Marcelo Castier

List of Publications by Year
in descending order

88	2,330	218677	233421
papers	citations	26 h-index	45 g-index

89	89	89	1856
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predicting the performance of spiral-wound membranes in pressure-retarded osmosis processes. Renewable Energy, 2022, 189, 66-77.	8.9	9
2	The role of cross-association between carbon dioxide and hydrogen sulfide using the SAFT-VR Mie equationÂof state. Fluid Phase Equilibria, 2022, 559, 113493.	2.5	5
3	Waterâ€“Hydrocarbon Phase Equilibria with SAFT-VR Mie Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 5278-5299.	3.7	8
4	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	6
5	Modeling of Gas Solubility in Aqueous Electrolyte Solutions with the eSAFT-VR Mie Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 15327-15342.	3.7	19
6	A tool for assessing the scalability of pressure-retarded osmosis (PRO) membranes. Renewable Energy, 2020, 149, 987-999.	8.9	23
7	Dynamics of gas flow between interconnected vessels: Experiments and simulations. Chemical Engineering Research and Design, 2020, 134, 381-391.	5.6	0
8	Energy recovery modeling of pressure-retarded osmosis systems with membrane modules compatible with high salinity draw streams. Desalination, 2020, 493, 114624.	8.2	10
9	Adsorption of Gases on Zeolitic Imidazolate Frameworks: Modeling with Equations of State for Confined Fluids and Pore Size Distribution Estimation. Industrial & Engineering Chemistry Research, 2019, 58, 19702-19708.	3.7	4
10	Shortcut modeling of natural gas supersonic separation. Journal of Natural Gas Science and Engineering, 2019, 65, 284-300.	4.4	14
11	Liquid Phase Density, Sound Speed, and Vapor Pressure of Linear Alkanes Using the Mattediâ€“Tavaresâ€“Castier Equation of State. Industrial & Engineering Chemistry Research, 2019, 58, 6767-6777.	3.7	2
12	Pore size distributions from extended Peng-Robinson equations of state for fluids confined in cylindrical and slit pores. Fluid Phase Equilibria, 2019, 493, 67-77.	2.5	8
13	Molecular dynamics simulation of electrolyte solutions confined by calcite mesopores. Fluid Phase Equilibria, 2019, 487, 24-32.	2.5	11
14	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	47
15	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.	2.8	47
16	Molecular Dynamics Simulation of n-Alkanes and CO₂ Confined by Calcite Nanopores. Energy & Fuels, 2018, 32, 1934-1941.	5.1	93
17	Cubic equations of state extended to confined fluids: New mixing rules and extension to spherical pores. Chemical Engineering Science, 2018, 184, 52-61.	3.8	19
18	Is it the time to say bye to the Ï•-factor?. Chemical Engineering Research and Design, 2018, 113, 193-203.	5.6	16

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19	On the Efficient Separation of Gas Mixtures with the Mixed-Linker Zeolitic-Imidazolate Framework-7-8. ACS Applied Materials & Interfaces, 2018, 10, 39631-39644.	8.0	32
20	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. Langmuir, 2017, 33, 11291-11298.	3.5	29
21	Computational Study of ZIF-8 and ZIF-67 Performance for Separation of Gas Mixtures. Journal of Physical Chemistry C, 2017, 121, 17999-18011.	3.1	70
22	Vaporâ€“Liquid Equilibrium of Carbon Dioxide + Ethyl Acetate + Oleic Acid Mixtures at High Pressures. Journal of Chemical & Engineering Data, 2017, 62, 2855-2860.	1.9	7
23	Two-body perturbation theory versus first order perturbation theory: A comparison based on the square-well fluid. Journal of Chemical Physics, 2017, 147, 214108.	3.0	11
24	Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study. Journal of Chemical Physics, 2016, 145, 084702.	3.0	51
25	Phase Equilibrium with External Fields: Application to Confined Fluids. Journal of Chemical & Engineering Data, 2016, 61, 2873-2885.	1.9	15
26	Effect of side streams on supersonic gas separations. Journal of Natural Gas Science and Engineering, 2016, 35, 299-308.	4.4	18
27	Diffusion in Homogeneous and in Inhomogeneous Media: A New Unified Approach. Journal of Chemical Theory and Computation, 2016, 12, 5247-5255.	5.3	34
28	Extending an equation of state to confined fluids with basis on molecular simulations. Chemical Engineering Science, 2016, 153, 212-220.	3.8	22
29	Volumetric properties of binary aqueous solutions of protic ionic liquids based on bis (2-hydroxyethyl) ammonium. Journal of Molecular Liquids, 2016, 222, 867-872.	4.9	14
30	Kenneth R. Hallâ€”A Distinguished Educator, Scientist, and University Administrator. Journal of Chemical & Engineering Data, 2016, 61, 2649-2650.	1.9	1
31	Experimental and DFT Approach on the Determination of Natural Gas Hydrate Equilibrium with the Use of Excess N₂ and Choline Chloride Ionic Liquid as an Inhibitor. Energy & Fuels, 2016, 30, 2821-2832.	5.1	36
32	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.	3.1	121
33	Simulation of venting and leaks from pressure vessels. Journal of Loss Prevention in the Process Industries, 2016, 40, 563-577.	3.3	16
34	Flash calculations with specified entropy and stagnation enthalpy. Fluid Phase Equilibria, 2016, 408, 196-204.	2.5	4
35	Molecular Simulation Studies of the Diffusion of Methane, Ethane, Propane, and Propylene in ZIF-8. Journal of Physical Chemistry C, 2015, 119, 27028-27037.	3.1	94
36	Thermodynamic properties of aqueous solutions of single and multiple salts using the Q-electrolattice equation of state. Fluid Phase Equilibria, 2014, 362, 268-280.	2.5	19

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37	Modeling and simulation of supersonic gas separations. Journal of Natural Gas Science and Engineering, 2014, 18, 304-311.	4.4	49
38	Modeling of pool spreading of LNG on land. Journal of Loss Prevention in the Process Industries, 2014, 30, 307-314.	3.3	23
39	Phase equilibrium of fluids confined in porous media from an extended Pengâ€“Robinson equation of state. Fluid Phase Equilibria, 2014, 362, 335-341.	2.5	122
40	Vaporâ€“Liquid Equilibrium Data for Carbon Dioxide + (R,S)-1,2-Isopropylidene Glycerol (Solketal) + Oleic Acid Systems at High Pressure. Journal of Chemical & Engineering Data, 2014, 59, 1494-1498.	1.9	11
41	Helmholtz function-based global phase stability test and its link to the isothermalâ€“isochoric flash problem. Fluid Phase Equilibria, 2014, 379, 104-111.	2.5	35
42	An empirical equation for the dielectric constant in aqueous and nonaqueous electrolyte mixtures. Fluid Phase Equilibria, 2014, 376, 116-123.	2.5	19
43	Biodiesel Production by Esterification of Hydrolyzed Soybean Oil with Ethanol in Reactive Distillation Columns: Simulation Studies. Industrial & Engineering Chemistry Research, 2013, 52, 9461-9469.	3.7	24
44	Pure saturated gases with predicted negative fundamental derivative of gas dynamics. Fluid Phase Equilibria, 2012, 334, 128-136.	2.5	3
45	Rigorous multiple utility targeting in heat exchanger networks. Energy Conversion and Management, 2012, 59, 74-85.	9.2	13
46	Computer Simulation of Fatty Acid Esterification in Reactive Distillation Columns. Industrial & Engineering Chemistry Research, 2011, 50, 10176-10184.	3.7	26
47	Vaporâ^'Liquid Equilibrium Calculations of Aqueous and Nonaqueous Binary Systems Using the Mattediâ^'Tavaresâ^'Castier Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 102-110.	3.7	4
48	Simulation of carbon dioxide recovery from flue gases in aqueous 2-amino-2-methyl-1-propanol solutions. International Journal of Greenhouse Gas Control, 2011, 5, 1478-1488.	4.6	13
49	Saturation points of specified entropy. Fluid Phase Equilibria, 2011, 301, 105-109.	2.5	0
50	Thermodynamic speed of sound in multiphase systems. Fluid Phase Equilibria, 2011, 306, 204-211.	2.5	36
51	Dynamic simulation of fluids in vessels via entropy maximization. Journal of Industrial and Engineering Chemistry, 2010, 16, 122-129.	5.8	16
52	Critical behavior of pure confined fluids from an extension of the van der Waals equation of state. Journal of Supercritical Fluids, 2010, 55, 455-461.	3.2	101
53	Thermodynamic modeling of confined fluids using an extension of the generalized van der Waals theory. Chemical Engineering Science, 2010, 65, 3088-3099.	3.8	135
54	Solution of the isochoricâ€“isoenergetic flash problem by direct entropy maximization. Fluid Phase Equilibria, 2009, 276, 7-17.	2.5	44

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55	Automatic Generation of Matlab Functions Using Mathematica and Thermath. Computing in Science and Engineering, 2008, 10, 41-49.	1.2	1
56	Differential-Algebraic Approach to Dynamic Simulations of Flash Drums with Rigorous Evaluation of Physical Properties. Oil and Gas Science and Technology, 2008, 63, 677-686.	1.4	18
57	Computational quantum mechanics: An underutilized tool in thermodynamics. Pure and Applied Chemistry, 2007, 79, 1345-1359.	1.9	13
58	Pinch analysis revisited: New rules for utility targeting. Applied Thermal Engineering, 2007, 27, 1653-1656.	6.0	17
59	Critical points of hydrocarbon mixtures with the Pengâ€“Robinson, SAFT, and PC-SAFT equations of state. Fluid Phase Equilibria, 2007, 257, 78-101.	2.5	32
60	Evaluation of mixing and combining rules for asymmetric Lennardâ€“Jones chain mixtures: Effect of segment diameter, energy interaction, and chain length. Fluid Phase Equilibria, 2007, 259, 123-134.	2.5	3
61	Polymerization of 1-hexene using Î±-diimine nickel catalysts: Stochastic simulation of branch distribution. Polymer, 2007, 48, 5152-5160.	3.8	8
62	Critical points of adsorbed phases using a 2D lattice gas equation of state. Fluid Phase Equilibria, 2006, 244, 2-10.	2.5	0
63	Thermodynamic equilibrium of adsorbed phases. Fluid Phase Equilibria, 2005, 233, 66-72.	2.5	7
64	Effect of combining rules for cubic equations of state on the prediction of double retrograde vaporization. Fluid Phase Equilibria, 2005, 230, 1-8.	2.5	5
65	Thermodynamic equilibrium in systems with multiple adsorbed and bulk phases. Chemical Engineering Science, 2005, 60, 1773-1782.	3.8	22
66	Modeling and simulation of reactive distillation columns using computer algebra. Computers and Chemical Engineering, 2005, 29, 1875-1884.	3.8	15
67	Centrifugation equilibrium of natural gas. Chemical Engineering Science, 2005, 60, 2927-2935.	3.8	9
68	Modeling and simulation of supercritical extraction columns using computer algebra. Journal of Supercritical Fluids, 2005, 34, 203-208.	3.2	5
69	Influence of particle shape on the packing and on the segregation of spherocylinders via Monte Carlo simulations. Powder Technology, 2003, 134, 167-180.	4.2	165
70	Monte Carlo Simulations of the Adsorption of Chainlike Molecules on Two-Dimensional Heterogeneous Surfaces. Langmuir, 2003, 19, 1429-1438.	3.5	14
71	Energy Targeting in Heat Exchanger Network Synthesis Using Rigorous Physical Property Calculations. Industrial & Engineering Chemistry Research, 2002, 41, 1511-1515.	3.7	17
72	Automatic generation of procedures for the simulation of multistage separators using computer algebra. Chemical Engineering Communications, 2002, 189, 657-674.	2.6	5

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73	High pressure phase equilibrium calculations for hydrocarbon systems using an equation of state based on the lattice fluid theory. Fluid Phase Equilibria, 2002, 194-197, 599-607.	2.5	3
74	Automatic implementation of thermodynamic models for reliable parameter estimation using computer algebra. Computers and Chemical Engineering, 2002, 26, 1473-1479.	3.8	17
75	Calculations of thermodynamic equilibrium in systems subject to gravitational fields. Chemical Engineering Science, 2000, 55, 3495-3504.	3.8	35
76	Phase Equilibrium Calculations for Semicontinuous Mixtures Subject to Gravitational Fields. Industrial & Engineering Chemistry Research, 2000, 39, 4415-4421.	3.7	3
77	Reliable Computation of High-Pressure Solidâ^'Fluid Equilibrium. Industrial & Engineering Chemistry Research, 2000, 39, 1624-1636.	3.7	51
78	Automatic implementation of thermodynamic models using computer algebra. Computers and Chemical Engineering, 1999, 23, 1229-1245.	3.8	43
79	A phase stability analysis of the combinatorial term of the UNIQUAC model. Chemical Engineering Science, 1999, 54, 893-896.	3.8	5
80	Monte Carlo simulation of particle segregation. Powder Technology, 1998, 97, 200-207.	4.2	15
81	Group contribution equation of state based on the lattice fluid theory: Alkaneâ€“alkanol systems. Fluid Phase Equilibria, 1998, 142, 33-54.	2.5	29
82	Predictions of critical behavior using the Wongâ€“Sandler mixing rule. Journal of Supercritical Fluids, 1998, 13, 49-54.	3.2	9
83	Critical points with the Wong-Sandler mixing ruleâ€”I. Calculations with the van der Waals equation of state. Chemical Engineering Science, 1997, 52, 3393-3399.	3.8	21
84	Critical point calculations for semi-continuous mixtures. Fluid Phase Equilibria, 1997, 139, 137-153.	2.5	13
85	Critical points with the Wong-Sandler mixing ruleâ€”II. Calculations with a modified Peng-Robinson equation of state. Chemical Engineering Science, 1997, 52, 3579-3588.	3.8	39
86	Equations of state for chainlike polar fluids: a comparison of reference terms. Fluid Phase Equilibria, 1994, 99, 87-103.	2.5	6
87	Calculation of simultaneous chemical and phase equilibria in nonideal systems. Chemical Engineering Science, 1989, 44, 237-248.	3.8	75
88	Reactive Distillation Applied to Biodiesel Production by Esterification: Simulation Studies. , 0, , .		0