapor–liquid equilibrium of ethylene and ethylene mixtures with equations of state. *Fluid Phase Equilibria*, **2018**, 470, 149-163	2.5	15
100	Molecular simulations of imidazolium-based tricyanomethanide ionic liquids using an optimized classical force field. *Physical Chemistry Chemical Physics*, **2016**, 18, 6850-60	3.6	15
99	CO2QUEST: Techno-economic Assessment of CO2 Quality Effect on Its Storage and Transport. *Energy Procedia*, **2014**, 63, 2622-2629	2.3	15
98	Molecular simulation and macroscopic modeling of the diffusion of hydrogen, carbon monoxide and water in heavy n-alkane mixtures. *Physical Chemistry Chemical Physics*, **2012**, 14, 4133-41	3.6	15
97	Molecular simulation of the hydration Gibbs energy of barbiturates. *Fluid Phase Equilibria*, **2010**, 289, 148-155	2.5	15
96	Temperature-induced crystallization in concentrated suspensions of multiarm star polymers: a molecular dynamics study. *Journal of Chemical Physics*, **2006**, 124, 044905	3.9	15
95	Thermophysical properties of diphenylmethane and dicyclohexylmethane as a reference liquid organic hydrogen carrier system from experiments and molecular simulations. *International Journal of Hydrogen Energy*, **2020**, 45, 28903-28919	6.7	15
94	The effect of lattice constant on the storage capacity of hydrogen hydrates: a Monte Carlo study. *Molecular Physics*, **2016**, 114, 2664-2671	1.7	15
93	Lattice constants of pure methane and carbon dioxide hydrates at low temperatures. Implementing quantum corrections to classical molecular dynamics studies. *Journal of Chemical Physics*, **2016**, 144, 124512	2.9	15
92	Identification of conditions for increased methane storage capacity in sII and sH clathrate hydrates from Monte Carlo simulations. *Journal of Chemical Thermodynamics*, **2018**, 117, 128-137	2.9	14

91	Modeling of CO2 solubility in single and mixed electrolyte solutions using statistical associating fluid theory. *Geochimica Et Cosmochimica Acta*, **2016**, 176, 185-197	5.5	14
90	Solubility of gases and solvents in silicon polymers: molecular simulation and equation of state modeling. *Molecular Simulation*, **2007**, 33, 851-860	2	14
89	Estimation of endoglucanase and lysozyme effective diffusion coefficients in polysulphone membranes. *Journal of Biotechnology*, **1999**, 72, 77-83	3.7	14
88	Thermodynamic inconsistencies in and accuracy of chemical equations of state for associating fluids. *Industrial & Engineering Chemistry Research*, **1992**, 31, 1203-1211	3.9	14
87	Quantifying Pore Width Effects on Diffusivity via a Novel 3D Stochastic Approach with Input from Atomistic Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 6907-6922	5.4	13
86	Analysis of the heterogeneous dynamics of imidazolium-based [Tf2N] ionic liquids using molecular simulation. *Molecular Physics*, **2014**, 112, 2694-2706	1.7	13
85	Industrial use of thermodynamics workshop: Round table discussion on 8 July 2014. *Chemical Engineering Research and Design*, **2014**, 92, 2795-2796	5.5	13
84	A Study of the Dynamic Response of Emergency Shutdown Valves Following Full Bore Rupture of Gas Pipelines. *Chemical Engineering Research and Design*, **1997**, 75, 201-209	5.5	13
83	Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation. *Fluid Phase Equilibria*, **2005**, 228-229, 15-20	2.5	13
82	Phase Equilibria Prediction of Hydrogen Fluoride Systems from an Associating Model. *Industrial & Engineering Chemistry Research*, **1995**, 34, 1868-1872	3.9	13
81	Effect of hard-sphere structure on pure-component equation of state calculations. *Fluid Phase Equilibria*, **1992**, 73, 39-55	2.5	13
80	On the validity of the Stokes Einstein relation for various water force fields. *Molecular Physics*, **2020**, 118, e1702729	1.7	13
79	Storage of H2 in Clathrate Hydrates: Evaluation of Different Force-Fields used in Monte Carlo Simulations. *Molecular Physics*, **2017**, 115, 1274-1285	1.7	12
78	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. *Nanomaterials*, **2020**, 10,	5.4	12
77	Two- and three-phase equilibrium experimental measurements for the ternary CH 4 + CO 2 + H 2 O mixture. *Fluid Phase Equilibria*, **2017**, 451, 96-105	2.5	12
76	Lattice-Fluid Theory Prediction of High-Density Polyethylene Branched Polyolefin Blend Miscibility. *Macromolecules*, **2000**, 33, 4954-4960	5.5	12
75	Equation-of-State Modeling of Solid Liquid Gas Equilibrium of CO2 Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2016**, 55, 6213-6226	3.9	12
74	Molecular Simulation of n-Octacosane Water Mixture in Titania Nanopores at Elevated Temperature and Pressure. *Journal of Physical Chemistry C*, **2016**, 120, 24743-24753	3.8	12

73	CO2 selective metal organic framework ZIF-8 modified through ionic liquid encapsulation: A computational study. *Journal of Computational Science*, **2018**, 27, 183-191	3.4	12
72	Using clathrate hydrates for gas storage and gas-mixture separations: experimental and computational studies at multiple length scales. *Molecular Physics*, **2018**, 116, 2041-2060	1.7	12
71	Recent Advances in Experimental Measurements of Mixed-Gas Three-Phase Hydrate Equilibria for Gas Mixture Separation and Energy-Related Applications. *Journal of Chemical & Engineering Data*, **2019**, 64, 4991-5016	2.8	11
70	Prediction of microscopic structure and physical properties of complex fluid mixtures based on molecular simulation. *Fluid Phase Equilibria*, **2010**, 296, 125-132	2.5	11
69	Molecular simulation of structure and thermodynamic properties of pure tri- and tetra-ethylene glycols and their aqueous mixtures. *Fluid Phase Equilibria*, **2006**, 248, 134-146	2.5	11
68	Phase Equilibrium with External Fields: Application to Confined Fluids. *Journal of Chemical & Engineering Data*, **2016**, 61, 2873-2885	2.8	11
67	Monte Carlo simulations of the separation of a binary gas mixture (CH + CO) using hydrates. *Physical Chemistry Chemical Physics*, **2018**, 20, 28026-28038	3.6	11
66	Molecular dynamics simulation of electrolyte solutions confined by calcite mesopores. *Fluid Phase Equilibria*, **2019**, 487, 24-32	2.5	10
65	Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures. *Computers and Chemical Engineering*, **2016**, 95, 49-57	4	10
64	Two-body perturbation theory versus first order perturbation theory: A comparison based on the square-well fluid. *Journal of Chemical Physics*, **2017**, 147, 214108	3.9	10
63	Influence of combining rules on the cavity occupancy of clathrate hydrates using van der Waals□Platteeuw-theory-based modelling. *Chemical Engineering Research and Design*, **2014**, 92, 2992-3007	5.5	10
62	Phase equilibrium of colloidal suspensions with particle size dispersity: a Monte Carlo study. *Journal of Chemical Physics*, **2009**, 130, 194902	3.9	10
61	Modeling of Liquid□Liquid Phase Equilibria in Aqueous Solutions of Poly(ethylene glycol) with a UNIFAC-Based Model. *Industrial & Engineering Chemistry Research*, **2003**, 42, 5399-5408	3.9	10
60	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. *AICHE Journal*, **2019**, 65, 792-803	3.6	10
59	Defining New Limits in Gas Separations Using Modified ZIF Systems. *ACS Applied Materials & Interfaces*, **2020**, 12, 20536-20547	9.5	10
58	Computational investigation of the performance of ZIF-8 with encapsulated ionic liquids towards CO2 capture** This publication is dedicated to Professor Peter Cummings on the occasion of his 65th birthday. Professor Cummings has been an international leader in the field of computational	1.7	9
57	Solubility of Methane and Carbon Dioxide in the Aqueous Phase of the Ternary (Methane + Carbon Dioxide + Water) Mixture: Experimental Measurements and Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data*, **2018**, 63, 1027-1035	2.8	9
56	Characterization of Water Solubility in n-Octacosane Using Raman Spectroscopy. *Journal of Physical Chemistry B*, **2017**, 121, 10665-10673	3.4	9

55	Molecular Simulation of the Pure n-Hexadecane Vapor–Liquid Equilibria at Elevated Temperature. *Macromolecules*, **1998**, 31, 1430-1431	5.5	9
54	Calculation of the phase envelope of multicomponent mixtures with the bead spring method. *AICHE Journal*, **2016**, 62, 868-879	3.6	9
53	Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends. *Macromolecules*, **2007**, 40, 2904-2914	5.5	8
52	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs with Unsubstituted Imidazolate Linkers for Propylene/Propane and n-Butane/i-Butane Separations. *Angewandte Chemie - International Edition*, **2021**, 60, 10103-10111	16.4	8
51	Encapsulation of [bmim+][Tf2N–] in different ZIF-8 metal analogues and evaluation of their CO2 selectivity over CH4 and N2 using molecular simulation. *Molecular Systems Design and Engineering*, **2020**, 5, 1230-1238	4.6	7
50	Development of a novel experimental apparatus for hydrate equilibrium measurements. *Fluid Phase Equilibria*, **2016**, 424, 152-161	2.5	7
49	Calculation of the effect of macromolecular architecture on structure and thermodynamic properties of linear–tri-arm polyethylene blends from Monte Carlo simulation. *Polymer*, **2007**, 48, 3883-3892	3.9	6
48	Modeling the thermodynamic properties of CFC and HCFC compounds, and the vapor-liquid equilibria of CFC and HCFC mixtures and CFC/HCFC-hydrocarbon mixtures, with the perturbed anisotropic chain theory (PACT). *Fluid Phase Equilibria*, **1994**, 97, 13-28	2.5	6
47	Hydrogen bonding in polymer-solvent mixtures. *Macromolecules*, **1991**, 24, 5058-5067	5.5	6
46	Solid–liquid–Gas Equilibrium of Methane–n-Alkane Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2018**, 57, 8566-8583	3.9	5
45	Structural and dynamical analysis of monodisperse and polydisperse colloidal systems. *Journal of Chemical Physics*, **2010**, 133, 224901	3.9	5
44	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. *Journal of Supercritical Fluids*, **2010**, 55, 503-509	4.2	5
43	Assessment of the Perturbed Chain-Statistical Associating Fluid Theory Equation of State against a Benchmark Database of High-Quality Binary-System Data. *Industrial & Engineering Chemistry Research*, **2021**, 60, 8935-8946	3.9	5
42	Evaluation of the Efficiency of Clathrate Hydrates in Storing Energy Gases. *Journal of Physics: Conference Series*, **2015**, 640, 012026	0.3	4
41	Comments on "Thermodynamic inconsistencies in and accuracy of chemical equations of state for associating fluids". *Industrial & Engineering Chemistry Research*, **1993**, 32, 245-246	3.9	4
40	Measurement of infinite dilution activity coefficients using high performance liquid chromatography. *Fluid Phase Equilibria*, **1991**, 68, 131-149	2.5	4
39	A Practical Methodology to Estimate the H2 Storage Capacity of Pure and Binary Hydrates Based on Monte Carlo Simulations. *Journal of Chemical & Engineering Data*, **2020**, 65, 1289-1299	2.8	4
38	Thermodynamics 2011 Conference Athens, Greece, 31 August– September 2011 http://www.thermodynamics2011.org/. *Molecular Physics*, **2012**, 110, 1053-1056	1.7	3

37	Peculiarities of electric field alignment of nonlinear optical chromophores incorporated into thin film polymer matrix. *Theoretical Chemistry Accounts*, **2005**, 114, 153-158	1.9	3
36	Phase behavior of the binary refrigerant mixture chlorodifluoro-ethane (R22)-1,1,1,2-tetrafluoro-ethane (R134a): experimental investigation and theoretical modelling using the perturbed-anisotropic-chain theory (PACT). *Fluid Phase Equilibria*, **1995**, 111, 239-252	2.5	3
35	Closed-form expressions for chemical theory of associating mixtures. *AICHE Journal*, **1992**, 38, 611-614	3.6	3
34	What Is the Optimal Activity Coefficient Model To Be Combined with the translated-consistent Peng-Robinson Equation of State through Advanced Mixing Rules? Cross-Comparison and Grading of the Wilson, UNIQUAC, and NRTL aE Models against a Benchmark Database Involving 200 Binary Systems. *Industrial & Engineering Chemistry Research*, **2021**, 60, 17228-17247	3.9	3
33	Modeling of Gas Solubility in Aqueous Electrolyte Solutions with the eSAFT-VR Mie Equation of State. *Industrial & Engineering Chemistry Research*, **2021**, 60, 15327-15342	3.9	3
32	Chapter 4:Cubic and Generalized van der Waals Equations of State **2010**, 53-83		3
31	On the calculation of the chemical potential using the particle deletion scheme		3
30	Water-Hydrocarbon Phase Equilibria with SAFT-VR Mie Equation of State. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5278-5299	3.9	3
29	Modeling confined fluids with the multicomponent potential theory of adsorption and the SAFT-VR Mie equation of state. *Fluid Phase Equilibria*, **2021**, 534, 112941	2.5	3
28	Monte Carlo Molecular Simulation Study of Carbon Dioxide Sequestration into Dry and Wet Calcite Pores Containing Methane. *Energy & Fuels*, **2021**, 35, 11393-11402	4.1	3
27	Molecular Simulation Methods for CO2 Capture and Gas Separation with Emphasis on Ionic Liquids **2017**, 79-111		2
26	Thermodynamics 2015 Conference Copenhagen, Denmark, 15-18 September 2015. *Molecular Physics*, **2016**, 114, 2569-2573	1.7	2
25	Efficient and robust methods for direct saturation point calculations. *Fluid Phase Equilibria*, **2019**, 500, 112242	2.5	2
24	Phase Equilibria in Binary Mixtures of Propane and Phenanthrene: Experimental Data and Modeling with the GC-EoS. *Journal of Chemical & Engineering Data*, **2011**, 56, 1407-1413	2.8	2
23	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain-Statistical Associating Fluid Theory (sPC-SAFT). 2. Liquid-Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems. *Industrial & Engineering Chemistry Research*, **2009**, 48, 7860-7860	3.9	2
22	Partition coefficients of organic molecules in squalane and water/ethanol mixtures by molecular dynamics simulations. *Fluid Phase Equilibria*, **2011**, 306, 162-170	2.5	2
21	Amorphous and crystalline states of ultrasoft colloids: a molecular dynamics study. *Rheologica Acta*, **2007**, 46, 755-764	2.3	2
20	Investigation of the physicochemical characteristics of ancient mortars by static and dynamic studies. *Cement and Concrete Research*, **2000**, 30, 1151-1155	10.3	2

19	Equation-of-state calculations of chemical reaction equilibrium in nonideal systems. *International Journal of Thermophysics*, **1993**, 14, 199-213	2.1	2
18	13 The Role of Molecular Thermodynamics in Developing Industrial Processes and Novel Products That Meet the Needs for a Sustainable Future. *Green Chemistry and Chemical Engineering*, **2017**, 633-660		2
17	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs with Unsubstituted Imidazolate Linkers for Propylene/Propane and n-Butane/i-Butane Separations. *Angewandte Chemie*, **2021**, 133, 10191-10199	3.6	2
16	Construction of phase envelopes for binary and multicomponent mixtures with Euler-Newton predictor-corrector methods. *Fluid Phase Equilibria*, **2020**, 505, 112338	2.5	2
15	Molecular Dynamics Simulation of the n-Octacosane–Water Mixture Confined in Graphene Mesopores: Comparison of Atomistic and Coarse-Grained Calculations and the Effect of Catalyst Nanoparticle. *Energy & Fuels*, **2021**, 35, 4313-4332	4.1	2
14	**2018**,		2
13	Molecular dynamics simulation of the n-octacosane-water mixture confined in hydrophilic and hydrophobic mesopores: The effect of oxygenates. *Fluid Phase Equilibria*, **2020**, 526, 112816	2.5	1
12	Novel methodology for the calculation of the enthalpy of enclathration of methane hydrates using molecular dynamics simulations. *Molecular Physics*, **2020**, 118, e1711976	1.7	1
11	Determination of liquid–gas partition coefficients of BuA and MMA by headspace-gas chromatography utilizing the phase ratio variation method. *Fluid Phase Equilibria*, **2008**, 266, 21-30	2.5	1
10	Molecular Simulation of Phase Equilibria for Industrial Applications. *Computer Aided Chemical Engineering*, **2004**, 279-307	0.6	1
9	Multi-Scale Models for the Prediction of Microscopic Structure and Physical Properties of Chemical Systems Related to Natural Gas Technology **2018**, 463-497		1
8	Atomistic Simulations of Clathrate Hydrates **2015**, 351-359		0
7	Rigorous Phase Equilibrium Calculation Methods for Strong Electrolyte Solutions: The Isothermal Flash. *Fluid Phase Equilibria*, **2022**, 558, 113441	2.5	0
6	Gas Solubility in Aqueous Solutions Under Two-Phase (H–w) Hydrate Equilibrium Conditions **2015**, 205-212		
5	The Role of Molecular Thermodynamics and Simulation in Natural Gas Sustainable Processes **2010**, 299-309		
4	Inductive construction of 2-connected graphs for calculating the virial coefficients. *Journal of Physics A: Mathematical and Theoretical*, **2010**, 43, 315004	2	
3	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design **2015**, 361-370		
2	Molecular Modeling of Gas Treatment Processes with Emphasis to GTL Process **2012**, 319-325		

List of Publications

1 Thermodynamic Modeling of Relevance to Natural Gas Processing **2018**, 341-378