Claire Adjiman

List of Publications by Year
in descending order

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173 papers	12,952 citations	36203 51 h-index	23472 111 g-index
193 all docs	193 docs citations	193 times ranked	9864 citing authors

#	Article	IF	Citations
1	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
2	An overview of CO2 capture technologies. Energy and Environmental Science, 2010, 3, 1645.	15.6	1,376
3	Anode-supported intermediate temperature direct internal reforming solid oxide fuel cell. I: model-based steady-state performance. Journal of Power Sources, 2004, 138, 120-136.	4.0	613
4	A global optimization method, Î±BB, for general twice-differentiable constrained NLPs â€" I. Theoretical advances. Computers and Chemical Engineering, 1998, 22, 1137-1158.	2.0	454
5	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
6	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	1.2	382
7	Handbook of Test Problems in Local and Global Optimization. Nonconvex Optimization and Its Applications, 1999, , .	0.1	379
8	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
9	A global optimization method, Î±BB, for general twice-differentiable constrained NLPsâ€"II. Implementation and computational results. Computers and Chemical Engineering, 1998, 22, 1159-1179.	2.0	295
10	Anode-supported intermediate-temperature direct internal reforming solid oxide fuel cell. Journal of Power Sources, 2005, 147, 136-147.	4.0	251
11	Global optimization of mixed-integer nonlinear problems. AICHE Journal, 2000, 46, 1769-1797.	1.8	241
12	Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. Journal of Chemical Physics, 2014, 140, 054107.	1.2	225
13	A group contribution method for associating chain molecules based on the statistical associating fluid theory (SAFT-Î³). Journal of Chemical Physics, 2007, 127, 234903.	1.2	213
14	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 1. A Single-Site Coarse Grained Model of Carbon Dioxide. Journal of Physical Chemistry B, 2011, 115, 11154-11169.	1.2	200
15	Modelling system efficiencies and costs of two biomass-fuelled SOFC systems. Journal of Power Sources, 2004, 131, 96-106.	4.0	153
16	Rigorous convex underestimators for general twice-differentiable problems. Journal of Global Optimization, 1996, 9, 23-40.	1.1	143
17	Computer-aided molecular design of solvents for accelerated reaction kinetics. Nature Chemistry, 2013, 5, 952-957.	6.6	141
18	Modeling the Fluid Phase Behavior of Carbon Dioxide in Aqueous Solutions of Monoethanolamine Using Transferable Parameters with the SAFT-VR Approach. Industrial & Engineering Chemistry Research, 2010, 49, 1883-1899.	1.8	129

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19	A generalisation of the SAFT- group contribution method for groups comprising multiple spherical segments. Fluid Phase Equilibria, 2008, 274, 85-104.	1.4	128
20	SAFT-Î³ Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Greenhouse Gases, Refrigerants, and Long Alkanes. Journal of Physical Chemistry B, 2013, 117, 2717-2733.	1.2	126
21	A hierarchical method to integrated solvent and process design of physical <scp>CO</scp>₂ absorption using the <scp>SAFT</scp>â€Î³ <scp>M</scp>ie approach. AICHE Journal, 2015, 61, 3249-3269.	1.8	120
22	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? 2. Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2009, 5, 1432-1448.	2.3	118
23	Comparison of two IT DIR-SOFC models: Impact of variable thermodynamic, physical, and flow properties. Steady-state and dynamic analysis. Chemical Engineering Science, 2005, 60, 2963-2975.	1.9	117
24	A spatially explicit whole-system model of the lignocellulosic bioethanol supply chain: an assessment of decentralised processing potential. Biotechnology for Biofuels, 2008, 1, 13.	6.2	110
25	Efficient Handling of Molecular Flexibility in Lattice Energy Minimization of Organic Crystals. Journal of Chemical Theory and Computation, 2011, 7, 1998-2016.	2.3	110
26	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. International Journal of Pharmaceutics, 2011, 418, 168-178.	2.6	110
27	A global optimization method, Î±BB, for process design. Computers and Chemical Engineering, 1996, 20, S419-S424.	2.0	108
28	Prediction of Thermodynamic Properties and Phase Behavior of Fluids and Mixtures with the SAFT-Î³ Mie Group-Contribution Equation of State. Journal of Chemical & Engineering Data, 2014, 59, 3272-3288.	1.0	107
29	A Rigorous Global Optimization Algorithm for Problems with Ordinary Differential Equations. Journal of Global Optimization, 2002, 24, 1-33.	1.1	106
30	The effect of feed spacer geometry on membrane performance and concentration polarisation based on 3D CFD simulations. Journal of Membrane Science, 2017, 527, 78-91.	4.1	106
31	Microstructural analysis of a solid oxide fuel cell anode using focused ion beam techniques coupled with electrochemical simulation. Journal of Power Sources, 2010, 195, 4804-4810.	4.0	96
32	Modelling the 3D microstructure and performance of solid oxide fuel cell electrodes: Computational parameters. Electrochimica Acta, 2011, 56, 5804-5814.	2.6	88
33	Integrated solvent and process design using a SAFT-VR thermodynamic description: High-pressure separation of carbon dioxide and methane. Computers and Chemical Engineering, 2011, 35, 474-491.	2.0	83
34	Modelling the fluid phase behaviour of aqueous mixtures of multifunctional alkanolamines and carbon dioxide using transferable parameters with the SAFT-VR approach. Molecular Physics, 2012, 110, 1325-1348.	0.8	83
35	SAFT-Î³force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models ofn-decylbenzene. Molecular Physics, 2012, 110, 1189-1203.	0.8	82
36	Transferable SAFT-VR Models for the Calculation of the Fluid Phase Equilibria in Reactive Mixtures of Carbon Dioxide, Water, and n-Alkylamines in the Context of Carbon Capture. Journal of Physical Chemistry B, 2011, 115, 8155-8168.	1.2	79

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37	Solid oxide fuel cell micro combined heat and power system operating strategy: Options for provision of residential space and water heating. Journal of Power Sources, 2007, 164, 260-271.	4.0	76
38	Microstructural Modeling of Solid Oxide Fuel Cell Anodes. Industrial & Engineering Chemistry Research, 2008, 47, 7693-7699.	1.8	74
39	Global Optimization of MINLP Problems in Process Synthesis and Design. Computers and Chemical Engineering, 1997, 21, S445-S450.	2.0	72
40	Global optimization of dynamic systems. Computers and Chemical Engineering, 2004, 28, 403-415.	2.0	70
41	Optimal solvent design for batch separation based on economic performance. AICHE Journal, 2003, 49, 3095-3109.	1.8	67
42	Design of solvents for optimal reaction rate constants. AICHE Journal, 2007, 53, 1240-1256.	1.8	67
43	Modelling of the thermodynamic and solvation properties of electrolyte solutions with the statistical associating fluid theory for potentials of variable range. Molecular Physics, 2014, 112, 2339-2364.	0.8	65
44	Prediction of the crystal structures of axitinib, a polymorphic pharmaceutical molecule. Chemical Engineering Science, 2015, 121, 60-76.	1.9	64
45	Application of the SAFT-Î³ Mie group contribution equation of state to fluids of relevance to the oil and gas industry. Fluid Phase Equilibria, 2016, 416, 104-119.	1.4	62
46	Techno-economic modelling of a solid oxide fuel cell stack for micro combined heat and power. Journal of Power Sources, 2006, 156, 321-333.	4.0	59
47	The polymorphs of ROY: application of a systematic crystal structure prediction technique. Acta Crystallographica Section B: Structural Science, 2012, 68, 677-685.	1.8	59
48	Efficient Handling of Molecular Flexibility in Ab Initio Generation of Crystal Structures. Journal of Chemical Theory and Computation, 2015, 11, 1957-1969.	2.3	58
49	Solvents for ring-closing metathesis reactions. Chemical Communications, 2008, , 2806.	2.2	56
50	Computer-aided molecular design and selection of CO₂ capture solvents based on thermodynamics, reactivity and sustainability. Molecular Systems Design and Engineering, 2016, 1, 313-334.	1.7	56
51	Simultaneous prediction of vapourâ€“liquid and liquidâ€“liquid equilibria (VLE and LLE) of aqueous mixtures with the SAFT-Î³ group contribution approach. Fluid Phase Equilibria, 2011, 306, 82-96.	1.4	55
52	Optimal control strategies for hydrogen production when coupling solid oxide electrolysers with intermittent renewable energies. Journal of Power Sources, 2014, 268, 212-224.	4.0	54
53	Investigation of the active thickness of solid oxide fuel cell electrodes using a 3D microstructure model. Electrochimica Acta, 2011, 56, 10809-10819.	2.6	53
54	Computer-Aided Solvent Design for Reactions: Maximizing Product Formation. Industrial & Engineering Chemistry Research, 2008, 47, 5190-5202.	1.8	48

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55	Outer approximation algorithm with physical domain reduction for computerâ€aided molecular and separation process design. AICHE Journal, 2016, 62, 3484-3504.	1.8	47
56	The Effects of Operating Conditions on the Performance of a Solid Oxide Steam Electrolyser: A Modelâ€Based Study. Fuel Cells, 2010, 10, 1114-1128.	1.5	46
57	Predicting the Solvation of Organic Compounds in Aqueous Environments: From Alkanes and Alcohols to Pharmaceuticals. Industrial & Engineering Chemistry Research, 2017, 56, 10856-10876.	1.8	43
58	How many more polymorphs of ROY remain undiscovered. Chemical Science, 2022, 13, 1288-1297.	3.7	41
59	Pure component properties from group contribution: Hydrogen-bond basicity, hydrogen-bond acidity, Hildebrand solubility parameter, macroscopic surface tension, dipole moment, refractive index and dielectric constant. Fluid Phase Equilibria, 2005, 231, 27-37.	1.4	40
60	Development of intermolecular potential models for electrolyte solutions using an electrolyte SAFT-VR Mie equation of state. Molecular Physics, 2016, 114, 2724-2749.	0.8	40
61	The formulation of optimal mixtures with generalized disjunctive programming: A solvent design case study. AICHE Journal, 2016, 62, 1616-1633.	1.8	40
62	A generalization of the Branch-and-Sandwich algorithm: From continuous to mixed-integer nonlinear bilevel problems. Computers and Chemical Engineering, 2015, 72, 373-386.	2.0	39
63	A QM-CAMD approach to solvent design for optimal reaction rates. Chemical Engineering Science, 2017, 159, 69-83.	1.9	39
64	Modelling the phase and chemical equilibria of aqueous solutions of alkanolamines and carbon dioxide using the SAFT-Î³ SW group contribution approach. Fluid Phase Equilibria, 2016, 407, 280-297.	1.4	37
65	Predicting enhanced absorption of light gases in polyethylene using simplified PC-SAFT and SAFT-VR. Fluid Phase Equilibria, 2006, 243, 74-91.	1.4	36
66	Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation. Fluid Phase Equilibria, 2011, 306, 129-136.	1.4	35
67	Molecules Matter. Computer Aided Chemical Engineering, 2014, , 55-64.	0.3	33
68	Hybrid QSPR models for the prediction of the free energy of solvation of organic solute/solvent pairs. Physical Chemistry Chemical Physics, 2019, 21, 13706-13720.	1.3	33
69	A duality-based optimisation approach for the reliable solution of (P, T) phase equilibrium in volume-composition space. Fluid Phase Equilibria, 2010, 299, 1-23.	1.4	32
70	The development of unlike induced association-site models to study the phase behaviour of aqueous mixtures comprising acetone, alkanes and alkyl carboxylic acids with the SAFT-Î³ Mie group contribution methodology. Fluid Phase Equilibria, 2016, 407, 39-57.	1.4	32
71	Expanding the Applications of the SAFT-Î³ Mie Group-Contribution Equation of State: Prediction of Thermodynamic Properties and Phase Behavior of Mixtures. Journal of Chemical & Engineering Data, 2020, 65, 5862-5890.	1.0	32
72	General Computational Algorithms for Ab Initio Crystal Structure Prediction for Organic Molecules. Topics in Current Chemistry, 2014, 345, 25-58.	4.0	31

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73	An approach for simultaneous computer-aided molecular design with holistic sustainability assessment: Application to phase-change CO2 capture solvents. Computers and Chemical Engineering, 2020, 135, 106769.	2.0	31
74	On the optimal design of gas-expanded liquids based on process performance. Chemical Engineering Science, 2014, 115, 19-30.	1.9	30
75	The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state. Computers and Chemical Engineering, 2012, 36, 99-118.	2.0	29
76	A predictive model for spiral wound reverse osmosis membrane modules: The effect of winding geometry and accurate geometric details. Computers and Chemical Engineering, 2017, 96, 248-265.	2.0	28
77	Crystal Structure Prediction Methods for Organic Molecules: State of the Art. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 593-623.	3.3	28
78	Quantitative framework for reliable safety analysis. AICHE Journal, 2002, 48, 78-96.	1.8	27
79	Branch-and-Sandwich: a deterministic global optimization algorithm for optimistic bilevel programming problems. Part II: Convergence analysis and numerical results. Journal of Global Optimization, 2014, 60, 459-481.	1.1	27
80	Branch-and-Sandwich: a deterministic global optimization algorithm for optimistic bilevel programming problems. Part I: Theoretical development. Journal of Global Optimization, 2014, 60, 425-458.	1.1	25
81	Designing optimal mixtures using generalized disjunctive programming: Hull relaxations. Chemical Engineering Science, 2017, 159, 106-130.	1.9	24
82	Process Systems Engineering Perspective on the Design of Materials and Molecules. Industrial & Engineering Chemistry Research, 2021, 60, 5194-5206.	1.8	22
83	The design of optimal mixtures from atom groups using Generalized Disjunctive Programming. Computers and Chemical Engineering, 2018, 116, 401-421.	2.0	21
84	Two results on bounding the roots of interval polynomials. Computers and Chemical Engineering, 1999, 23, 1333-1339.	2.0	20
85	Solvent Design Using a Quantum Mechanical Continuum Solvation Model. Industrial & Engineering Chemistry Research, 2006, 45, 1128-1140.	1.8	20
86	Toward Sustainable Solvent-Based Postcombustion CO2 Capture. Computer Aided Chemical Engineering, 2015, , 279-310.	0.3	20
87	Beyond a heuristic analysis: integration of process and working-fluid design for organic Rankine cycles. Molecular Systems Design and Engineering, 2020, 5, 493-510.	1.7	20
88	Mixed-Integer Nonlinear Optimization in Process Synthesis. , 1998, , 1-76.		19
89	Accurate and efficient representation of intramolecular energy inab initiogeneration of crystal structures. I. Adaptive local approximate models. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 864-874.	0.5	18
90	Computer Aided Design of Solvent Blends for Hybrid Cooling and Antisolvent Crystallization of Active Pharmaceutical Ingredients. Organic Process Research and Development, 2021, 25, 1123-1142.	1.3	18

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91	Modelling the dynamic response of a solid oxide steam electrolyser to transient inputs during renewable hydrogen production. Frontiers of Energy and Power Engineering in China, 2010, 4, 211-222.	0.4	17
92	Computer-aided design of optimal environmentally benign solvent-based adhesive products. Computers and Chemical Engineering, 2019, 130, 106518.	2.0	17
93	A comparative study of multi-objective optimization methodologies for molecular and process design. Computers and Chemical Engineering, 2020, 136, 106802.	2.0	17
94	Towards the 3D modeling of the effective conductivity of solid oxide fuel cell electrodes: I. Model development. Chemical Engineering Science, 2013, 99, 161-170.	1.9	16
95	Molecular engineering of sustainable phase-change solvents: From digital design to scaling-up for CO2 capture. Chemical Engineering Journal, 2021, 420, 127624.	6.6	15
96	Description of the thermodynamic properties and fluidâ€phase behavior of aqueous solutions of linear, branched, and cyclic amines. AICHE Journal, 2021, 67, e17194.	1.8	14
97	Correlations for Concentration Polarization and Pressure Drop in Spacer-Filled RO Membrane Modules Based on CFD Simulations. Membranes, 2021, 11, 338.	1.4	14
98	Efficient Screening of Coformers for Active Pharmaceutical Ingredient Cocrystallization. Crystal Growth and Design, 2022, 22, 4513-4527.	1.4	14
99	Predictive models for the phase behaviour and solution properties of weak electrolytes: nitric, sulphuric, and carbonic acids. Physical Chemistry Chemical Physics, 2020, 22, 15248-15269.	1.3	13
100	On the impact of using volume as an independent variable for the solution of P â€“ T fluid-phase equilibrium with equations of state. Computers and Chemical Engineering, 2014, 71, 67-76.	2.0	12
101	On the use of molecular-based thermodynamic models to assess the performance of solvents for CO₂ capture processes: monoethanolamine solutions. Faraday Discussions, 2016, 192, 337-390.	1.6	12
102	Modelling and prediction of the thermophysical properties of aqueous mixtures of choline geranate and geranic acid (CAGE) using SAFT-Î³ Mie. RSC Advances, 2019, 9, 38017-38031.	1.7	12
103	Global optimization for clusters of flexible moleculesâ€”solventâ€“solute interaction energy calculations. Fluid Phase Equilibria, 2002, 194-197, 169-183.	1.4	11
104	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 79-94.	1.4	11
105	Fluid phase stability and equilibrium calculations in binary mixtures. Fluid Phase Equilibria, 2009, 275, 95-104.	1.4	11
106	Towards the 3D modeling of the effective conductivity of solid oxide fuel cell electrodes â€“ II. Computational parameters. Chemical Engineering Science, 2014, 116, 781-792.	1.9	10
107	Mechanism, kinetics and selectivity of a Williamson ether synthesis: elucidation under different reaction conditions. Reaction Chemistry and Engineering, 2021, 6, 1195-1211.	1.9	10
108	Extending the SAFT-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mi>Î³</mml:mi></mml:math> Mie approach to model benzoic acid, diphenylamine, and mefenamic acid: Solubility prediction and experimental measurement. Fluid Phase Equilibria, 2021, 540, 113002.	1.4	10

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109	The design of solvents for optimal reaction rates. Computer Aided Chemical Engineering, 2004, 18, 175-180.	0.3	9
110	An optimization framework to combine operable space maximization with design of experiments. AICHE Journal, 2018, 64, 3944-3957.	1.8	9
111	Accurate and efficient representation of intramolecular energy in ab initio generation of crystal structures. II. Smoothed intramolecular potentials. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 423-433.	0.5	9
112	Computer-aided Design of Solvent Blends for the Cooling and Anti-solvent Crystallisation of Ibuprofen. Computer Aided Chemical Engineering, 2019, , 949-954.	0.3	9
113	Optimization Methods in CAMD â€“ II. Computer Aided Chemical Engineering, 2003, 12, 63-93.	0.3	8
114	Development of Predictive Models of the Kinetics of a Hydrogen Abstraction Reaction Combining Quantum-Mechanical Calculations and Experimental Data. Industrial & Engineering Chemistry Research, 2017, 56, 815-831.	1.8	8
115	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	1.6	8
116	Global optimization and modeling techniques for planar multilayered dielectric structures. Applied Optics, 2006, 45, 5910.	2.1	7
117	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
118	Repulsionâ€“dispersion parameters for the modelling of organic molecular crystals containing N, O, S and Cl. Faraday Discussions, 2018, 211, 297-323.	1.6	7
119	Intramolecular bonding in a statistical associating fluid theory of ring aggregates. Molecular Physics, 2019, 117, 3884-3912.	0.8	7
120	Proof of Convergence for a Global Optimization Algorithm for Problems with Ordinary Differential Equations. Journal of Global Optimization, 2005, 33, 83-107.	1.1	6
121	An algorithm for the estimation of parameters in models with stochastic differential equations. Chemical Engineering Science, 2008, 63, 4820-4833.	1.9	6
122	Refrigerant Design Case Study. Computer Aided Chemical Engineering, 2003, 12, 289-301.	0.3	5
123	A comparison of the performance of multi-objective optimization methodologies for solvent design. Computer Aided Chemical Engineering, 2019, 46, 37-42.	0.3	5
124	A computer-aided methodology with robust design criteria for selection of solvents for reactions. Computer Aided Chemical Engineering, 2006, , 787-792.	0.3	4
125	Arbitrarily tight $$alpha $$ Î± BB underestimators of general non-linear functions over sub-optimal domains. Journal of Global Optimization, 2018, 71, 815-844.	1.1	4
126	Multi-Objective Computer-Aided Solvent Design for Selectivity and Rate in Reactions. Computer Aided Chemical Engineering, 2018, , 2437-2442.	0.3	4

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127	Optimal design of post combustion CO2 capture processes based on phase-change solvents. Computer Aided Chemical Engineering, 2019, , 463-468.	0.3	4
128	Global optimization of nonconvex bilevel problems: implementation and computational study of the Branch-and-Sandwich algorithm. Computer Aided Chemical Engineering, 2016, 38, 1977-1982.	0.3	4
129	Assessment of a two-step approach for global optimization of mixed-integer polynomial programs using quadratic reformulation. Computers and Chemical Engineering, 2022, 165, 107909.	2.0	4
130	Safety verification in chemical plants: A new quantitative approach. Computers and Chemical Engineering, 1999, 23, S581-S584.	2.0	3
131	Micro-structural Modelling of SOFC Anodes. ECS Transactions, 2007, 7, 2041-2047.	0.3	3
132	Model-Based Evaluation of the Production of Pure Oxygen through SOFC/SOEC Integration. ECS Transactions, 2011, 35, 2997-3006.	0.3	3
133	Solid Oxide Fuel Cell Electrode 3D Microstructure and Performance Modeling. ECS Transactions, 2011, 35, 1097-1105.	0.3	3
134	Microstructural Characterization of SOFC Electrodes: Observations and Simulations. ECS Transactions, 2011, 35, 1367-1377.	0.3	3
135	Hydrogen production through steam electrolysis. Computer Aided Chemical Engineering, 2012, 30, 257-261.	0.3	3
136	Globie. Computer Aided Chemical Engineering, 2014, 34, 669-674.	0.3	3
137	A feasibility-based algorithm for Computer Aided Molecular and Process Design of solvent-based separation systems. Computer Aided Chemical Engineering, 2016, 38, 73-78.	0.3	3
138	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
139	Computer-aided Solvent Mixture Design for the Crystallisation and Isolation of Mefenamic Acid. Computer Aided Chemical Engineering, 2020, 48, 649-654.	0.3	3
140	A Deterministic Global Optimization Algorithm for Problems with Nonlinear Dynamics. Nonconvex Optimization and Its Applications, 2004, , 1-23.	0.1	3
141	New bounding schemes and algorithmic options for the Branch-and-Sandwich algorithm. Journal of Global Optimization, 2020, 77, 197-225.	1.1	3
142	Towards the identification of optimal solvents for long chain alkanes with the SAFT equation of state. Computer Aided Chemical Engineering, 2003, 14, 137-142.	0.3	2
143	A computer-aided methodology for optimal solvent design for reactions with experimental verification. Computer Aided Chemical Engineering, 2005, 20, 1651-1656.	0.3	2
144	Design of polyolefin reactor mixtures. Computer Aided Chemical Engineering, 2006, 22, 301-332.	0.3	2

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145	An integrated framework for model-based flow assurance in deep-water oil and gas production. Computer Aided Chemical Engineering, 2008, 25, 787-792.	0.3	2
146	Integrated Modeling of Mixture Fluid Phase Equilibrium Experiments Using SAFT-VR Applied to Xenon + Diborane, Xenon + Cyclopropane, Xenon + Boron Trifluoride. Industrial & Engineering Chemistry Research, 2009, 48, 2188-2198.	1.8	2
147	Ab Initio Crystal Structure Prediction for Flexible Molecules. Computer Aided Chemical Engineering, 2010, 28, 817-822.	0.3	2
148	Solvent design for a Menschutkin reaction by using CAMD and DFT calculations. Computer Aided Chemical Engineering, 2010, 28, 1291-1296.	0.3	2
149	Enclosure of all index-1 saddle points of general nonlinear functions. Journal of Global Optimization, 2017, 67, 451-474.	1.1	2
150	An interval-matrix branch-and-bound algorithm for bounding eigenvalues. Optimization Methods and Software, 2017, 32, 872-891.	1.6	2
151	A Comprehensive Approach for the Design of Solvent-based Adhesive Products using Generalized Disjunctive Programming. Computer Aided Chemical Engineering, 2018, , 427-432.	0.3	2
152	Tighter $$alpha $$ Î± BB relaxations through a refinement scheme for the scaled Gerschgorin theorem. Journal of Global Optimization, 2019, 73, 467-483.	1.1	2
153	Efficient Parameterization of a Surrogate Model of Molecular Interactions in Crystals. Computer Aided Chemical Engineering, 2020, , 493-498.	0.3	2
154	Integrated Design of a Reactor and a Gas-Expanded Solvent. Computer Aided Chemical Engineering, 2011, , 316-320.	0.3	2
155	Enhancement of optical extraction from OLEDs using scattering layers. , 2005, 5724, 191.		1
156	Chapter 1 Parameter estimation for stochastic differential equations: algorithm and application to polymer melt rheology. Computer Aided Chemical Engineering, 2006, 21, 143-148.	0.3	1
157	State estimation for dynamic prediction of hydrate formation in oil and gas production systems. Computer Aided Chemical Engineering, 2008, 25, 507-512.	0.3	1
158	Robust algorithms for the calculation of phase equilibrium. Computer Aided Chemical Engineering, 2010, 28, 79-84.	0.3	1
159	Validation of a Process Model of CO2 Capture in an Aqueous Solvent, Using an Implicit Molecular Based Treatment of The Reactions. Energy Procedia, 2013, 37, 1566-1571.	1.8	1
160	Deterministic Global Optimization and Transition States. Computer Aided Chemical Engineering, 2015, , 851-856.	0.3	1
161	An approach for simultaneous computer-aided solvent design and process design for CO2 chemical absorption processes. Computer Aided Chemical Engineering, 2021, , 167-172.	0.3	1
162	Optimal Solvent Design Approaches. , 2008, , 2750-2757.		1

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163	The Î±BB Global Optimization Algorithm for Nonconvex Problems: An Overview. Nonconvex Optimization and Its Applications, 2001, , 155-186.	0.1	1
164	A Convex Hull Formulation for the Design of Optimal Mixtures. Computer Aided Chemical Engineering, 2016, 38, 2325-2330.	0.3	1
165	Branch-and-Sandwich. Computer Aided Chemical Engineering, 2011, 29, 602-606.	0.3	1
166	Model-based safety verification under uncertainty. Computer Aided Chemical Engineering, 2000, , 793-798.	0.3	0
167	A method for the systematic estimation of parameters for a stochastic reptation model. Computer Aided Chemical Engineering, 2006, 22, 69-83.	0.3	0
168	Integrating advanced thermodynamics and process and solvent design for gas separation. Computer Aided Chemical Engineering, 2006, 21, 743-748.	0.3	0
169	A heteronuclear group contribution method for associating chain molecules (SAFT-Î³). Computer Aided Chemical Engineering, 2008, 25, 871-876.	0.3	0
170	Thermal Management Issues in Fuel Cell Technology. , 2010, , .		0
171	Simultaneous prediction of phase behaviour and second derivative properties with a group contribution approach (SAFT-Î³ Mie). Computer Aided Chemical Engineering, 2011, , 1593-1597.	0.3	0
172	Modelling â€“ from molecules to mega-scale: general discussion. Faraday Discussions, 2016, 192, 493-509.	1.6	0
173	International Programming Committee. Computer Aided Chemical Engineering, 2014, 34, xvi-xvii.	0.3	0