Ioannis Economou

List of Publications by Year in descending order

236 papers	8,618 citations	38660 50 h-index	69108 77 g-index
252 all docs	252 docs citations	252 times ranked	5251 citing authors

#	Article	IF	Citations
1	Statistical Associating Fluid Theory:Â A Successful Model for the Calculation of Thermodynamic and Phase Equilibrium Properties of Complex Fluid Mixtures. Industrial & Engineering Chemistry Research, 2002, 41, 953-962.	1.8	320
2	Industrial Requirements for Thermodynamics and Transport Properties. Industrial & Engineering Chemistry Research, 2010, 49, 11131-11141.	1.8	211
3	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, 9262-9269.	1.2	166
4	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. Journal of Physical Chemistry B, 1998, 102, 1029-1035.	1.2	159
5	Associating models and mixing rules in equations of state for water/hydrocarbon mixtures. Chemical Engineering Science, 1997, 52, 511-525.	1.9	139
6	Chemical, quasi-chemical and perturbation theories for associating fluids. AICHE Journal, 1991, 37, 1875-1894.	1.8	132
7	Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies. Molecular Simulation, 2019, 45, 425-453.	0.9	130
8	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.	1.6	125
9	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.	1.5	121
10	Water/Hydrocarbon Phase Equilibria Using the Thermodynamic Perturbation Theory. Industrial & Engineering Chemistry Research, 2000, 39, 797-804.	1.8	120
11	Extended statistical associating fluid theory (SAFT) equations of state for dipolar fluids. AICHE Journal, 2005, 51, 2328-2342.	1.8	118
12	Molecular Simulation of Phase Equilibria for Waterâ^'Methane and Waterâ^'Ethane Mixtures. Journal of Physical Chemistry B, 1998, 102, 8865-8873.	1.2	115
13	1-Octanol/Water Partition Coefficients of n-Alkanes from Molecular Simulations of Absolute Solvation Free Energies. Journal of Chemical Theory and Computation, 2009, 5, 2436-2446.	2.3	115
14	Prediction of the phase equilibria of methane hydrates using the direct phase coexistence methodology. Journal of Chemical Physics, 2015, 142, 044501.	1.2	111
15	Perturbed Chain-Statistical Associating Fluid Theory Extended to Dipolar and Quadrupolar Molecular Fluids. Journal of Physical Chemistry B, 2006, 110, 9252-9261.	1.2	110
16	Transferable Potentials for Phase Equilibriaâ€"United Atom Description of Five- and Six-Membered Cyclic Alkanes and Ethers. Journal of Physical Chemistry B, 2012, 116, 11234-11246.	1.2	106
17	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.	2.5	105
18	Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 1. Pure Fluids. Industrial & Engineering Chemistry Research, 2004, 43, 6592-6606.	1.8	103

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19	Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 2. Multicomponent Mixtures. Industrial & Engineering Chemistry Research, 2007, 46, 2628-2636.	1.8	102
20	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.	1.2	101
21	Evaluation of Cubic, SAFT, and PC-SAFT Equations of State for the Vaporâ€“Liquid Equilibrium Modeling of CO₂ Mixtures with Other Gases. Industrial & Engineering Chemistry Research, 2013, 52, 3933-3942.	1.8	100
22	Molecular Simulation Studies of the Diffusion of Methane, Ethane, Propane, and Propylene in ZIF-8. Journal of Physical Chemistry C, 2015, 119, 27028-27037.	1.5	94
23	tPC-PSAFT Modeling of Gas Solubility in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry C, 2007, 111, 15487-15492.	1.5	93
24	Molecular Dynamics Simulation of n-Alkanes and CO₂ Confined by Calcite Nanopores. Energy & Fuels, 2018, 32, 1934-1941.	2.5	93
25	Molecular Modeling of Imidazolium-Based [Tf₂N^{â^’}] Ionic Liquids: Microscopic Structure, Thermodynamic and Dynamic Properties, and Segmental Dynamics. Journal of Physical Chemistry B, 2009, 113, 7211-7224.	1.2	92
26	Industrial Requirements for Thermodynamic and Transport Properties: 2020. Industrial & Engineering Chemistry Research, 2021, 60, 4987-5013.	1.8	90
27	Mutual solubilities of hydrocarbons and water: III. 1-hexene; 1-octene; C10ï£¿C12 hydrocarbons. AICHE Journal, 1997, 43, 535-546.	1.8	85
28	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.	2.3	83
29	Atomistic Molecular Dynamics Simulations of CO₂ Diffusivity in H₂O for a Wide Range of Temperatures and Pressures. Journal of Physical Chemistry B, 2014, 118, 5532-5541.	1.2	83
30	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.	2.2	82
31	Equation of state with multiple associating sites for water and water-hydrocarbon mixtures. Industrial & Engineering Chemistry Research, 1992, 31, 2388-2394.	1.8	73
32	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.	1.8	73
33	Computational Study of ZIF-8 and ZIF-67 Performance for Separation of Gas Mixtures. Journal of Physical Chemistry C, 2017, 121, 17999-18011.	1.5	70
34	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chainâ^’Statistical Associating Fluid Theory (sPC-SAFT). 1. Vaporâ^’Liquid Equilibria. Industrial & Engineering Chemistry Research, 2008, 47, 5636-5650.	1.8	68
35	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chainâ^’Statistical Associating Fluid Theory (sPC-SAFT). 2. Liquidâ^’Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems. Industrial & Engineering Chemistry Research, 2008, 47, 5651-5659.	1.8	68
36	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.	1.0	68

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37	Morphology and Organization of Poly(propylene imine) Dendrimers in the Melt from Molecular Dynamics Simulation. Macromolecules, 2002, 35, 1814-1821.	2.2	66
38	On the calculation of the chemical potential using the particle deletion scheme. Molecular Physics, 1999, 96, 905-913.	0.8	64
39	Molecular Simulation of Diffusion of Hydrogen, Carbon Monoxide, and Water in Heavy n-Alkanes. Journal of Physical Chemistry B, 2011, 115, 1429-1439.	1.2	63
40	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. Journal of Chemical Physics, 2014, 141, 234507.	1.2	63
41	Thermodynamic and Transport Properties of H₂O + NaCl from Polarizable Force Fields. Journal of Chemical Theory and Computation, 2015, 11, 3802-3810.	2.3	63
42	The role of intermolecular interactions in the prediction of the phase equilibria of carbon dioxide hydrates. Journal of Chemical Physics, 2015, 143, 094506.	1.2	58
43	Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. Physical Review Letters, 1998, 80, 4466-4469.	2.9	57
44	Thermodynamics of pharmaceuticals: Prediction of solubility in pure and mixed solvents with PC-SAFT. Fluid Phase Equilibria, 2011, 302, 331-337.	1.4	56
45	Molecular Dynamics Simulation of Pure n-Alkanes and Their Mixtures at Elevated Temperatures Using Atomistic and Coarse-Grained Force Fields. Journal of Physical Chemistry B, 2019, 123, 6229-6243.	1.2	56
46	Use of monomer fraction data in the parametrization of association theories. Fluid Phase Equilibria, 2010, 296, 219-229.	1.4	55
47	Transport Properties of Shale Gas in Relation to Kerogen Porosity. Journal of Physical Chemistry C, 2018, 122, 6166-6177.	1.5	55
48	Molecular Dynamics Simulations of Electric Field Poled Nonlinear Optical Chromophores Incorporated in a Polymer Matrix. Journal of Physical Chemistry B, 2004, 108, 588-596.	1.2	54
49	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.	1.2	53
50	A transient outflow model for pipeline puncture. Chemical Engineering Science, 2003, 58, 4591-4604.	1.9	52
51	Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study. Journal of Chemical Physics, 2016, 145, 084702.	1.2	51
52	Equations of state: From the ideas of van der Waals to association theories. Journal of Supercritical Fluids, 2010, 55, 421-437.	1.6	50
53	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. Energy & Fuels, 2017, 31, 6004-6018.	2.5	49
54	Thermodynamics of Chain Fluids from Atomistic Simulation:â€‰ A Test of the Chain Increment Method for Chemical Potential. Macromolecules, 1997, 30, 4744-4755.	2.2	47

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55	Molecular Simulation of Phase Equilibria for Waterâˆ'n-Butane and Waterâˆ'n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	1.2	47
56	A thermodynamic model for strong aqueous electrolytes based on the eSAFT-VR Mie equation of state. Fluid Phase Equilibria, 2018, 464, 47-63.	1.4	47
57	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.	1.3	47
58	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.	2.2	46
59	Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents. Journal of Physical Chemistry B, 2009, 113, 6446-6458.	1.2	46
60	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.	1.2	46
61	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.	1.0	45
62	Equations of state for hydrogen bonding systems. Fluid Phase Equilibria, 1996, 116, 518-529.	1.4	44
63	Equation of state modeling of the phase equilibria of ionic liquid mixtures at low and high pressure. Physical Chemistry Chemical Physics, 2008, 10, 6160.	1.3	44
64	Prediction of the nâ€hexane/water and 1â€octanol/water partition coefficients for environmentally relevant compounds using molecular simulation. AICHE Journal, 2012, 58, 1929-1938.	1.8	44
65	Modeling the phase equilibria of a H₂Oâ€“CO₂mixture with PC-SAFT and tPC-PSAFT equations of state. Molecular Physics, 2012, 110, 1205-1212.	0.8	42
66	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. Journal of Chemical Physics, 2001, 115, 8231-8237.	1.2	41
67	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, 3981-3990.	1.2	41
68	Fast numerical simulation for full bore rupture of pressurized pipelines. AICHE Journal, 1999, 45, 1191-1201.	1.8	40
69	Phase equilibrium calculations for multi-component polar fluid mixtures with tPC-PSAFT. Fluid Phase Equilibria, 2007, 261, 265-271.	1.4	40
70	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. Molecular Simulation, 2013, 39, 1135-1142.	0.9	40
71	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.	2.3	40
72	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. Journal of Physical Chemistry B, 2016, 120, 12358-12370.	1.2	40

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73	Thermophysical Properties of the Ionic Liquids [EMIM][B(CN)₄] and [HMIM][B(CN)₄]. Journal of Physical Chemistry B, 2013, 117, 8512-8523.	1.2	39
74	Direct phase coexistence molecular dynamics study of the phase equilibria of the ternary methaneâ€“carbon dioxideâ€“water hydrate system. Physical Chemistry Chemical Physics, 2016, 18, 23538-23548.	1.3	39
75	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.	1.4	39
76	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.	2.2	38
77	Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon. Molecular Physics, 2012, 110, 1153-1160.	0.8	38
78	Atomistic molecular dynamics simulations of H₂O diffusivity in liquid and supercritical CO₂. Molecular Physics, 2015, 113, 2805-2814.	0.8	38
79	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.	3.8	38
80	Methane solubility in aqueous solutions under two-phase (Hâ€“Lw) hydrate equilibrium conditions. Fluid Phase Equilibria, 2014, 371, 106-120.	1.4	37
81	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.	1.2	36
82	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.	2.7	36
83	Optimization of Intermolecular Potential Parameters for the CO₂/H₂O Mixture. Journal of Physical Chemistry B, 2014, 118, 11504-11511.	1.2	35
84	Modeling the solidâ€“liquid equilibrium in pharmaceuticalâ€“solvent mixtures: Systems with complex hydrogen bonding behavior. AIChE Journal, 2009, 55, 756-770.	1.8	34
85	Diffusion in Homogeneous and in Inhomogeneous Media: A New Unified Approach. Journal of Chemical Theory and Computation, 2016, 12, 5247-5255.	2.3	34
86	Gaussian-Charge Polarizable and Nonpolarizable Models for CO₂. Journal of Physical Chemistry B, 2016, 120, 984-994.	1.2	34
87	Atomistic Simulation of Poly(dimethylsiloxane):Â Force Field Development, Structure, and Thermodynamic Properties of Polymer Melt and Solubility ofn-Alkanes,n-Perfluoroalkanes, and Noble and Light Gases. Macromolecules, 2007, 40, 1720-1729.	2.2	33
88	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. Journal of Physical Chemistry C, 2018, 122, 17170-17183.	1.5	33
89	Equation of State Description of Thermodynamic Properties of Near-Critical and Supercritical Water. The Journal of Physical Chemistry, 1994, 98, 12080-12085.	2.9	32
90	Influence of combining rules on the cavity occupancy of clathrate hydrates by Monte Carlo simulations. Molecular Physics, 2014, 112, 2258-2274.	0.8	32

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91	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.	1.4	32
92	On the Efficient Separation of Gas Mixtures with the Mixed-Linker Zeolitic-Imidazolate Framework-7-8. ACS Applied Materials & Interfaces, 2018, 10, 39631-39644.	4.0	32
93	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.	1.8	32
94	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, 8583-8592.	1.2	31
95	Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 23121-23138.	1.3	31
96	Using molecular simulation to predict solute solvation and partition coefficients in solvents of different polarity. Physical Chemistry Chemical Physics, 2011, 13, 9155.	1.3	30
97	Hydrate â€“ fluid phase equilibria modeling using PC-SAFT and Pengâ€“Robinson equations of state. Fluid Phase Equilibria, 2016, 413, 209-219.	1.4	30
98	Enthalpy of dissociation of methane hydrates at a wide pressure and temperature range. Fluid Phase Equilibria, 2019, 489, 30-40.	1.4	30
99	Phase behavior of LCST and UCST solutions of branchy copolymers: experiment and SAFT modelling. Fluid Phase Equilibria, 1993, 83, 391-398.	1.4	29
100	Molecular Simulation of Î±-Olefins Using a New United-Atom Potential Model:â€‰ Vaporâ€“Liquid Equilibria of Pure Compounds and Mixtures. Journal of the American Chemical Society, 1999, 121, 3407-3413.	6.6	29
101	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.	1.4	29
102	CO2PipeHaz: Quantitative Hazard Assessment for Next Generation CO2 Pipelines. Energy Procedia, 2014, 63, 2510-2529.	1.8	29
103	Molecular Dynamics Simulation of Highly Confined Glassy Ionic Liquids. Journal of Physical Chemistry C, 2016, 120, 1013-1024.	1.5	29
104	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. Langmuir, 2017, 33, 11291-11298.	1.6	29
105	Mean field calculations of thermodynamic properties of supercritical fluids. AICHE Journal, 1990, 36, 1920-1925.	1.8	28
106	Equations of state and activity coefficient models for vapor-liquid equilibria of polymer solutions. AICHE Journal, 1994, 40, 1711-1727.	1.8	28
107	Development of a united-atom force field for 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid. Molecular Physics, 2012, 110, 1115-1126.	0.8	28
108	Diffusivities of Ternary Mixtures of n-Alkanes with Dissolved Gases by Dynamic Light Scattering. Journal of Physical Chemistry B, 2016, 120, 10808-10823.	1.2	28

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109	Monte Carlo simulation studies of clathrate hydrates: A review. Journal of Supercritical Fluids, 2018, 134, 51-60.	1.6	28
110	Computation of partial molar properties using continuous fractional component Monte Carlo. Molecular Physics, 2018, 116, 3331-3344.	0.8	28
111	Modeling fluid phase transition effects on dynamic behavior of ESDV. AICHE Journal, 2000, 46, 997-1006.	1.8	27
112	Thermodynamics of Lewis acid-base mixtures. AICHE Journal, 1990, 36, 1851-1864.	1.8	26
113	Water-Salt Phase Equilibria at Elevated Temperatures and Pressures: Model Development and Mixture Predictions. The Journal of Physical Chemistry, 1995, 99, 6182-6193.	2.9	26
114	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.	1.0	26
115	Phase Equilibria of Water/CO₂ and Water/n-Alkane Mixtures from Polarizable Models. Journal of Physical Chemistry B, 2017, 121, 1386-1395.	1.2	26
116	Molecular Modeling of Thermodynamic and Transport Properties for CO₂ and Aqueous Brines. Accounts of Chemical Research, 2017, 50, 751-758.	7.6	26
117	Transport properties of silmethylene homo-polymers and random copolymers: experimental measurements and molecular simulation. Polymer, 2004, 45, 6933-6944.	1.8	25
118	Techno-economic assessment of CO 2 quality effect on its storage and transport: CO 2 QUEST. International Journal of Greenhouse Gas Control, 2016, 54, 662-681.	2.3	25
119	Molecular dynamics simulations of pure methane and carbon dioxide hydrates: lattice constants and derivative properties. Molecular Physics, 2016, 114, 2672-2687.	0.8	24
120	Evaluation of SAFT and PC-SAFT models for the description of homo- and co-polymer solution phase equilibria. Polymer, 2005, 46, 10772-10781.	1.8	23
121	Atomistic Simulation of Poly(dimethylsiloxane) Permeability Properties to Gases and n-Alkanes. Macromolecules, 2008, 41, 5899-5907.	2.2	23
122	Structure, thermodynamic and transport properties of imidazolium-based bis(trifluoromethylsulfonyl)imide ionic liquids from molecular dynamics simulations. Molecular Physics, 2012, 110, 1139-1152.	0.8	23
123	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs withâ€‰Unsubstituted Imidazolate Linkers for Propylene/Propane and nâ€Butane/iâ€Butane Separations. Angewandte Chemie - International Edition, 2021, 60, 10103-10111.	7.2	23
124	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.	1.8	22
125	Modeling of multicomponent vaporâ€“liquid equilibria for polymerâ€“solvent systems. Fluid Phase Equilibria, 2004, 220, 11-20.	1.4	22
126	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.	1.3	22

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127	Modeling of CO2 solubility in single and mixed electrolyte solutions using statistical associating fluid theory. Geochimica Et Cosmochimica Acta, 2016, 176, 185-197.	1.6	22
128	On the validity of the Stokesâ€“Einstein relation for various water force fields. Molecular Physics, 2020, 118, e1702729.	0.8	22
129	Defining New Limits in Gas Separations Using Modified ZIF Systems. ACS Applied Materials & Interfaces, 2020, 12, 20536-20547.	4.0	22
130	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, 16047-16058.	1.2	21
131	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.	1.0	21
132	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.	2.3	21
133	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. Nanomaterials, 2020, 10, 771.	1.9	21
134	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. Macromolecules, 2008, 41, 6228-6238.	2.2	20
135	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.	1.4	20
136	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.	1.2	20
137	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.	1.8	20
138	Monte Carlo simulation of phase equilibria of aqueous systems. Fluid Phase Equilibria, 2001, 183-184, 259-269.	1.4	19
139	CO2QUEST: Techno-economic Assessment of CO2 Quality Effect on Its Storage and Transport. Energy Procedia, 2014, 63, 2622-2629.	1.8	19
140	Modeling of Gas Solubility in Aqueous Electrolyte Solutions with the eSAFT-VR Mie Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 15327-15342.	1.8	19
141	Molecular simulation of absolute hydration Gibbs energies of polar compounds. Fluid Phase Equilibria, 2010, 296, 110-115.	1.4	18
142	The effect of lattice constant on the storage capacity of hydrogen hydrates: a Monte Carlo study. Molecular Physics, 2016, 114, 2664-2671.	0.8	18
143	Using clathrate hydrates for gas storage and gas-mixture separations: experimental and computational studies at multiple length scales. Molecular Physics, 2018, 116, 2041-2060.	0.8	18
144	Solubility of gases and solvents in silicon polymers: molecular simulation and equation of state modeling. Molecular Simulation, 2007, 33, 851-860.	0.9	17

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145	Molecular simulation of the hydration Gibbs energy of barbiturates. Fluid Phase Equilibria, 2010, 289, 148-155.	1.4	17
146	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.	2.6	17
147	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.	1.3	17
148	Modeling of physical properties and vapor â€“ liquid equilibrium of ethylene and ethylene mixtures with equations of state. Fluid Phase Equilibria, 2018, 470, 149-163.	1.4	17
149	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.	1.0	17
150	Monte Carlo simulations of the separation of a binary gas mixture (CH₄ +) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 542 Td (C	1.3	17
151	CO2 selective metal organic framework ZIF-8 modified through ionic liquid encapsulation: A computational study. Journal of Computational Science, 2018, 27, 183-191.	1.5	17
152	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.	1.0	17
153	Thermodynamic inconsistencies in and accuracy of chemical equations of state for associating fluids. Industrial & Engineering Chemistry Research, 1992, 31, 1203-1211.	1.8	16
154	Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation. Fluid Phase Equilibria, 2005, 228-229, 15-20.	1.4	16
155	Monte Carlo Simulation of the Phase Behavior of Model Dendrimers. Macromolecules, 2006, 39, 6298-6305.	2.2	16
156	Storage of H₂ in Clathrate Hydrates: Evaluation of Different Force-Fields used in Monte Carlo Simulations. Molecular Physics, 2017, 115, 1274-1285.	0.8	16
157	Thermophysical Properties of Homologous Tetracyanoborate-Based Ionic Liquids Using Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 4145-4157.	1.2	16
158	Effect of hard-sphere structure on pure-component equation of state calculations. Fluid Phase Equilibria, 1992, 73, 39-55.	1.4	15
159	Phase Equilibria Prediction of Hydrogen Fluoride Systems from an Associating Model. Industrial & Engineering Chemistry Research, 1995, 34, 1868-1872.	1.8	15
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