## Andres Mejia

List of Publications by Year in descending order

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100 papers	2,217 citations	25 h-index	276539 41 g-index
102	102	102	1093
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	Force Fields for Coarse-Grained Molecular Simulations from a Corresponding States Correlation. Industrial & Description of the Research, 2014, 53, 4131-4141.	1.8	109
2	Interfacial properties of selected binary mixtures containing n-alkanes. Fluid Phase Equilibria, 2009, 282, 68-81.	1.4	98
3	Use of Equations of State and Coarse Grained Simulations to Complement Experiments: Describing the Interfacial Properties of Carbon Dioxide + Decane and Carbon Dioxide + Eicosane Mixtures. Journal of Chemical & Chemical	1.0	85
4	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
5	Unnoticed Pitfalls of Soave-Type Alpha Functions in Cubic Equations of State. Industrial & Description of State. Industri	1.8	71
6	SAFT- $\hat{I}^3$ force field for the simulation of molecular fluids 6: Binary and ternary mixtures comprising water, carbon dioxide, and n -alkanes. Journal of Chemical Thermodynamics, 2016, 93, 320-336.	1.0	71
7	Interfacial tensions of industrial fluids from a molecularâ€based square gradient theory. AICHE Journal, 2016, 62, 1781-1794.	1.8	66
8	Simultaneous prediction of interfacial tension and phase equilibria in binary mixtures. Fluid Phase Equilibria, 2005, 227, 225-238.	1.4	63
9	High-pressure densities and interfacial tensions of binary systems containing carbon dioxide+n-alkanes: (n-Dodecane, n-tridecane, n-tetradecane). Fluid Phase Equilibria, 2014, 380, 82-92.	1.4	60
10	Early regimes of water capillary flow in slit silica nanochannels. Physical Chemistry Chemical Physics, 2015, 17, 14731-14739.	1.3	59
11	Comprehensive Characterization of Interfacial Behavior for the Mixture CO <sub>2</sub> + H <sub>2</sub> O + CH <sub>4</sub> : Comparison between Atomistic and Coarse Grained Molecular Simulation Models and Density Gradient Theory. Journal of Physical Chemistry C, 2014, 118, 24504-24519.	1.5	52
12	Comparison of United-Atom Potentials for the Simulation of Vapor–Liquid Equilibria and Interfacial Properties of Long-Chain <i>n</i> -Alkanes up to <i>n</i> -C <sub>100</sub> . Journal of Physical Chemistry B, 2011, 115, 12822-12834.	1.2	46
13	Combined Experimental, Theoretical, and Molecular Simulation Approach for the Description of the Fluid-Phase Behavior of Hydrocarbon Mixtures within Shale Rocks. Energy & Energy & 2018, 32, 5750-5762.	2.5	46
14	Wounding prior to challenge substantially improves infectivity of cottontail rabbit papillomavirus and allows for standardization of infection. Journal of Virological Methods, 2008, 148, 34-39.	1.0	45
15	Resolving Discrepancies in the Measurements of the Interfacial Tension for the CO <sub>2</sub> + H <sub>2</sub> O Mixture by Computer Simulation. Journal of Physical Chemistry Letters, 2014, 5, 1267-1271.	2.1	43
16	Interfacial tensions of binary mixtures of ethanol with octane, decane, dodecane, and tetradecane. Journal of Chemical Thermodynamics, 2011, 43, 1395-1400.	1.0	42
17	Prediction of the water/oil interfacial tension from molecular simulations using the coarse-grained SAFT-Î <sup>3</sup> Mie force field. Fluid Phase Equilibria, 2018, 476, 9-15.	1.4	40
18	A rigorous approach for predicting the slope and curvature of the temperature–entropy saturation boundary of pure fluids. Energy, 2012, 45, 888-899.	4.5	38

#	Article	IF	Citations
19	Bottled SAFT: A Web App Providing SAFT- $\hat{l}^3$ Mie Force Field Parameters for Thousands of Molecular Fluids. Journal of Chemical Information and Modeling, 2016, 56, 1609-1614.	2.5	36
20	Assessing salt-surfactant synergistic effects on interfacial tension from molecular dynamics simulations. Journal of Molecular Liquids, 2020, 299, 112223.	2.3	35
21	Vapor–Liquid Equilibrium, Densities, and Interfacial Tensions of the System Hexane + 2,5-Dimethylfuran. Journal of Chemical & Engineering Data, 2012, 57, 2681-2688.	1.0	32
22	Atmospheric densities and interfacial tensions for 1-alkanol (1-butanol to 1-octanol)+water and ether (MTBE, ETBE, DIPE, TAME and THP)+water demixed mixtures. Fluid Phase Equilibria, 2015, 396, 88-97.	1.4	31
23	Correlation and prediction of interface tension for fluid mixtures: An approach based on cubic equations of state with the wong-sandler mixing rule. Journal of Phase Equilibria and Diffusion, 2005, 26, 215-224.	0.5	29
24	SGTPy: A Python Code for Calculating the Interfacial Properties of Fluids Based on the Square Gradient Theory Using the SAFT-VR Mie Equation of State. Journal of Chemical Information and Modeling, 2021, 61, 1244-1250.	2.5	27
25	High-pressure interfacial tensions for nitrogen+ethanol, or hexane or 2-methoxy-2-methylbutane: A comparison between experimental tensiometry and Monte Carlo simulations. Journal of Supercritical Fluids, 2014, 89, 78-88.	1.6	26
26	Estimation of interfacial behavior using the global phase diagram approach I. Carbon dioxide–n-alkanes. Thermochimica Acta, 2004, 411, 171-176.	1.2	25
27	Perfect wetting along a three-phase line: Theory and molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 244505.	1.2	25
28	Extension of the SAFT-VR Mie EoS To Model Homonuclear Rings and Its Parametrization Based on the Principle of Corresponding States. Langmuir, 2017, 33, 11518-11529.	1.6	25
29	Measurement and modeling of isobaric vapor – Liquid equilibrium and isothermal interfacial tensions of ethanol + hexane + 2,5 – Dimethylfuran mixture. Fuel, 2018, 229, 105-115.	3.4	24
30	Coarse-grained theoretical modeling and molecular simulations of nitrogen + n -alkanes: ( n -pentane,) Tj ETQq0 (	0 0 rgBT /0	Overlock 10 T
31	Isobaric Vapor–Liquid Equilibrium and Isothermal Interfacial Tensions for the System Ethanol + 2,5-Dimethylfuran. Journal of Chemical & Engineering Data, 2013, 58, 3226-3232.	1.0	21
32	Understanding the interfacial behavior in isopycnic Lennard-Jones mixtures by computer simulations. Physical Chemistry Chemical Physics, 2016, 18, 1114-1124.	1.3	21
33	Interfacial Behavior in Type IV Systems. International Journal of Thermophysics, 2004, 25, 1395-1414.	1.0	20
34	Experimental determination and theoretical modeling of the vapor–liquid equilibrium and surface tensions of hexane+tetrahydro-2H-pyran. Fluid Phase Equilibria, 2012, 316, 55-65.	1.4	20
35	Experimental determination and theoretical prediction of the vapor–liquid equilibrium and interfacial tensions of the system methyl-tert-butyl ether + 2,5-dimethylfuran. Fuel, 2014, 116, 183-190.	3.4	19
36	Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl) Tj ETQq0 0 0 rgBT	/Overlock 1.0	10 Tf 50 67 1

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Thermodynamics, 2018, 121, 121-128.

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37	On the Interfacial Behavior about the Shield Region. International Journal of Thermophysics, 2005, 26, 13-29.	1.0	18
38	Association and molecular chain length effects on interfacial behavior§. Physics and Chemistry of Liquids, 2006, 44, 45-59.	0.4	18
39	Vapor–liquid equilibrium, densities, and interfacial tensions for the system ethyl 1,1-dimethylethyl ether (ETBE)+propan-1-ol. Fluid Phase Equilibria, 2007, 255, 121-130.	1.4	18
40	Vaporâ <sup>°</sup> Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylpropane. Journal of Chemical & Chemica	1.0	18
41	Measurement and theoretical prediction of the vaporâ€"liquid equilibrium, densities and interfacial tensions of the system hexane+2-methoxy-2-methylbutane. Fluid Phase Equilibria, 2011, 308, 15-24.	1.4	18
42	An accurate direct technique for parametrizing cubic equations of state. Fluid Phase Equilibria, 2008, 264, 201-210.	1.4	17
43	Vaporâ^'Liquid Equilibrium in the Binary Systems 2-Butanol + <i>tert</i> -Amyl Methyl Ether, 2-Butanol + Heptane, and Heptane + <i>tert</i> -Amyl Methyl Ether. Journal of Chemical & Engineering Data, 2011, 56, 2256-2265.	1.0	17
44	Vapor–Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylbutane. Journal of Chemical & Data, 2011, 56, 3142-3148.	1.0	17
45	Isobaric vapor–liquid equilibrium and isothermal surface tensions of 2,2′-oxybis[propane]+2,5-Dimethylfuran. Fluid Phase Equilibria, 2013, 345, 60-67.	1.4	17
46	A rigorous and accurate approach for predicting the wet-to-dry transition for working mixtures in organic Rankine cycles. Energy, 2018, 156, 509-519.	4.5	17
47	A Guide to Computing Interfacial Properties of Fluids from Molecular Simulations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	17
48	Vapor–liquid equilibria and interfacial tensions for the ternary system acetone+2,2′-oxybis[propane]+cyclohexane and its constituent binary systems. Fluid Phase Equilibria, 2008, 270, 75-86.	1.4	16
49	On the phase and interface behavior along the three-phase line of ternary Lennard-Jones mixtures: A collaborative approach based on square gradient theory and molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 014503.	1.2	16
50	Modelling of solubility of vitamin K3 derivatives in supercritical carbon dioxide using cubic and SAFT equations of state. Journal of Supercritical Fluids, 2021, 167, 105040.	1.6	16
51	Isobaric Vapor-Liquid Equilibria and Densities for the Binary Systems Oxolane + Ethyl 1,1-Dimethylethyl Ether, Oxolane + 2-Propanol and Propan-2-One + Trichloromethane. Physics and Chemistry of Liquids, 2003, 41, 283-301.	0.4	15
52	Phase behaviour and interfacial properties of ternary system CO <sub>2</sub> + n-butane + n-decane: coarse-grained theoretical modelling and molecular simulations. Molecular Physics, 2016, 114, 2627-2640.	0.8	15
53	Prediction of azeotropic behavior using equations of state. Fluid Phase Equilibria, 1999, 166, 141-162.	1.4	14
54	A Model-Free Approach Data Treatment of Vaporâ-'Liquid Equilibrium Data in Ternary Systems. 2. Applications. Industrial & Data Treatment of Vaporâ-'Liquid Equilibrium Data in Ternary Systems. 2. Applications. Industrial & Data Treatment of Vaporâ-'Liquid Equilibrium Data in Ternary Systems. 2.	1.8	14

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55	Phase equilibria and interfacial tensions in the systems methyl tert-butyl ether+acetone+cyclohexane, methyl tert-butyl ether+acetone and methyl tert-butyl ether+cyclohexane. Fluid Phase Equilibria, 2008, 273, 68-77.	1.4	14
56	Molar isopycnicity in heterogeneous binary mixtures. Fluid Phase Equilibria, 2012, 336, 84-97.	1.4	14
57	A topological approach to mass barotropic phenomena in asymmetric mixtures. Fluid Phase Equilibria, 2012, 313, 171-181.	1.4	14
58	A Model-Free Approach Data Treatment of Vaporâ°'Liquid Equilibrium Data in Ternary Systems. 1. Theory and Numerical Procedures. Industrial & Data to Chemistry Research, 2001, 40, 2134-2148.	1.8	13
59	An accurate direct technique for parameterizing cubic equations of state. Fluid Phase Equilibria, 2008, 265, 155-172.	1.4	13
60	Experimental measurements and theoretical modeling of high-pressure mass densities and interfacial tensions of carbon dioxide + n-heptane + toluene and its carbon dioxide binary systems. Fuel, 2018, 228 92-102.	3,3.4	13
61	Phasepy: A Python based framework for fluid phase equilibria and interfacial properties computation. Journal of Computational Chemistry, 2020, 41, 2504-2526.	1.5	13
62	Surface Tension of 1-Ethyl-3-methylimidazolium Ethyl Sulfate or 1-Butyl-3-methylimidazolium Hexafluorophosphate with Argon and Carbon Dioxide. Journal of Chemical & Dioxide, 2013, 58, 1203-1211.	1.0	12
63	Phase Equilibria and Interfacial Properties of the Tetrahydrofuran + Methane Binary Mixture from Experiment and Computer Simulation. Journal of Physical Chemistry C, 2019, 123, 20960-20970.	1.5	12
64	Experimental Determination of Isobaric Vapor–Liquid Equilibrium and Isothermal Interfacial Tensions for the Binary Ethanol + Cyclopentyl Methyl Ether Mixture. Journal of Chemical & Engineering Data, 2019, 64, 1970-1977.	1.0	12
65	Isobaric vapor–liquid equilibrium and isothermal surface tension for hexaneÂ+ cyclopentyl methyl ether binary mixture: Experimental determinations and theoretical predictions. Fluid Phase Equilibria, 2020, 520, 112654.	1.4	12
66	Comments on "Experimental Measurements of Vapor–Liquid Equilibrium Data for the Binary Systems of Methanol + 2-Butyl Acetate, 2-Butyl Alcohol + 2-Butyl Acetate, and Methyl Acetate + 2-Butyl Acetate at 101.33 kPa― Journal of Chemical & Data, 2013, 58, 3563-3566.	1.0	11
67	Phase equilibria and interfacial tensions in the systems ethanol+2-methoxy-2-methylbutane+hexane. Fuel, 2014, 117, 996-1003.	3.4	11
68	Vapour–liquid phase equilibria and interfacial properties of fatty acid methyl esters from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 4974-4983.	1.3	11
69	Rebuttal to the Comments of Paul M. Mathias on "Unnoticed Pitfalls of Soave-Type Alpha Functions in Cubic Equations of State― Industrial & Engineering Chemistry Research, 2004, 43, 1895-1896.	1.8	10
70	An accurate direct technique for parameterizing cubic equations of state. Fluid Phase Equilibria, 2008, 265, 66-83.	1.4	10
71	Vapor–liquid equilibrium, densities, and interfacial tensions for the system benzene <b>+</b> propan-1-ol. Physics and Chemistry of Liquids, 2008, 46, 175-190.	0.4	10
72	Vapor–Liquid Equilibrium and Interfacial Tension for the 1-Butanol + Cyclopentyl Methyl Ether Binary Mixture. Journal of Chemical & Engineering Data, 2020, 65, 4142-4149.	1.0	10

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73	Vapor–liquid equilibrium at 94ÂkPa and surface tension at 298.15ÂK for hexaneÂ+ÂethanolÂ+Âcyclopentyl methyl ether mixture. Fuel, 2020, 279, 118415.	3.4	10
74	Barotropic phenomena in binary mixtures. Fluid Phase Equilibria, 2015, 394, 175-185.	1.4	9
75	Probing the Interfacial Behavior of Type Illa Binary Mixtures Along the Three-Phase Line Employing Molecular Thermodynamics. Molecules, 2020, 25, 1499.	1.7	9
76	Isobaric Vapor-Liquid Equilibria and Densities for the System Ethyl 1,1-Dimethylethyl Ether + 2-Propanol. Physics and Chemistry of Liquids, 2002, 40, 685-702.	0.4	8
77	Isobaric vapor – liquid – liquid equilibrium for waterÂ+ÂMTBEÂ+Âalcohol (ethanol or 1-butanol) mixtures. Fluid Phase Equilibria, 2020, 523, 112768.	1.4	8
78	Interfacial Properties of Tetrahydrofuran and Carbon Dioxide Mixture from Computer Simulation. Journal of Physical Chemistry C, 2018, 122, 16142-16153.	1.5	7
79	Comments "On The Consistency and Correctness of Thermodynamics Phase Equilibria Modeling and Correlations Reports Published In Fuel Journalâ€, Fuel, 2015, 140, 812-813.	3.4	6
80	Measurements and modeling of the phase equilibria for the n-hexaneÂ+ÂethanolÂ+Âdibutyl ether ternary mixture and its dibutyl ether sub-binary mixtures at 94ÂkPa. Fuel, 2021, 297, 120361.	3.4	6
81	Phase equilibria and interfacial properties of selected methaneÂ+Ân-alkane binary mixtures. Journal of Molecular Liquids, 2021, 341, 116918.	2.3	6
82	Density and viscosity of liquid mixtures formed by n-hexane, ethanol, and cyclopentyl methyl ether. Journal of Molecular Liquids, 2022, 359, 119353.	2.3	6
83	Vapor–Liquid Equilibrium, Densities, and Interfacial Tensions of the System Ethanol + Tetrahydro-2 <i>H</i> -pyran. Journal of Chemical & Engineering Data, 2012, 57, 561-567.	1.0	5
84	Experimental determination and theoretical modeling of the vapor–liquid equilibrium and densities of the binary system butan-2-ol+tetrahydro-2H-pyran. Fluid Phase Equilibria, 2013, 342, 52-59.	1.4	5
85	Vapor–liquid equilibrium and interfacial tensions of the system ethanol+hexane+tetrahydro-2H-Pyran. Fluid Phase Equilibria, 2014, 361, 229-236.	1.4	5
86	A Novel Experimental Procedure to Measure the Bulk Mass Densities and Interfacial Tensions for Mixtures at Vapor–Liquid–Liquid Equilibria. Journal of Chemical & Engineering Data, 2020, 65, 3344-3356.	1.0	5
87	Impact of morphology on the interfacial tension of liquid-liquid equilibrium interfaces in asymmetric mixtures. Chemical Physics, 2022, 557, 111498.	0.9	5
88	Vapor-liquid phase equilibria, liquid densities, liquid viscosities and surface tensions for the ternary n-hexaneÂ+Âcyclopentyl methyl etherÂ+Â1-butanol mixture. Fluid Phase Equilibria, 2022, 558, 113444.	1.4	5
89	Coarse-grained molecular dynamic simulations of selected thermophysical properties for 1-Butyl-3-methylimidazolium hexafluorophosphate. Journal of Molecular Liquids, 2013, 186, 106-115.	2.3	4
90	Measurement and modeling of high pressure density and interfacial tension of carbon dioxide + tetrahydrofuran mixture. Journal of Supercritical Fluids, 2017, 128, 359-369.	1.6	4

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91	Vapor–Liquid Equilibrium, Surface Tension, and Dynamic Viscosity for the Propan-1-ol + Dibutyl Ether Binary Mixture. Journal of Chemical & Engineering Data, 2021, 66, 2783-2792.	1.0	4
92	Measurement of phase equilibrium and interfacial tension for the (1-propanolÂ+Âcyclopentyl methyl) Tj ETQq0 C	0 0 <sub>[gB</sub> T /C	verlock 10 Tf
93	Preferential Orientations and Anomalous Interfacial Tensions in Aqueous Solutions of Alcohols. Journal of Physical Chemistry B, 2020, 124, 8388-8401.	1.2	3
94	ISOBARIC VAPOR—LIQUID EQUILIBRIA FOR THE TERNARY SYSTEM OXOLANE + ETHYL 1, 1-DIMETHYLETHYL ETHER + 2-PROPANOL AT 50kPa. Physics and Chemistry of Liquids, 2003, 41, 493-501.	0.4	3
95	The additivity of surface and volumetric properties of $\hat{l}_{\pm}$ , $\hat{l}_{\infty}$ -dihalogenoalkanes. Journal of Chemical Thermodynamics, 2019, 132, 222-228.	1.0	2
96	Comments on "isobaric (vapor + liquid) equilibria for three binary systems (toluene + anisole, n) Tj ETQq0 0 C	rgBŢ /Ov	erlgck 10 Tf 50
97	Comments on "Vapor–Liquid Equilibrium for Ternary and Binary Systems of Tetrahydrofuran, Cyclohexane, and 1,2-Propanediol at 101.3 kPa― Journal of Chemical & Engineering Data, 2016, 61, 1961-1963.	1.0	1
98	Molecular dynamics of liquid–liquid equilibrium and interfacial properties of aqueous solutions of methyl esters. Physical Chemistry Chemical Physics, 2022, 24, 5371-5382.	1.3	1
99	Comment on "lsobaric Vapor + Liquid Equilibrium Measurements and Calculations for Using Nontraditional Models for the Association Systems of Ethyl Acetate + 2-Ethylhexanoic Acid and Propyl Acetate + 2-Ethylhexanoic Acid at Atmospheric Pressureâ€, Journal of Chemical & Data, 2021. 66. 848-851.	1.0	O
100	Correlation and Prediction of Interface Tension for Fluid Mixtures: An Approach Based on Cubic Equations of State with the Wong-Sandler Mixing Rule. Journal of Phase Equilibria and Diffusion, 2005, 26, 215-224.	0.5	0