Ioannis Economou

List of Publications by Year in Descending Order

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	Rigorous Phase Equilibrium Calculation Methods for Strong Electrolyte Solutions: The Isothermal Flash. *Fluid Phase Equilibria*, **2022**, 558, 113441	2.5	0
233	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
232	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
231	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
230	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
229	Industrial Requirements for Thermodynamic and Transport Properties: 2020. *Industrial & Engineering Chemistry Research*, **2021**, 60, 4987-5013	3.9	30
228	Water-Hydrocarbon Phase Equilibria with SAFT-VR Mie Equation of State. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5278-5299	3.9	3
227	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
226	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
225	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
224	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
223	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
222	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
221	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
220	Kirkwood-Buff Integrals Using Molecular Simulation: Estimation of Surface Effects. *Nanomaterials*, **2020**, 10,	5.4	12
219	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
218	On the validity of the Stokes-Einstein relation for various water force fields. *Molecular Physics*, **2020**, 118, e1702729	1.7	13

217	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
216	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
215	Construction of phase envelopes for binary and multicomponent mixtures with Euler-Newton predictor-corrector methods. *Fluid Phase Equilibria*, **2020**, 505, 112338	2.5	2
214	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
213	Defining New Limits in Gas Separations Using Modified ZIF Systems. *ACS Applied Materials & Interfaces*, **2020**, 12, 20536-20547	9.5	10
212	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 chemistry, statistical mechanics and molecular simulation for many decades and a great mentor for	1.7	9
211	Enthalpy of dissociation of methane hydrates at a wide pressure and temperature range. *Fluid Phase Equilibria*, **2019**, 489, 30-40 *Molecular Physics*, **2019**, 117, 3791-3805	2.5	19
210	Molecular dynamics simulation of electrolyte solutions confined by calcite mesopores. *Fluid Phase Equilibria*, **2019**, 487, 24-32	2.5	10
209	Efficient and robust methods for direct saturation point calculations. *Fluid Phase Equilibria*, **2019**, 500, 112242	2.5	2
208	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
207	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
206	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
205	Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies. *Molecular Simulation*, **2019**, 45, 425-453	2	69
204	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. *AICHE Journal*, **2019**, 65, 792-803	3.6	10
203	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
202	Transport Properties of Shale Gas in Relation to Kerogen Porosity. *Journal of Physical Chemistry C*, **2018**, 122, 6166-6177	3.8	32
201	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
200	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

199	Molecular Dynamics Simulation of n-Alkanes and CO2 Confined by Calcite Nanopores. *Energy & Fuels*, **2018**, 32, 1934-1941	4.1	73
198	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
197	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
196	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
195	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. *Journal of Physical Chemistry C*, **2018**, 122, 17170-17183	3.8	19
194	Computation of partial molar properties using continuous fractional component Monte Carlo. *Molecular Physics*, **2018**, 116, 3331-3344	1.7	19
193	Solid□iquid□Gas Equilibrium of Methane□-Alkane Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2018**, 57, 8566-8583	3.9	5
192	Monte Carlo simulation studies of clathrate hydrates: A review. *Journal of Supercritical Fluids*, **2018**, 134, 51-60	4.2	19
191	**2018**,		2
190	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
189	Thermodynamic Modeling of Relevance to Natural Gas Processing **2018**, 341-378		
188	Multi-Scale Models for the Prediction of Microscopic Structure and Physical Properties of Chemical Systems Related to Natural Gas Technology **2018**, 463-497		1
187	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
186	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
185	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
184	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
183	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
182	Molecular Modeling of Thermodynamic and Transport Properties for CO and Aqueous Brines. *Accounts of Chemical Research*, **2017**, 50, 751-758	24.3	16

181	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
180	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. *Energy & Fuels*, **2017**, 31, 6004-6018	4.1	35
179	Molecular Simulation Methods for CO2 Capture and Gas Separation with Emphasis on Ionic Liquids **2017**, 79-111		2
178	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. *Langmuir* , **2017**, 33, 11291-11298	4	25
177	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
176	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
175	Characterization of Water Solubility in n-Octacosane Using Raman Spectroscopy. *Journal of Physical Chemistry B*, **2017**, 121, 10665-10673	3.4	9
174	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
173	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
172	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
171	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
170	Thermodynamics 2015 Conference Copenhagen, Denmark, 15–18 September 2015. *Molecular Physics*, **2016**, 114, 2569-2573	1.7	2
169	Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures. *Computers and Chemical Engineering*, **2016**, 95, 49-57	4	10
168	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
167	Molecular dynamics simulations of pure methane and carbon dioxide hydrates: lattice constants and derivative properties. *Molecular Physics*, **2016**, 114, 2672-2687	1.7	17
166	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
165	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370	3.4	28
164	Development of a novel experimental apparatus for hydrate equilibrium measurements. *Fluid Phase Equilibria*, **2016**, 424, 152-161	2.5	7

163	Hydrate–fluid phase equilibria modeling using PC-SAFT and Peng–Robinson equations of state. *Fluid Phase Equilibria*, **2016**, 413, 209-219	2.5	21
162	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
161	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
160	Gaussian-Charge Polarizable and Nonpolarizable Models for CO2. *Journal of Physical Chemistry B*, **2016**, 120, 984-94	3.4	25
159	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
158	Molecular Dynamics Simulation of Highly Confined Glassy Ionic Liquids. *Journal of Physical Chemistry C*, **2016**, 120, 1013-1024	3.8	27
157	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
156	Calculation of the phase envelope of multicomponent mixtures with the bead spring method. *AICHE Journal*, **2016**, 62, 868-879	3.6	9
155	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
154	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	3.9	15
153	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
152	Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study. *Journal of Chemical Physics*, **2016**, 145, 084702	3.9	40
151	Equation-of-State Modeling of Solid–Liquid–Gas Equilibrium of CO2 Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2016**, 55, 6213-6226	3.9	12
150	Phase Equilibrium with External Fields: Application to Confined Fluids. *Journal of Chemical & Engineering Data*, **2016**, 61, 2873-2885	2.8	11
149	Diffusion in Homogeneous and in Inhomogeneous Media: A New Unified Approach. *Journal of Chemical Theory and Computation*, **2016**, 12, 5247-5255	6.4	24
148	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
147	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
146	Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 23121-38	3.6	25

145	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
144	Gas Solubility in Aqueous Solutions Under Two-Phase (H□w) Hydrate Equilibrium Conditions **2015**, 205-212		
143	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
142	Thermodynamic and Transport Properties of H2O + NaCl from Polarizable Force Fields. *Journal of Chemical Theory and Computation*, **2015**, 11, 3802-10	6.4	49
141	Atomistic molecular dynamics simulations of H2O diffusivity in liquid and supercritical CO2. *Molecular Physics*, **2015**, 113, 2805-2814	1.7	27
140	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
139	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
138	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
137	Atomistic Simulations of Clathrate Hydrates **2015**, 351-359		0
136	Prediction of the phase equilibria of methane hydrates using the direct phase coexistence methodology. *Journal of Chemical Physics*, **2015**, 142, 044501	3.9	81
135	Evaluation of the Efficiency of Clathrate Hydrates in Storing Energy Gases. *Journal of Physics: Conference Series*, **2015**, 640, 012026	0.3	4
134	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design **2015**, 361-370		
133	Methane solubility in aqueous solutions under two-phase (H□w) hydrate equilibrium conditions. *Fluid Phase Equilibria*, **2014**, 371, 106-120	2.5	30
132	Analysis of the heterogeneous dynamics of imidazolium-based [Tf2N□ionic liquids using molecular simulation. *Molecular Physics*, **2014**, 112, 2694-2706	1.7	13
131	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
130	Optimization of intermolecular potential parameters for the CO2/H2O mixture. *Journal of Physical Chemistry B*, **2014**, 118, 11504-11	3.4	27
129	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
128	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

127	CO2PipeHaz: Quantitative Hazard Assessment for Next Generation CO2 Pipelines. *Energy Procedia*, **2014**, 63, 2510-2529	2.3	25
126	CO2QUEST: Techno-economic Assessment of CO2 Quality Effect on Its Storage and Transport. *Energy Procedia*, **2014**, 63, 2622-2629	2.3	15
125	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	2.5	10
124	Industrial use of thermodynamics workshop: Round table discussion on 8 July 2014. *Chemical Engineering Research and Design*, **2014**, 92, 2795-2796	2.5	13
123	Influence of combining rules on the cavity occupancy of clathrate hydrates by Monte Carlo simulations. *Molecular Physics*, **2014**, 112, 2258-2274	1.7	30
122	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. *Journal of Chemical Physics*, **2014**, 141, 234507	3.9	49
121	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
120	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. *Molecular Simulation*, **2013**, 39, 1135-1142	2	36
119	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	2.5	28
118	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
117	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
116	Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon. *Molecular Physics*, **2012**, 110, 1153-1160	1.7	29
115	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
114	Thermodynamics 2011 Conference Athens, Greece, 31 August−3 September 2011 http://www.thermodynamics2011.org/. *Molecular Physics*, **2012**, 110, 1053-1056	1.7	3
113	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
112	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
111	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
110	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

109	Development of a united-atom force field for 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid. *Molecular Physics*, **2012**, 110, 1115-1126	1.7	26
108	Molecular Modeling of Gas Treatment Processes with Emphasis to GTL Process **2012**, 319-325		
107	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
106	Thermodynamics of pharmaceuticals: Prediction of solubility in pure and mixed solvents with PC-SAFT. *Fluid Phase Equilibria*, **2011**, 302, 331-337	2.5	42
105	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
104	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
103	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
102	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
101	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
100	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
99	The Role of Molecular Thermodynamics and Simulation in Natural Gas Sustainable Processes **2010**, 299-309		
98	Inductive construction of 2-connected graphs for calculating the virial coefficients. *Journal of Physics A: Mathematical and Theoretical*, **2010**, 43, 315004	2	
97	Industrial Requirements for Thermodynamics and Transport Properties. *Industrial & Engineering Chemistry Research*, **2010**, 49, 11131-11141	3.9	186
96	Structural and dynamical analysis of monodisperse and polydisperse colloidal systems. *Journal of Chemical Physics*, **2010**, 133, 224901	3.9	5
95	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
94	Molecular simulation of the hydration Gibbs energy of barbiturates. *Fluid Phase Equilibria*, **2010**, 289, 148-155	2.5	15
93	Molecular simulation of absolute hydration Gibbs energies of polar compounds. *Fluid Phase Equilibria*, **2010**, 296, 110-115	2.5	16
92	Use of monomer fraction data in the parametrization of association theories. *Fluid Phase Equilibria*, **2010**, 296, 219-229	2.5	49

91	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
90	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. *Journal of Supercritical Fluids*, **2010**, 55, 503-509	4.2	5
89	Equations of state: From the ideas of van der Waals to association theories. *Journal of Supercritical Fluids*, **2010**, 55, 421-437	4.2	41
88	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
87	Chapter 4:Cubic and Generalized van der Waals Equations of State **2010**, 53-83		3
86	Phase equilibrium of colloidal suspensions with particle size dispersity: a Monte Carlo study. *Journal of Chemical Physics*, **2009**, 130, 194902	3.9	10
85	Modeling the solid□liquid equilibrium in pharmaceutical-solvent mixtures: Systems with complex hydrogen bonding behavior. *AICHE Journal*, **2009**, 55, 756-770	3.6	28
84	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
83	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
82	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
81	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
80	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
79	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
78	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
77	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. *Macromolecules*, **2008**, 41, 6228-6238	5.5	16
76	Atomistic Simulation of Poly(dimethylsiloxane) Permeability Properties to Gases and n-Alkanes. *Macromolecules*, **2008**, 41, 5899-5907	5.5	17
75	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
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List of Publications