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	Rigorous Phase Equilibrium Calculation Methods for Strong Electrolyte Solutions: The Isothermal Flash. Fluid Phase Equilibria, 2022, 558, 113441.	1.4	4
2	Data mining for predicting gas diffusivity in zeolitic-imidazolate frameworks (ZIFs). Journal of Materials Chemistry A, 2022, 10, 13697-13703.	5.2	11
3	Diffusion of fluids confined in carbonate minerals: A molecular dynamics simulation study for carbon dioxide and methaneâ€“ethane mixture within calcite. Fuel, 2022, 325, 124800.	3.4	4
4	Molecular Dynamics Simulation of the n-Octacosaneâ€“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.	2.5	5
5	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs withâ€‰Unsubstituted Imidazolate Linkers for Propylene/Propane and nâ€Butane/iâ€Butane Separations. Angewandte Chemie, 2021, 133, 10191-10199.	1.6	5
6	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
7	Industrial Requirements for Thermodynamic and Transport Properties: 2020. Industrial & Engineering Chemistry Research, 2021, 60, 4987-5013.	1.8	90
8	Waterâ€“Hydrocarbon Phase Equilibria with SAFT-VR Mie Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 5278-5299.	1.8	8
9	Modeling confined fluids with the multicomponent potential theory of adsorption and the SAFT-VR Mie equation of state. Fluid Phase Equilibria, 2021, 534, 112941.	1.4	6
10	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
11	Monte Carlo Molecular Simulation Study of Carbon Dioxide Sequestration into Dry and Wet Calcite Pores Containing Methane. Energy & Fuels, 2021, 35, 11393-11402.	2.5	7
12	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
13	What Is the Optimal Activity Coefficient Model To Be Combined with the translatedâ€“consistent Pengâ€“Robinson Equation of State through Advanced Mixing Rules? Cross-Comparison and Grading of the Wilson, UNIQUAC, and NRTL a^E Models against a Benchmark Database Involving 200 Binary Systems. Industrial & Engineering Chemistry Research, 2021, 60, 17228-17247.	1.8	12
14	Construction of phase envelopes for binary and multicomponent mixtures with Euler-Newton predictor-corrector methods. Fluid Phase Equilibria, 2020, 505, 112338.	1.4	5
15	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.	1.0	10
16	On the validity of the Stokesâ€“Einstein relation for various water force fields. Molecular Physics, 2020, 118, e1702729.	0.8	22
17	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
18	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

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19	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.	1.4	3
20	Encapsulation of [bmim⁺][Tf₂N^{â^'}] 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.	1.7	9
21	Novel methodology for the calculation of the enthalpy of enclathration of methane hydrates using molecular dynamics simulations. Molecular Physics, 2020, 118, e1711976.	0.8	1
22	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. Nanomaterials, 2020, 10, 771.	1.9	21
23	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
24	Defining New Limits in Gas Separations Using Modified ZIF Systems. ACS Applied Materials & Interfaces, 2020, 12, 20536-20547.	4.0	22
25	Efficient and robust methods for direct saturation point calculations. Fluid Phase Equilibria, 2019, 500, 112242.	1.4	4
26	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
27	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
28	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
29	Computational investigation of the performance of ZIF-8 with encapsulated ionic liquids towards CO₂ capture. Molecular Physics, 2019, 117, 3791-3805.	0.8	13
30	Enthalpy of dissociation of methane hydrates at a wide pressure and temperature range. Fluid Phase Equilibria, 2019, 489, 30-40.	1.4	30
31	Molecular dynamics simulation of electrolyte solutions confined by calcite mesopores. Fluid Phase Equilibria, 2019, 487, 24-32.	1.4	11
32	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
33	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. AICHE Journal, 2019, 65, 792-803.	1.8	11
34	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
35	Transport Properties of Shale Gas in Relation to Kerogen Porosity. Journal of Physical Chemistry C, 2018, 122, 6166-6177.	1.5	55
36	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

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37	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
38	Molecular Dynamics Simulation of n-Alkanes and CO₂ Confined by Calcite Nanopores. Energy & Fuels, 2018, 32, 1934-1941.	2.5	93
39	Solubility of Methane and Carbon Dioxide in the Aqueous Phase of the Ternary (Methane + Carbon) Tj ETQq1 1 0.784314 rgBT /Overlock of Chemical & Engineering Data, 2018, 63, 1027-1035.	1.0	15
40	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
41	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
42	Monte Carlo simulation studies of clathrate hydrates: A review. Journal of Supercritical Fluids, 2018, 134, 51-60.	1.6	28
43	Monte Carlo simulations of the separation of a binary gas mixture (CH₄ +) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	1.3	17
44	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
45	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
46	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
47	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. Journal of Physical Chemistry C, 2018, 122, 17170-17183.	1.5	33
48	Computation of partial molar properties using continuous fractional component Monte Carlo. Molecular Physics, 2018, 116, 3331-3344.	0.8	28
49	Solidâ€“Liquidâ€“Gas Equilibrium of Methaneâ€“n-Alkane Binary Mixtures. Industrial & Engineering Chemistry Research, 2018, 57, 8566-8583.	1.8	5
50	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
51	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
52	Molecular Modeling of Thermodynamic and Transport Properties for CO₂ and Aqueous Brines. Accounts of Chemical Research, 2017, 50, 751-758.	7.6	26
53	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
54	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. Energy & Fuels, 2017, 31, 6004-6018.	2.5	49

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55	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. Langmuir, 2017, 33, 11291-11298.	1.6	29
56	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
57	Two- and three-phase equilibrium experimental measurements for the ternary CH 4 Â+ CO 2 Â+ H 2 O mixture. Fluid Phase Equilibria, 2017, 451, 96-105.	1.4	15
58	Characterization of Water Solubility in n-Octacosane Using Raman Spectroscopy. Journal of Physical Chemistry B, 2017, 121, 10665-10673.	1.2	13
59	Two-body perturbation theory versus first order perturbation theory: A comparison based on the square-well fluid. Journal of Chemical Physics, 2017, 147, 214108.	1.2	11
60	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.	0.0	2
61	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
62	Calculation of the phase envelope of multicomponent mixtures with the bead spring method. AICHE Journal, 2016, 62, 868-879.	1.8	14
63	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
64	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
65	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
66	Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study. Journal of Chemical Physics, 2016, 145, 084702.	1.2	51
67	Equation-of-State Modeling of Solidâ€“Liquidâ€“Gas Equilibrium of CO₂ Binary Mixtures. Industrial & Engineering Chemistry Research, 2016, 55, 6213-6226.	1.8	15
68	Phase Equilibrium with External Fields: Application to Confined Fluids. Journal of Chemical & Engineering Data, 2016, 61, 2873-2885.	1.0	15
69	Diffusion in Homogeneous and in Inhomogeneous Media: A New Unified Approach. Journal of Chemical Theory and Computation, 2016, 12, 5247-5255.	2.3	34
70	Molecular Simulation of n-Octacosaneâ€“Water Mixture in Titania Nanopores at Elevated Temperature and Pressure. Journal of Physical Chemistry C, 2016, 120, 24743-24753.	1.5	14
71	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
72	Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 23121-23138.	1.3	31

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73	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
74	Thermodynamics 2015 Conference Copenhagen, Denmark, 15â€“18 September 2015. Molecular Physics, 2016, 114, 2569-2573.	0.8	3
75	Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures. Computers and Chemical Engineering, 2016, 95, 49-57.	2.0	13
76	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
77	Molecular dynamics simulations of pure methane and carbon dioxide hydrates: lattice constants and derivative properties. Molecular Physics, 2016, 114, 2672-2687.	0.8	24
78	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
79	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. Journal of Physical Chemistry B, 2016, 120, 12358-12370.	1.2	40
80	Kenneth R. Hallâ€”A Distinguished Educator, Scientist, and University Administrator. Journal of Chemical & Engineering Data, 2016, 61, 2649-2650.	1.0	1
81	Development of a novel experimental apparatus for hydrate equilibrium measurements. Fluid Phase Equilibria, 2016, 424, 152-161.	1.4	10
82	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
83	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
84	Molecular simulations of imidazolium-based tricyanomethanide ionic liquids using an optimized classical force field. Physical Chemistry Chemical Physics, 2016, 18, 6850-6860.	1.3	15
85	Gaussian-Charge Polarizable and Nonpolarizable Models for CO₂. Journal of Physical Chemistry B, 2016, 120, 984-994.	1.2	34
86	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
87	Molecular Dynamics Simulation of Highly Confined Glassy Ionic Liquids. Journal of Physical Chemistry C, 2016, 120, 1013-1024.	1.5	29
88	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
89	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
90	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

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91	Atomistic Simulations of Clathrate Hydrates. , 2015, , 351-359.		2
92	Prediction of the phase equilibria of methane hydrates using the direct phase coexistence methodology. Journal of Chemical Physics, 2015, 142, 044501.	1.2	111
93	Evaluation of the Efficiency of Clathrate Hydrates in Storing Energy Gases. Journal of Physics: Conference Series, 2015, 640, 012026.	0.3	4
94	Gas Solubility in Aqueous Solutions Under Two-Phase (Hâ€“Lw) Hydrate Equilibrium Conditions. , 2015, , 205-212.		0
95	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
96	Thermodynamic and Transport Properties of H₂O + NaCl from Polarizable Force Fields. Journal of Chemical Theory and Computation, 2015, 11, 3802-3810.	2.3	63
97	Atomistic molecular dynamics simulations of H₂O diffusivity in liquid and supercritical CO₂. Molecular Physics, 2015, 113, 2805-2814.	0.8	38
98	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
99	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
100	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design. , 2015, , 361-370.		0
101	CO2PipeHaz: Quantitative Hazard Assessment for Next Generation CO2 Pipelines. Energy Procedia, 2014, 63, 2510-2529.	1.8	29
102	CO2QUEST: Techno-economic Assessment of CO2 Quality Effect on Its Storage and Transport. Energy Procedia, 2014, 63, 2622-2629.	1.8	19
103	Influence of combining rules on the cavity occupancy of clathrate hydrates using van der Waalsâ€“Platteeuw-theory-based modelling. Chemical Engineering Research and Design, 2014, 92, 2992-3007.	2.7	12
104	Industrial use of thermodynamics workshop: Round table discussion on 8 July 2014. Chemical Engineering Research and Design, 2014, 92, 2795-2796.	2.7	14
105	Influence of combining rules on the cavity occupancy of clathrate hydrates by Monte Carlo simulations. Molecular Physics, 2014, 112, 2258-2274.	0.8	32
106	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. Journal of Chemical Physics, 2014, 141, 234507.	1.2	63
107	Methane solubility in aqueous solutions under two-phase (Hâ€“Lw) hydrate equilibrium conditions. Fluid Phase Equilibria, 2014, 371, 106-120.	1.4	37
108	Analysis of the heterogeneous dynamics of imidazolium-based [Tf₂N^{â^'}] ionic liquids using molecular simulation. Molecular Physics, 2014, 112, 2694-2706.	0.8	14

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109	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
110	Optimization of Intermolecular Potential Parameters for the CO₂/H₂O Mixture. Journal of Physical Chemistry B, 2014, 118, 11504-11511.	1.2	35
111	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
112	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
113	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
114	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. Molecular Simulation, 2013, 39, 1135-1142.	0.9	40
115	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
116	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
117	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
118	Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon. Molecular Physics, 2012, 110, 1153-1160.	0.8	38
119	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
120	Thermodynamics 2011 Conference Athens, Greece, 31 Augustâ€“3 September 2011 http://www.thermodynamics2011.org/. Molecular Physics, 2012, 110, 1053-1056.	0.8	5
121	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
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	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
124	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
125	Development of a united-atom force field for 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid. Molecular Physics, 2012, 110, 1115-1126.	0.8	28
126	Molecular Modeling of Gas Treatment Processes with Emphasis to GTL Process. , 2012, , 319-325.		0

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127	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
128	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.	1.0	2
129	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
130	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
131	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
132	Thermodynamics of pharmaceuticals: Prediction of solubility in pure and mixed solvents with PC-SAFT. Fluid Phase Equilibria, 2011, 302, 331-337.	1.4	56
133	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
134	Partition coefficients of organic molecules in squalane and water/ethanol mixtures by molecular dynamics simulations. Fluid Phase Equilibria, 2011, 306, 162-170.	1.4	2
135	Structural and dynamical analysis of monodisperse and polydisperse colloidal systems. Journal of Chemical Physics, 2010, 133, 224901.	1.2	6
136	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
137	Molecular simulation of the hydration Gibbs energy of barbiturates. Fluid Phase Equilibria, 2010, 289, 148-155.	1.4	17
138	Molecular simulation of absolute hydration Gibbs energies of polar compounds. Fluid Phase Equilibria, 2010, 296, 110-115.	1.4	18
139	Use of monomer fraction data in the parametrization of association theories. Fluid Phase Equilibria, 2010, 296, 219-229.	1.4	55
140	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
141	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. Journal of Supercritical Fluids, 2010, 55, 503-509.	1.6	7
142	Equations of state: From the ideas of van der Waals to association theories. Journal of Supercritical Fluids, 2010, 55, 421-437.	1.6	50
143	Prediction of microscopic structure and physical properties of complex fluid mixtures based on molecular simulation. Fluid Phase Equilibria, 2010, 296, 125-132.	1.4	11
144	The Role of Molecular Thermodynamics and Simulation in Natural Gas Sustainable Processes. , 2010, , 299-309.		0

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145	Inductive construction of 2-connected graphs for calculating the virial coefficients. Journal of Physics A: Mathematical and Theoretical, 2010, 43, 315004.	0.7	0
146	Industrial Requirements for Thermodynamics and Transport Properties. Industrial & Engineering Chemistry Research, 2010, 49, 11131-11141.	1.8	211
147	Cubic and Generalized van der Waals Equations of State. , 2010, , 53-83.		5
148	Phase equilibrium of colloidal suspensions with particle size dispersity: A Monte Carlo study. Journal of Chemical Physics, 2009, 130, 194902.	1.2	11
149	Modeling the solidâ€“liquid equilibrium in pharmaceuticalâ€“solvent mixtures: Systems with complex hydrogen bonding behavior. AICHE Journal, 2009, 55, 756-770.	1.8	34
150	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
151	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain-Statistical Associating Fluid Theory (sPC-SAFT). 2. Liquidâ^'Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems. Industrial & Engineering Chemistry Research, 2009, 48, 7860-7860.	1.8	3
152	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
153	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
154	Determination of liquidâ€“gas partition coefficients of BuA and MMA by headspace-gas chromatography utilizing the phase ratio variation method. Fluid Phase Equilibria, 2008, 266, 21-30.	1.4	1
155	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
156	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
157	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
158	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. Macromolecules, 2008, 41, 6228-6238.	2.2	20
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