Lourdes F Vega

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6036866/publications.pdf

Version: 2024-02-01

225	8,957	36203	58464
papers	citations	51 h-index	82 g-index

230	230	230	5467
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modifying absorption process configurations to improve their performance for Post-Combustion CO2 capture â€“ What have we learned and what is still Missing?. Chemical Engineering Journal, 2022, 430, 133096.	6.6	34
2	Systematic study of the effect of the co-solvent on the performance of amine-based solvents for CO2 capture. Separation and Purification Technology, 2022, 282, 120093.	3.9	23
3	Critical assessment of the performance of next-generation carbon-based adsorbents for CO2 capture focused on their structural properties. Science of the Total Environment, 2022, 810, 151720.	3.9	17
4	Accurate Predictions of the Effect of Hydrogen Composition on the Thermodynamics and Transport Properties of Natural Gas. Industrial & Engineering Chemistry Research, 2022, 61, 6214-6234.	1.8	7
5	Encapsulated Protic Ionic Liquids as Sustainable Materials for CO₂ Separation. Industrial & Engineering Chemistry Research, 2022, 61, 4046-4057.	1.8	4
6	Understanding the Absorption of Fluorinated Gases in Fluorinated Ionic Liquids for Recovering Purposes Using Soft-SAFT. Journal of Chemical & Engineering Data, 2022, 67, 1951-1963.	1.0	2
7	Molecular Thermodynamic Modeling of Hybrid Ionic Liquids for Biogas Upgrading. Industrial & Engineering Chemistry Research, 2022, 61, 12190-12207.	1.8	1
8	The Hydrogen Economy Preface. Industrial & Engineering Chemistry Research, 2022, 61, 6065-6066.	1.8	7
9	Understanding the phase and solvation behavior of fluorinated ionic liquids. Journal of Molecular Liquids, 2022, 359, 119285.	2.3	8
10	Searching for Sustainable Refrigerants by Bridging Molecular Modeling with Machine Learning. Industrial & Engineering Chemistry Research, 2022, 61, 7414-7429.	1.8	16
11	Insights into the thermal stability and conversion of carbon-based materials by using ReaxFF reactive force field: Recent advances and future directions. Carbon, 2022, 196, 840-866.	5.4	32
12	Adhesion and Cohesion of Silica Surfaces with Quartz Cement: A Molecular Simulations Study. ACS Omega, 2022, 7, 22303-22316.	1.6	2
13	Insights into the performance of hybrid graphene oxide/MOFs for CO2 capture at process conditions by molecular simulations. Chemical Engineering Journal, 2022, 449, 137884.	6.6	10
14	Quantifying the effect of polarity on the behavior of mixtures of <scp>nâ€alkanes</scp> with dipolar solvents using polar <scp>softâ€</scp>statistical associating fluid theory (Polar softâ€SAFT). AICHE Journal, 2021, 67, e16649.	1.8	11
15	Assessing the effect of impurities on the thermophysical properties of methane-based energy systems using polar soft-SAFT. Fluid Phase Equilibria, 2021, 527, 112841.	1.4	16
16	Understanding the relationship between the structural properties of three corrosion inhibitors and their surface protectiveness ability in different environments. Applied Surface Science, 2021, 542, 148600.	3.1	25
17	A DFT study of the adsorption energy and electronic interactions of the SO₂ molecule on a CoP hydrotreating catalyst. RSC Advances, 2021, 11, 2947-2957.	1.7	49
18	Are we missing something when evaluating adsorbents for CO₂ capture at the system level?. Energy and Environmental Science, 2021, 14, 6360-6380.	15.6	16

#	Article	IF	Citations
19	Systematic Search of Suitable Metalâ€“Organic Frameworks for Thermal Energy-Storage Applications with Low Global Warming Potential Refrigerants. ACS Sustainable Chemistry and Engineering, 2021, 9, 3157-3171.	3.2	15
20	Editorial: Chemical Modification of Adsorbents for Enhanced Carbon Capture Performance. Frontiers in Chemistry, 2021, 9, 657669.	1.8	2
21	Strategies for Integrated Capture and Conversion of CO₂ from Dilute Flue Gases and the Atmosphere. ChemSusChem, 2021, 14, 1805-1820.	3.6	37
22	Searching for Suitable Lubricants for low Global Warming Potential Refrigerant R513A using Molecular-Based Models: Solubility and Performance in Refrigeration Cycles. International Journal of Refrigeration, 2021, 128, 252-252.	1.8	8
23	Quantifying the effect of polar interactions on the behavior of binary mixtures: Phase, interfacial, and excess properties. Journal of Chemical Physics, 2021, 154, 164503.	1.2	8
24	Development of a robust soft-SAFT model for protic ionic liquids using new high-pressure density data. Fluid Phase Equilibria, 2021, 539, 113036.	1.4	10
25	Salt-free synthesis of Cu-BTC metal-organic framework exhibiting mesoporosity and enhanced carbon dioxide adsorption. Microporous and Mesoporous Materials, 2021, 324, 111265.	2.2	18
26	Grand Canonical Monte Carlo Simulations to Determine the Optimal Interlayer Distance of a Graphene Slit-Shaped Pore for Adsorption of Methane, Hydrogen and their Equimolar Mixture. Nanomaterials, 2021, 11, 2534.	1.9	5
27	Hybrid â€“ Slurry/Nanofluid systems as alternative to conventional chemical absorption for carbon dioxide capture: A review. International Journal of Greenhouse Gas Control, 2021, 110, 103415.	2.3	23
28	Current and future perspectives on catalytic-based integrated carbon capture and utilization. Science of the Total Environment, 2021, 790, 148081.	3.9	67
29	Activated carbons from biomass-based sources for CO2 capture applications. Chemosphere, 2021, 282, 131111.	4.2	135
30	Sustainability criteria as a game changer in the search for hybrid solvents for CO2 and H2S removal. Separation and Purification Technology, 2021, 277, 119516.	3.9	11
31	Unveiling the phase behavior of C_iE_j non-ionic surfactants in water through coarse-grained molecular dynamics simulations. Soft Matter, 2021, 17, 5183-5196.	1.2	8
32	How Molecular Modelling Tools Can Help in Mitigating Climate Change. Molecular Modeling and Simulation, 2021, , 181-220.	0.2	2
33	Computational modeling of green hydrogen generation from photocatalytic H2S splitting: Overview and perspectives. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 49, 100456.	5.6	15
34	Assessment of Low Global Warming Potential Refrigerants for Drop-In Replacement by Connecting their Molecular Features to Their Performance. ACS Sustainable Chemistry and Engineering, 2021, 9, 17034-17048.	3.2	18
35	Modeling of Hierarchical Cathodes for Li-Air Batteries with Improved Discharge Capacity. Journal of the Electrochemical Society, 2021, 168, 120534.	1.3	5
36	Performance of non-aqueous amine hybrid solvents mixtures for CO2 capture: A study using a molecular-based model. Journal of CO2 Utilization, 2020, 35, 126-144.	3.3	52

#	Article	IF	Citations
37	Surface modification of antiâ€fouling novel cellulose/graphene oxide (GO) nanosheets (NS) microfiltration membranes for seawater desalination applications. Journal of Chemical Technology and Biotechnology, 2020, 95, 1915-1925.	1.6	26
38	Detailed surface characterization of highly fluorinated liquid alcohols: Experimental surface tensions, molecular simulations and soft-SAFT theory. Journal of Molecular Liquids, 2020, 300, 112294.	2.3	8
39	Perspectives and guidelines on thermodynamic modelling of deep eutectic solvents. Journal of Molecular Liquids, 2020, 298, 112183.	2.3	83
40	Predicting the density and viscosity of hydrophobic eutectic solvents: towards the development of sustainable solvents. Green Chemistry, 2020, 22, 8511-8530.	4.6	84
41	A Thermodynamic Robust Model to Assess Hybrid Solvents for CO2 Capture. , 2020, , .		0
42	A Comparative Assessment of Emerging Solvents and Adsorbents for Mitigating CO2 Emissions From the Industrial Sector by Using Molecular Modeling Tools. Frontiers in Energy Research, 2020, 8, .	1.2	20
43	Screening of Ionic Liquids and Deep Eutectic Solvents for Physical CO₂ Absorption by Soft-SAFT Using Key Performance Indicators. Journal of Chemical & Engineering Data, 2020, 65, 5844-5861.	1.0	40
44	Polar soft-SAFT: theory and comparison with molecular simulations and experimental data of pure polar fluids. Physical Chemistry Chemical Physics, 2020, 22, 13171-13191.	1.3	25
45	Assessment on Separating Hydrofluoroolefins from Hydrofluorocarbons at the Azeotropic Mixture R513A by Using Fluorinated Ionic Liquids: A Soft-SAFT Study. Industrial & Engineering Chemistry Research, 2020, 59, 13315-13324.	1.8	23
46	Design of Subâ€Nanochannels between Graphene Oxide Sheets via Crown Ether Intercalation to Selectively Regulate Cation Permeation. Advanced Materials Interfaces, 2020, 7, 1901876.	1.9	17
47	Synthesis and characterization of activated carbon from biomass date seeds for carbon dioxide adsorption. Journal of Environmental Chemical Engineering, 2020, 8, 104257.	3.3	94
48	Isobaric vapor-liquid equilibrium of waterÂ+ glymes binary mixtures: Experimental measurements and molecular thermodynamic modelling. Fluid Phase Equilibria, 2020, 513, 112547.	1.4	9
49	A consistent thermodynamic molecular model of n-hydrofluoroolefins and blends for refrigeration applications. International Journal of Refrigeration, 2020, 113, 145-155.	1.8	25
50	Functionalization of fluorinated ionic liquids: A combined experimental-theoretical study. Journal of Molecular Liquids, 2020, 302, 112489.	2.3	15
51	Performance of Activated Carbons Derived from Date Seeds in CO₂ Swing Adsorption Determined by Combining Experimental and Molecular Simulation Data. Industrial & Engineering Chemistry Research, 2020, 59, 7161-7173.	1.8	25
52	Effect of Amine Functionalization of MOF Adsorbents for Enhanced CO2 Capture and Separation: A Molecular Simulation Study. Frontiers in Chemistry, 2020, 8, 574622.	1.8	16
53	Systematic study of the influence of the molecular structure of fluorinated ionic liquids on the solubilization of atmospheric gases using a soft-SAFT based approach. Journal of Molecular Liquids, 2019, 294, 111645.	2.3	17
54	Insights into the Transport Properties of Electrolyte Solutions in a Hierarchical Carbon Electrode by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 27273-27285.	1.5	11

#	Article	IF	Citations
55	Molecular simulations of phenol and ibuprofen removal from water using multilayered graphene oxide membranes. Molecular Physics, 2019, 117, 3703-3714.	0.8	15
56	Molecular modeling of the solubility of low global warming potential refrigerants in polyol ester lubricants. International Journal of Refrigeration, 2019, 103, 145-154.	1.8	25
57	A methodology to parameterize SAFT-type equations of state for solid precursors of deep eutectic solvents: the example of cholinium chloride. Physical Chemistry Chemical Physics, 2019, 21, 15046-15061.	1.3	32
58	Molecular simulations of carbon-based materials for selected CO2 separation and water treatment processes. Fluid Phase Equilibria, 2019, 492, 10-25.	1.4	19
59	110th Anniversary: Accurate Modeling of the Simultaneous Absorption of H2S and CO2 in Aqueous Amine Solvents. Industrial & Engineering Chemistry Research, 2019, 58, 6870-6886.	1.8	18
60	Insights into the influence of the molecular structures of fluorinated ionic liquids on their thermophysical properties. A soft-SAFT based approach. Physical Chemistry Chemical Physics, 2019, 21, 6362-6380.	1.3	28
61	Interfacial anomaly in low global warming potential refrigerant blends as predicted by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 22092-22102.	1.3	23
62	Applications of fly ash for CO2 capture, utilization, and storage. Journal of CO2 Utilization, 2019, 29, 82-102.	3.3	234
63	Energetic evaluation of swing adsorption processes for CO 2 capture in selected MOFs and zeolites: Effect of impurities. Chemical Engineering Journal, 2018, 342, 458-473.	6.6	76
64	Measurement and Modeling of Isobaric Vaporâ€“Liquid Equilibrium of Water + Glycols. Journal of Chemical & Engineering Data, 2018, 63, 2394-2401.	1.0	13
65	Perspectives on molecular modeling of supercritical fluids: From equations of state to molecular simulations. Recent advances, remaining challenges and opportunities. Journal of Supercritical Fluids, 2018, 134, 41-50.	1.6	24
66	Crystallization processes in bicomponent thin film depositions: Towards a realistic kinetic Monte Carlo simulation. Surface and Coatings Technology, 2018, 343, 38-48.	2.2	3
67	Thermodynamic characterisation of aqueous alkanolamine and amine solutions for acid gas processing by transferable molecular models. Applied Energy, 2018, 222, 687-703.	5.1	29
68	High-pressure solubility of CO2 in glymes. Fuel, 2018, 219, 120-125.	3.4	13
69	Next generation of low global warming potential refrigerants: Thermodynamic properties molecular modeling. AICHE Journal, 2018, 64, 250-262.	1.8	58
70	Transport properties of HFC and HFO based refrigerants using an excess entropy scaling approach. Journal of Supercritical Fluids, 2018, 131, 106-116.	1.6	52
71	Amine-functionalized hierarchical zeolites for carbon dioxide capture. , 2018, , .		1
72	A systematic approach for the thermodynamic modelling of CO2-amine absorption process using molecular-based models. Applied Energy, 2018, 232, 273-291.	5.1	31

#	Article	IF	Citations
73	On the anomalous composition dependence of viscosity and surface tension in refrigerant blends. Journal of Molecular Liquids, 2018, 268, 190-200.	2.3	22
74	Vapor Liquid Equilibria of Binary Mixtures of 1-Butyl-3-methylimidazolium Triflate (C₄mimTfO) and Molecular Solvents: n-Alkyl Alcohols and Water. Journal of Physical Chemistry B, 2018, 122, 6017-6032.	1.2	20
75	Physical synthesis and characterization of activated carbon from date seeds for CO2 capture. Journal of Environmental Chemical Engineering, 2018, 6, 4245-4252.	3.3	96
76	Development of predictive molecular models to describe thermodynamic and transport properties of hydrocarbons and their mixtures present in petroleum fractions. , 2018, , .		0
77	Accurate viscosity predictions of carbonated aqueous MEA Solutions for CO2 capture processes. , 2018, , .		0
78	Exploring alternative solvents for gas processing using the soft-SAFT EoS. , 2018, , .		0
79	New measurements and modeling of high pressure thermodynamic properties of glycols. Fluid Phase Equilibria, 2017, 436, 113-123.	1.4	38
80	Evaluation of the solvent structural effect upon the vapor â€“liquid equilibrium of [C4C1im][Cl]Â+ alcohols. Fluid Phase Equilibria, 2017, 440, 36-44.	1.4	6
81	Thermophysical Characterization of Ionic Liquids Based on the Perfluorobutanesulfonate Anion: Experimental and Softâ€SAFT Modeling Results. ChemPhysChem, 2017, 18, 2012-2023.	1.0	23
82	Accurate description of thermophysical properties of Tetraalkylammonium Chloride Deep Eutectic Solvents with the soft-SAFT equation of state. Fluid Phase Equilibria, 2017, 448, 81-93.	1.4	56
83	New Experimental Data and Modeling of Glymes: Toward the Development of a Predictive Model for Polyethers. Industrial & Engineering Chemistry Research, 2017, 56, 7830-7844.	1.8	18
84	Computational study of ibuprofen removal from water by adsorption in realistic activated carbons. Journal of Colloid and Interface Science, 2017, 498, 323-334.	5.0	64
85	The phase and interfacial properties of azeotropic refrigerants: the prediction of aneotropes from molecular theory. Physical Chemistry Chemical Physics, 2017, 19, 8977-8988.	1.3	36
86	Accurate viscosity predictions of linear polymers from n-alkanes data. Journal of Molecular Liquids, 2017, 243, 115-123.	2.3	14
87	Pharmaceutical Removal from Water Effluents by Adsorption on Activated Carbons: A Monte Carlo Simulation Study. Langmuir, 2017, 33, 11146-11155.	1.6	36
88	Soft-SAFT Equation of State as a Valuable Tool for the Design of new CO2 Capture Technologies.. , 2017, , .		1
89	Pharmaceuticals removal from water effluents by adsorption in activated carbons using Monte Carlo simulations. Computer Aided Chemical Engineering, 2017, 40, 2695-2700.	0.3	11
90	New Procedure for Enhancing the Transferability of Statistical Associating Fluid Theory (SAFT) Molecular Parameters: The Role of Derivative Properties. Industrial & Engineering Chemistry Research, 2016, 55, 10011-10024.	1.8	27

#	Article	IF	Citations
91	Comparative Study of MOFs and Zeolites For CO2 Capture and Separation at Process Conditions. , 2016, , .		3
92	Review and new insights into the application of molecular-based equations of state to water and aqueous solutions. Fluid Phase Equilibria, 2016, 416, 150-173.	1.4	66
93	Microscale Characterization of Surface Recombination at the Vicinity of Laser-Processed Regions in c-Si Solar Cells. IEEE Journal of Photovoltaics, 2016, 6, 426-431.	1.5	6
94	High pressure solubility of CH4, N2O and N2 in 1-butyl-3-methylimidazolium dicyanamide: Solubilities, selectivities and soft-SAFT modeling. Journal of Supercritical Fluids, 2016, 110, 56-64.	1.6	38
95	Life cycle assessment of CaO looping versus amine-based absorption for capturing CO2 in a subcritical coal power plant. International Journal of Greenhouse Gas Control, 2016, 46, 18-27.	2.3	24
96	Systematic evaluation of materials for post-combustion CO 2 capture in a Temperature Swing Adsorption process. Chemical Engineering Journal, 2016, 284, 438-447.	6.6	118
97	Incorporating critical divergence of isochoric heat capacity into the softâ€SAFT equation of state. AICHE Journal, 2015, 61, 3073-3080.	1.8	15
98	Microscale Spatially Resolved Characterization of Highly Doped Regions in Laser-Fired Contacts for High-Efficiency Crystalline Si Solar Cells. IEEE Journal of Photovoltaics, 2015, 5, 545-551.	1.5	15
99	Hybrid aminopolymerâ€“silica materials for efficient CO₂adsorption. RSC Advances, 2015, 5, 104943-104953.	1.7	22
100	Analysis of CO₂ Adsorption in Amine-Functionalized Porous Silicas by Molecular Simulations. Energy & Fuels, 2015, 29, 3855-3862.	2.5	36
101	Solubility of greenhouse and acid gases on the [C4mim][MeSO4] ionic liquid for gas separation and CO2 conversion. Catalysis Today, 2015, 255, 87-96.	2.2	34
102	Accurate modeling of supercritical CO2 for sustainable processes: Water+CO2 and CO2+fatty acid esters mixtures. Journal of Supercritical Fluids, 2015, 96, 86-95.	1.6	21
103	A novel solventless coating method to graft low-molecular weight polyethyleneimine on silica fine powders. Journal of Polymer Science Part A, 2014, 52, 2760-2768.	2.5	9
104	On the observation of electron-hole liquid luminescence under low excitation in Al2O3-passivated c-Si wafers. Physica Status Solidi - Rapid Research Letters, 2014, 8, 943-947.	1.2	4
105	Assessing the N2O/CO2 high pressure separation using ionic liquids with the soft-SAFT EoS. Journal of Supercritical Fluids, 2014, 92, 231-241.	1.6	40
106	Regenerable solid CO2 sorbents prepared by supercritical grafting of aminoalkoxysilane into low-cost mesoporous silica. Journal of Supercritical Fluids, 2014, 85, 68-80.	1.6	31
107	Engineering the TiO2 outermost layers using magnesium for carbon dioxide photoreduction. Applied Catalysis B: Environmental, 2014, 150-151, 57-62.	10.8	57
108	New Experimental Density Data and Soft-SAFT Models of Alkylimidazolium ([C_nC₁im]⁺) Chloride (Cl^{â€“}), Methylsulfate ([MeSO₄]^{â¯}), and Dimethylphosphate ([Me₂PO₄]^{â¯}) Based Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 6206-6221.	1.2	65

#	Article	IF	Citations
109	Understanding the Performance of New Amine-Functionalized Mesoporous Silica Materials for CO₂ Adsorption. Industrial & Engineering Chemistry Research, 2014, 53, 15611-15619.	1.8	25
110	Assessing Ionic Liquids Experimental Data Using Molecular Modeling: [C_nmim][BF₄] Case Study. Journal of Chemical & Engineering Data, 2014, 59, 3220-3231.	1.0	47
111	Development of simple and transferable molecular models for biodiesel production with the soft-SAFT equation of state. Chemical Engineering Research and Design, 2014, 92, 2898-2911.	2.7	40
112	Phase equilibria description of biodiesels with water and alcohols for the optimal design of the production and purification process. Fuel, 2014, 129, 116-128.	3.4	20
113	The toxicity effects of atmospheres with high content of carbon dioxide with addition of sulphur dioxide on two stored-product pest species: Sitophilus oryzae and Tribolium confusum. Journal of Stored Products Research, 2014, 57, 58-62.	1.2	14
114	CO2 capture efficiency and carbonation/calcination kinetics of micro and nanosized particles of supercritically precipitated calcium carbonate. Chemical Engineering Journal, 2013, 226, 357-366.	6.6	28
115	Modeling the Self-Assembly of Nano Objects: Applications to Supramolecular Organic Monolayers Adsorbed on Metal Surfaces. Journal of Chemical Theory and Computation, 2013, 9, 2161-2169.	2.3	23
116	Free-Volume Theory Coupled with Soft-SAFT for Viscosity Calculations: Comparison with Molecular Simulation and Experimental Data. Journal of Physical Chemistry B, 2013, 117, 8159-8171.	1.2	95
117	Water+1-alkanol systems: Modeling the phase, interface and viscosity properties. Fluid Phase Equilibria, 2013, 360, 367-378.	1.4	44
118	A new method using compressed CO2 for the in situ functionalization of mesoporous silica with hyperbranched polymers. Chemical Communications, 2013, 49, 11776.	2.2	20
119	High pressure separation of greenhouse gases from air with 1-ethyl-3-methylimidazolium methyl-phosphonate. International Journal of Greenhouse Gas Control, 2013, 19, 299-309.	2.3	46
120	Effect of high carbon dioxide atmosphere packaging and soluble gas stabilization pre-treatment on the shelf-life and quality of chicken drumsticks. Meat Science, 2013, 94, 1-8.	2.7	59
121	Transport Properties of Mixtures by the Soft-SAFT + Free-Volume Theory: Application to Mixtures of n-Alkanes and Hydrofluorocarbons. Journal of Physical Chemistry B, 2013, 117, 5195-5205.	1.2	64
122	Effect of Immobilized Amines on the Sorption Properties of Solid Materials: Impregnation versus Grafting. Langmuir, 2013, 29, 199-206.	1.6	44
123	Understanding CO₂ Capture in Amine-Functionalized MCM-41 by Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 3017-3024.	1.5	40
124	Alkylsilane-Functionalized Microporous and Mesoporous Materials: Molecular Simulation and Experimental Analysis of Gas Adsorption. Journal of Physical Chemistry C, 2012, 116, 10150-10161.	1.5	25
125	Surface Tension of Binary Mixtures of 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquids: Experimental Measurements and Soft-SAFT Modeling. Journal of Physical Chemistry B, 2012, 116, 12133-12141.	1.2	61
126	Flexible operation of solvent regeneration systems for CO2 capture processes using advanced control techniques: Towards operational cost minimisation. International Journal of Greenhouse Gas Control, 2012, 11, 236-250.	2.3	75

#	Article	IF	Citations
127	Thermodynamic Modeling of Imidazolium-Based Ionic Liquids with the [PF₆]^{â^'}Anion for Separation Purposes. Separation Science and Technology, 2012, 47, 399-410.	1.3	49
128	Modeling the [NTf₂] Pyridinium Ionic Liquids Family and Their Mixtures with the Soft Statistical Associating Fluid Theory Equation of State. Journal of Physical Chemistry B, 2012, 116, 9089-9100.	1.2	55
129	An equation of state for poreâ€confined fluids. AICHE Journal, 2012, 58, 3597-3600.	1.8	3
130	Modeling the Absorption of Weak Electrolytes and Acid Gases with Ionic Liquids Using the Soft-SAFT Approach. Journal of Physical Chemistry B, 2012, 116, 7709-7718.	1.2	62
131	Sorption of tryalkoxysilane in low-cost porous silicates using a supercritical CO2 method. Microporous and Mesoporous Materials, 2012, 148, 15-24.	2.2	28
132	Influence of the Concentration of CO₂ and SO₂ on the Absorption of CO₂ by a Lithium Orthosilicate-Based Absorbent. Environmental Science & Technology, 2011, 45, 7083-7088.	4.6	69
133	Microporous carbon adsorbents with high CO2 capacities for industrial applications. Physical Chemistry Chemical Physics, 2011, 13, 16063.	1.3	53
134	Monitoring the Effect of Mineral Precursor, Fluid Phase CO₂â€“H₂O Composition, and Stirring on CaCO₃ Crystallization in a Supercriticalâ€”Ultrasound Carbonation Process. Crystal Growth and Design, 2011, 11, 5324-5332.	1.4	18
135	Application of a renormalization-group treatment to the statistical associating fluid theory for potentials of variable range (SAFT-VR). Journal of Chemical Physics, 2011, 134, 154102.	1.2	42
136	Modeling Complex Associating Mixtures with [C_n-mim][Tf₂N] Ionic Liquids: Predictions from the Soft-SAFT Equation. Journal of Physical Chemistry B, 2011, 115, 4387-4398.	1.2	99
137	Direct calculation of interfacial properties of fluids close to the critical region by a molecular-based equation of state. Fluid Phase Equilibria, 2011, 306, 4-14.	1.4	50
138	Optimization of the separation of sulfur hexafluoride and nitrogen by selective adsorption using monte carlo simulations. AICHE Journal, 2011, 57, 962-974.	1.8	42
139	Soft-SAFT modeling of vaporâ€“liquid equilibria of nitriles and their mixtures. Fluid Phase Equilibria, 2010, 289, 191-200.	1.4	13
140	Modeling ionic liquids and the solubility of gases in them: Recent advances and perspectives. Fluid Phase Equilibria, 2010, 294, 15-30.	1.4	222
141	A breakthrough technique for the preparation of high-yield precipitated calcium carbonate. Journal of Supercritical Fluids, 2010, 52, 298-305.	1.6	45
142	Phase equilibria, surface tensions and heat capacities of hydrofluorocarbons and their mixtures including the critical region. Journal of Supercritical Fluids, 2010, 55, 755-768.	1.6	62
143	Investigating the Compatibility of Ruthenium Liners with Copper Interconnects. ECS Transactions, 2010, 33, 181-187.	0.3	11
144	Thermodynamic characterization of pure perfluoroalkanes, including interfacial and second order derivative properties, using the crossover soft-SAFT EoS. Fluid Phase Equilibria, 2009, 286, 134-143.	1.4	50

#	Article	IF	Citations
145	Selective Paraffin Removal from Ethane/Ethylene Mixtures by Adsorption into Aluminum Methylphosphonate-Î±: A Molecular Simulation Study. Langmuir, 2009, 25, 2148-2152.	1.6	38
146	Capturing the Solubility Minima ofn-Alkanes in Water by Soft-SAFT. Journal of Physical Chemistry B, 2009, 113, 7621-7630.	1.2	106
147	An accurate direct technique for parametrizing cubic equations of state. Fluid Phase Equilibria, 2008, 264, 201-210.	1.4	17
148	Modeling the vaporâ€“liquid equilibrium and association of nitrogen dioxide/dinitrogen tetroxide and its mixtures with carbon dioxide. Fluid Phase Equilibria, 2008, 266, 154-163.	1.4	20
149	Liquidâ€“liquid equilibrium of substituted perfluoro-n-octane+n-octane systems. Fluid Phase Equilibria, 2008, 268, 85-89.	1.4	7
150	An accurate direct technique for parameterizing cubic equations of state. Fluid Phase Equilibria, 2008, 265, 66-83.	1.4	10
151	An accurate direct technique for parameterizing cubic equations of state. Fluid Phase Equilibria, 2008, 265, 155-172.	1.4	13
152	Modeling the Solubility Behavior of CO₂, H₂, and Xe in [C_n-mim][Tf₂N] Ionic Liquids. Journal of Physical Chemistry B, 2008, 112, 15398-15406.	1.2	113
153	Modeling the phase equilibria of nitriles by the soft-SAFT Equation of State. Computer Aided Chemical Engineering, 2008, 25, 739-744.	0.3	3
154	Analysis of electron interactions in dielectric gases. Journal of Applied Physics, 2007, 101, 023308.	1.1	10
155	Capturing the Solubility Behavior of CO₂ in Ionic Liquids by a Simple Model. Journal of Physical Chemistry C, 2007, 111, 16028-16034.	1.5	126
156	Selective Adsorption of Volatile Organic Compounds in Micropore Aluminum Methylphosphonate-Î±:Â A Combined Molecular Simulationâ^'Experimental Approach. Langmuir, 2007, 23, 7299-7305.	1.6	26
157	Modeling the Phase Equilibria of Poly(ethylene glycol) Binary Mixtures with soft-SAFT EoS. Industrial & Engineering Chemistry Research, 2007, 46, 4678-4685.	1.8	19
158	Interaction between Coated Graphite Nanoparticles by Molecular Simulation. Journal of Physical Chemistry C, 2007, 111, 12328-12334.	1.5	6
159	Adsorption of Hydrogen and Methane Mixtures on Carbon Cylindrical Cavities. Journal of Physical Chemistry C, 2007, 111, 6473-6480.	1.5	19
160	Chapter 5 Structural characterization of nano- and mesoporous materials by molecular simulations. Theoretical and Computational Chemistry, 2007, 18, 101-126.	0.2	6
161	Predictions of Transport Properties in Gaseous Mixtures of Sulfur Hexafluoride and Nitrogenâ€. Journal of Physical Chemistry C, 2007, 111, 16013-16020.	1.5	7
162	Vaporâ^'Liquid and Critical Behavior of Binary Systems of Hydrogen Chloride and n-Alkanes:â€‰ Experimental Data and Soft-SAFT Modeling. Journal of Physical Chemistry B, 2007, 111, 10180-10188.	1.2	17

#	Article	IF	Citations
163	Optimized molecular force field for sulfur hexafluoride simulations. Journal of Chemical Physics, 2007, 126, 144502.	1.2	20
164	Phase equilibria, critical behavior and derivative properties of selected n-alkane/n-alkane and n-alkane/1-alkanol mixtures by the crossover soft-SAFT equation of state. Journal of Supercritical Fluids, 2007, 41, 204-216.	1.6	51
165	Effect of the flexibility and the anion in the structural and transport properties of ethyl-methyl-imidazolium ionic liquids. Fluid Phase Equilibria, 2007, 256, 62-69.	1.4	65
166	Liquidâ€“liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol+perfluoroalkane) binary mixtures. Fluid Phase Equilibria, 2007, 251, 33-40.	1.4	13
167	Global Fluid Phase Equilibria and Critical Phenomena of Selected Mixtures Using the Crossover Soft-SAFT Equation. Journal of Physical Chemistry B, 2006, 110, 1350-1362.	1.2	114
168	Phase Equilibria Calculations of Polyethylene Solutions from SAFT-Type Equations of State. Macromolecules, 2006, 39, 4240-4246.	2.2	38
169	Prediction of Thermodynamic Derivative Properties of Pure Fluids through the Soft-SAFT Equation of State. Journal of Physical Chemistry B, 2006, 110, 11427-11437.	1.2	96
170	Transport Properties of the Ionic Liquid 1-Ethyl-3-Methylimidazolium Chloride from Equilibrium Molecular Dynamics Simulation. The Effect of Temperature. Journal of Physical Chemistry B, 2006, 110, 14426-14435.	1.2	188
171	Nitrogen and Water Adsorption in Aluminum Methylphosphonate Î±:Â A Molecular Simulation Study. Langmuir, 2006, 22, 3097-3104.	1.6	11
172	Vaporâ^'Liquid Equilibrium of Carbon Dioxideâ^'Perfluoroalkane Mixtures:â€‰ Experimental Data and SAFT Modeling. Industrial & Engineering Chemistry Research, 2006, 45, 2341-2350.	1.8	107
173	Second-order thermodynamic derivative properties of selected mixtures by the soft-SAFT equation of state. Fluid Phase Equilibria, 2006, 248, 115-122.	1.4	55
174	Liquidâ€“liquid equilibrium of (perfluoroalkane+alkane) binary mixtures. Fluid Phase Equilibria, 2006, 242, 210-219.	1.4	47
175	Perfect wetting along a three-phase line: Theory and molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 244505.	1.2	25
176	Calculation of the force between surfaces coated with grafted molecules by molecular simulation. Journal of Chemical Physics, 2006, 124, 034703.	1.2	3
177	Precise Characterization of Selected Silica-Based Materials from Grand Canonical Monte Carlo Simulations. Materials Science Forum, 2006, 514-516, 1396-1400.	0.3	1
178	New insights into the adsorption isotherm interpretation by a coupled molecular simulationâ€”experimental procedure. Applied Surface Science, 2005, 252, 519-528.	3.1	17
179	Search for a reliable methodology for PSD determination based on a combined molecular simulationâ€“regularizationâ€“experimental approach. Applied Surface Science, 2005, 252, 538-547.	3.1	10
180	Simultaneous prediction of interfacial tension and phase equilibria in binary mixtures. Fluid Phase Equilibria, 2005, 227, 225-238.	1.4	63

#	Article	IF	Citations
181	Water liquid-vapor equilibria predicted by refined ab initio derived potentials. Journal of Chemical Physics, 2005, 123, 044506.	1.2	15
182	Phase and interface behaviors in type-I and type-V Lennard-Jones mixtures: Theory and simulations. Journal of Chemical Physics, 2005, 123, 034505.	1.2	77
183	Sulfur hexafluorideâ€™s liquid-vapor coexistence curve, interfacial properties, and diffusion coefficients as predicted by a simple rigid model. Journal of Chemical Physics, 2005, 123, 194508.	1.2	5
184	Phase Equilibria of Ethylene Glycol Oligomers and Their Mixtures. Industrial & Engineering Chemistry Research, 2005, 44, 7027-7037.	1.8	54
185	Densities and Vapor Pressures of Highly Fluorinated Compounds. Journal of Chemical & Engineering Data, 2005, 50, 1328-1333.	1.0	64
186	Pore Size Distribution Analysis of Selected Hexagonal Mesoporous Silicas by Grand Canonical Monte Carlo Simulations. Langmuir, 2005, 21, 8733-8742.	1.6	17
187	Some issues on the calculation of interfacial properties by molecular simulation. Journal of Chemical Physics, 2004, 121, 8611.	1.2	78
188	Thermodynamic properties of Lennard-Jones chain molecules: Renormalization-group corrections to a modified statistical associating fluid theory. Journal of Chemical Physics, 2004, 121, 10715-10724.	1.2	115
189	Thermodynamic properties of perfluoro-n-octane. Fluid Phase Equilibria, 2004, 225, 39-47.	1.4	48
190	SAFT Modeling of the Solubility of Gases in Perfluoroalkanes. Journal of Physical Chemistry B, 2004, 108, 1450-1457.	1.2	75
191	Interfacial properties of Lennard-Jones chains by direct simulation and density gradient theory. Journal of Chemical Physics, 2004, 121, 11395.	1.2	96
192	Thermodynamic properties and aggregate formation of surfactant-like molecules from theory and simulation. Journal of Chemical Physics, 2004, 120, 9822-9830.	1.2	9
193	Solubility of hydrogen in heavyn-alkanes: Experiments and saft modeling. AICHE Journal, 2003, 49, 3260-3269.	1.8	76
194	Pore Size Distribution of Porous Glasses:Â A Test of the Independent Pore Model. Langmuir, 2003, 19, 8592-8604.	1.6	32
195	Coexistence Densities of Methane and Propane by Canonical Molecular Dynamics and Gibbs Ensemble Monte Carlo Simulations. Molecular Simulation, 2003, 29, 463-470.	0.9	25
196	Application of the fundamental measure density functional theory to the adsorption in cylindrical pores. Journal of Chemical Physics, 2003, 118, 830-842.	1.2	31
197	Critical properties of homopolymer fluids studied by a Lennard-Jones statistical associating fluid theory. Molecular Physics, 2002, 100, 2519-2529.	0.8	31
198	Predictions of the Jouleâ^'Thomson Inversion Curve for then-Alkane Series and Carbon Dioxide from the Soft-SAFT Equation of Stateâ€. Industrial & Engineering Chemistry Research, 2002, 41, 1069-1075.	1.8	39

#	Article	IF	Citations
199	The influence of the density in the hydrophobic hydration of methane in supercritical water. Journal of Molecular Liquids, 2002, 101, 113-125.	2.3	3
200	Thermodynamic properties and phase equilibria of branched chain fluids using first- and second-order Wertheimâ€™s thermodynamic perturbation theory. Journal of Chemical Physics, 2001, 115, 3906-3915.	1.2	20
201	Vaporâ^'Liquid Equilibria and Critical Behavior of Heavy n-Alkanes Using Transferable Parameters from the Soft-SAFT Equation of State. Industrial & Engineering Chemistry Research, 2001, 40, 2532-2543.	1.8	143
202	The hydrophobic hydration of methane as a function of temperature from histogram reweighting Monte Carlo simulations. Journal of Chemical Physics, 2001, 114, 7527-7535.	1.2	17
203	Improved vaporâ€“liquid equilibria predictions for Lennard-Jones chains from the statistical associating fluid dimer theory: Comparison with Monte Carlo simulations. Journal of Chemical Physics, 2001, 115, 4355-4358.	1.2	44
204	Tricritical phenomena in chain-like mixtures from a molecular-based equation of state. Fluid Phase Equilibria, 2000, 171, 91-104.	1.4	29
205	Predicting Liquidâ€“Vapour Equilibria for Water Using anab-initioPotential from Histogram Reweighting Monte Carlo Simulations. Molecular Simulation, 2000, 24, 63-69.	0.9	4
206	Liquid vapor equilibria for an ab initio model for water. Journal of Chemical Physics, 1999, 111, 2103-2108.	1.2	18
207	Modeling new adsorbents for ethylene/ethane separations by adsorption via Ï€-complexation. Fluid Phase Equilibria, 1998, 150-151, 117-124.	1.4	27
208	Critical behavior and partial miscibility phenomena in binary mixtures of hydrocarbons by the statistical associating fluid theory. Journal of Chemical Physics, 1998, 109, 7405-7413.	1.2	62
209	Prediction of Binary and Ternary Diagrams Using the Statistical Associating Fluid Theory (SAFT) Equation of State. Industrial & Engineering Chemistry Research, 1998, 37, 660-674.	1.8	248
210	Molecular Modeling of Selective Adsorption from Mixtures. Materials Research Society Symposia Proceedings, 1997, 497, 231.	0.1	4
211	Thermodynamic behaviour of homonuclear and heteronuclear Lennard-Jones chains with association sites from simulation and theory. Molecular Physics, 1997, 92, 135-150.	0.8	333
212	Adsorption of Water on Activated Carbons:Â A Molecular Simulation Study. The Journal of Physical Chemistry, 1996, 100, 1189-1196.	2.9	353
213	Effect of surface active sites on adsorption of associating chain molecules in pores: A Monte Carlo study. Adsorption, 1996, 2, 59-68.	1.4	11
214	Adsorption Isotherms of Associating Fluids in Slit-Like Pores. A Monte Carlo Simulation Study. Kluwer International Series in Engineering and Computer Science, 1996, , 993-1000.	0.2	1
215	Molecular simulation and theory of associating chain molecules. International Journal of Thermophysics, 1995, 16, 705-713.	1.0	20
216	Phase equilibria in ternary Lennard-Jones systems. Fluid Phase Equilibria, 1995, 107, 31-43.	1.4	32

#	Article	IF	Citations
217	Mixtures of Associating and Non-associating Chains on Activated Surfaces: A Monte Carlo Approach. Molecular Simulation, 1995, 15, 141-154.	0.9	9
218	Adsorption isotherms of associating chain molecules from Monte Carlo simulations. Molecular Physics, 1995, 85, 9-21.	0.8	24
219	Chemical potentials and adsorption isotherms of polymers confined between parallel plates. Chemical Engineering Science, 1994, 49, 2921-2929.	1.9	20
220	A new algorithm for molecular dynamics simulations in the grand canonical ensemble. Molecular Physics, 1994, 82, 439-453.	0.8	19
221	Theory and simulation of associating fluids: Lennard-Jones chains with association sites. Molecular Physics, 1994, 83, 1209-1222.	0.8	40
222	Phase equilibria and critical behavior of squareâ€well fluids of variable width by Gibbs ensemble Monte Carlo simulation. Journal of Chemical Physics, 1992, 96, 2296-2305.	1.2	307
223	Hydrogen Technologies and Applications: Safety. Advances in Science and Technology, 0, , .	0.2	1
224	Synergetic Effect of Physicochemical and Electrostatic Strategies on Ion Sieving for Polymer Cross-linked Graphene Oxide Membrane. Environmental Science: Nano, 0, , .	2.2	2
225	Robust Thermodynamic Models to Describe the Physicochemical Behaviour of Deep Eutectic Solvents for Gas Separation. , 0, , .		0