Lourdes F Vega

List of Publications by Year
in descending order

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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	Adsorption of Water on Activated Carbons:Â A Molecular Simulation Study. The Journal of Physical Chemistry, 1996, 100, 1189-1196.	2.9	353
2	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
3	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
4	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
5	Applications of fly ash for CO2 capture, utilization, and storage. Journal of CO2 Utilization, 2019, 29, 82-102.	3.3	234
6	Modeling ionic liquids and the solubility of gases in them: Recent advances and perspectives. Fluid Phase Equilibria, 2010, 294, 15-30.	1.4	222
7	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
8	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
9	Activated carbons from biomass-based sources for CO2 capture applications. Chemosphere, 2021, 282, 131111.	4.2	135
10	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
11	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
12	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
13	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
14	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
15	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
16	Capturing the Solubility Minima ofn-Alkanes in Water by Soft-SAFT. Journal of Physical Chemistry B, 2009, 113, 7621-7630.	1.2	106
17	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
18	Interfacial properties of Lennard-Jones chains by direct simulation and density gradient theory. Journal of Chemical Physics, 2004, 121, 11395.	1.2	96

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19	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
20	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
21	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
22	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
23	Predicting the density and viscosity of hydrophobic eutectic solvents: towards the development of sustainable solvents. Green Chemistry, 2020, 22, 8511-8530.	4.6	84
24	Perspectives and guidelines on thermodynamic modelling of deep eutectic solvents. Journal of Molecular Liquids, 2020, 298, 112183.	2.3	83
25	Some issues on the calculation of interfacial properties by molecular simulation. Journal of Chemical Physics, 2004, 121, 8611.	1.2	78
26	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
27	Solubility of hydrogen in heavyn-alkanes: Experiments and saft modeling. AICHE Journal, 2003, 49, 3260-3269.	1.8	76
28	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
29	SAFT Modeling of the Solubility of Gases in Perfluoroalkanes. Journal of Physical Chemistry B, 2004, 108, 1450-1457.	1.2	75
30	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
31	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
32	Current and future perspectives on catalytic-based integrated carbon capture and utilization. Science of the Total Environment, 2021, 790, 148081.	3.9	67
33	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
34	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
35	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
36	Densities and Vapor Pressures of Highly Fluorinated Compounds. Journal of Chemical & Engineering Data, 2005, 50, 1328-1333.	1.0	64

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37	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
38	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
39	Simultaneous prediction of interfacial tension and phase equilibria in binary mixtures. Fluid Phase Equilibria, 2005, 227, 225-238.	1.4	63
40	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
41	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
42	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
43	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
44	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
45	Next generation of low global warming potential refrigerants: Thermodynamic properties molecular modeling. AICHE Journal, 2018, 64, 250-262.	1.8	58
46	Engineering the TiO2 outermost layers using magnesium for carbon dioxide photoreduction. Applied Catalysis B: Environmental, 2014, 150-151, 57-62.	10.8	57
47	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
48	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
49	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
50	Phase Equilibria of Ethylene Glycol Oligomers and Their Mixtures. Industrial & Engineering Chemistry Research, 2005, 44, 7027-7037.	1.8	54
51	Microporous carbon adsorbents with high CO2 capacities for industrial applications. Physical Chemistry Chemical Physics, 2011, 13, 16063.	1.3	53
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	Thermodynamic properties of perfluoro-n-octane. Fluid Phase Equilibria, 2004, 225, 39-47.	1.4	48
60	Liquidâ€"liquid equilibrium of (perfluoroalkane+alkane) binary mixtures. Fluid Phase Equilibria, 2006, 242, 210-219.	1.4	47
61	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
62	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
63	A breakthrough technique for the preparation of high-yield precipitated calcium carbonate. Journal of Supercritical Fluids, 2010, 52, 298-305.	1.6	45
64	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
65	Water+1-alkanol systems: Modeling the phase, interface and viscosity properties. Fluid Phase Equilibria, 2013, 360, 367-378.	1.4	44
66	Effect of Immobilized Amines on the Sorption Properties of Solid Materials: Impregnation versus Grafting. Langmuir, 2013, 29, 199-206.	1.6	44
67	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
68	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
69	Theory and simulation of associating fluids: Lennard-Jones chains with association sites. Molecular Physics, 1994, 83, 1209-1222.	0.8	40
70	Understanding CO₂ Capture in Amine-Functionalized MCM-41 by Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 3017-3024.	1.5	40
71	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
72	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

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73	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
74	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
75	Phase Equilibria Calculations of Polyethylene Solutions from SAFT-Type Equations of State. Macromolecules, 2006, 39, 4240-4246.	2.2	38
76	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
77	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
78	New measurements and modeling of high pressure thermodynamic properties of glycols. Fluid Phase Equilibria, 2017, 436, 113-123.	1.4	38
79	Strategies for Integrated Capture and Conversion of CO₂ from Dilute Flue Gases and the Atmosphere. ChemSusChem, 2021, 14, 1805-1820.	3.6	37
80	Analysis of CO₂ Adsorption in Amine-Functionalized Porous Silicas by Molecular Simulations. Energy & Fuels, 2015, 29, 3855-3862.	2.5	36
81	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
82	Pharmaceutical Removal from Water Effluents by Adsorption on Activated Carbons: A Monte Carlo Simulation Study. Langmuir, 2017, 33, 11146-11155.	1.6	36
83	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
84	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
85	Phase equilibria in ternary Lennard-Jones systems. Fluid Phase Equilibria, 1995, 107, 31-43.	1.4	32
86	Pore Size Distribution of Porous Glasses:Â A Test of the Independent Pore Model. Langmuir, 2003, 19, 8592-8604.	1.6	32
87	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
88	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
89	Critical properties of homopolymer fluids studied by a Lennard-Jones statistical associating fluid theory. Molecular Physics, 2002, 100, 2519-2529.	0.8	31
90	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

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91	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
92	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
93	Tricritical phenomena in chain-like mixtures from a molecular-based equation of state. Fluid Phase Equilibria, 2000, 171, 91-104.	1.4	29
94	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
95	Sorption of tryalkoxysilane in low-cost porous silicates using a supercritical CO2 method. Microporous and Mesoporous Materials, 2012, 148, 15-24.	2.2	28
96	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
97	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
98	Modeling new adsorbents for ethylene/ethane separations by adsorption via Ï€-complexation. Fluid Phase Equilibria, 1998, 150-151, 117-124.	1.4	27
99	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
100	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
101	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
102	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
103	Perfect wetting along a three-phase line: Theory and molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 244505.	1.2	25
104	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
105	Understanding the Performance of New Amine-Functionalized Mesoporous Silica Materials for CO₂ Adsorption. Industrial & Engineering Chemistry Research, 2014, 53, 15611-15619.	1.8	25
106	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
107	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
108	A consistent thermodynamic molecular model of n-hydrofluoroolefins and blends for refrigeration applications. International Journal of Refrigeration, 2020, 113, 145-155.	1.8	25

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109	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
110	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
111	Adsorption isotherms of associating chain molecules from Monte Carlo simulations. Molecular Physics, 1995, 85, 9-21.	0.8	24
112	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
113	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
114	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
115	Thermophysical Characterization of Ionic Liquids Based on the Perfluorobutanesulfonate Anion: Experimental and Softâ€SAFT Modeling Results. ChemPhysChem, 2017, 18, 2012-2023.	1.0	23
116	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
117	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
118	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
119	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
120	Hybrid aminopolymerâ€“silica materials for efficient CO₂adsorption. RSC Advances, 2015, 5, 104943-104953.	1.7	22
121	On the anomalous composition dependence of viscosity and surface tension in refrigerant blends. Journal of Molecular Liquids, 2018, 268, 190-200.	2.3	22
122	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
123	Chemical potentials and adsorption isotherms of polymers confined between parallel plates. Chemical Engineering Science, 1994, 49, 2921-2929.	1.9	20
124	Molecular simulation and theory of associating chain molecules. International Journal of Thermophysics, 1995, 16, 705-713.	1.0	20
125	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
126	Optimized molecular force field for sulfur hexafluoride simulations. Journal of Chemical Physics, 2007, 126, 144502.	1.2	20

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127	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
128	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
129	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
130	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
131	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
132	A new algorithm for molecular dynamics simulations in the grand canonical ensemble. Molecular Physics, 1994, 82, 439-453.	0.8	19
133	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
134	Adsorption of Hydrogen and Methane Mixtures on Carbon Cylindrical Cavities. Journal of Physical Chemistry C, 2007, 111, 6473-6480.	1.5	19
135	Molecular simulations of carbon-based materials for selected CO2 separation and water treatment processes. Fluid Phase Equilibria, 2019, 492, 10-25.	1.4	19
136	Liquid vapor equilibria for an ab initio model for water. Journal of Chemical Physics, 1999, 111, 2103-2108.	1.2	18
137	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
138	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
139	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
140	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
141	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
142	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
143	New insights into the adsorption isotherm interpretation by a coupled molecular simulationâ€”experimental procedure. Applied Surface Science, 2005, 252, 519-528.	3.1	17
144	Pore Size Distribution Analysis of Selected Hexagonal Mesoporous Silicas by Grand Canonical Monte Carlo Simulations. Langmuir, 2005, 21, 8733-8742.	1.6	17

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145	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
146	An accurate direct technique for parametrizing cubic equations of state. Fluid Phase Equilibria, 2008, 264, 201-210.	1.4	17
147	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
148	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
149	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
150	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
151	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
152	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
153	Searching for Sustainable Refrigerants by Bridging Molecular Modeling with Machine Learning. Industrial & Engineering Chemistry Research, 2022, 61, 7414-7429.	1.8	16
154	Water liquid-vapor equilibria predicted by refined ab initio derived potentials. Journal of Chemical Physics, 2005, 123, 044506.	1.2	15
155	Incorporating critical divergence of isochoric heat capacity into the softâ€SAFT equation of state. AICHE Journal, 2015, 61, 3073-3080.	1.8	15
156	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
157	Molecular simulations of phenol and ibuprofen removal from water using multilayered graphene oxide membranes. Molecular Physics, 2019, 117, 3703-3714.	0.8	15
158	Functionalization of fluorinated ionic liquids: A combined experimental-theoretical study. Journal of Molecular Liquids, 2020, 302, 112489.	2.3	15
159	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
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