AndrÃ© Bardow

List of Publications by Year
in descending order

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271	13,420	36271	51	26591	107
papers	citations		h-index		g-index

279	279	279	11511
all docs	docs citations	times ranked	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	Sustainable Conversion of Carbon Dioxide: An Integrated Review of Catalysis and Life Cycle Assessment. Chemical Reviews, 2018, 118, 434-504.	23.0	1,571
3	Climate change mitigation potential of carbon capture and utilization in the chemical industry. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 11187-11194.	3.3	384
4	Power-to-What? â€“ Environmental assessment of energy storage systems. Energy and Environmental Science, 2015, 8, 389-400.	15.6	373
5	Life-cycle assessment of carbon dioxide capture and utilization: avoiding the pitfalls. Energy and Environmental Science, 2013, 6, 2721.	15.6	325
6	Life cycle assessment of CO₂capture and utilization: a tutorial review. Chemical Society Reviews, 2014, 43, 7982-7994.	18.7	317
7	Life cycle assessment of polyols for polyurethane production using CO₂ as feedstock: insights from an industrial case study. Green Chemistry, 2014, 16, 3272-3280.	4.6	307
8	Life-cycle assessment of an industrial direct air capture process based on temperatureâ€“vacuum swing adsorption. Nature Energy, 2021, 6, 203-213.	19.8	238
9	Achieving net-zero greenhouse gas emission plastics by a circular carbon economy. Science, 2021, 374, 71-76.	6.0	222
10	Cleaner production of cleaner fuels: wind-to-wheel â€“ environmental assessment of CO₂-based oxymethylene ether as a drop-in fuel. Energy and Environmental Science, 2018, 11, 331-343.	15.6	195
11	Towards a circular economy for plastic packaging wastes â€“ the environmental potential of chemical recycling. Resources, Conservation and Recycling, 2020, 162, 105010.	5.3	188
12	Selecting CO₂ Sources for CO₂ Utilization by Environmental-Merit-Order Curves. Environmental Science & Technology, 2016, 50, 1093-1101.	4.6	164
13	Automated superstructure-based synthesis and optimization of distributed energy supply systems. Energy, 2013, 50, 374-388.	4.5	149
14	Life cycle assessment of CO₂-based C1-chemicals. Green Chemistry, 2017, 19, 2244-2259.	4.6	147
15	Efficient technologies for worldwide clean water supply. Chemical Engineering and Processing: Process Intensification, 2012, 51, 2-17.	1.8	128
16	Continuous-Molecular Targeting for Integrated Solvent and Process Design. Industrial & Engineering Chemistry Research, 2010, 49, 2834-2840.	1.8	126
17	Cononsolvency of poly-N-isopropyl acrylamide (PNIPAM): Microgels versus linear chains and macrogels. Current Opinion in Colloid and Interface Science, 2014, 19, 84-94.	3.4	125
18	Finite-Size Effects of Binary Mutual Diffusion Coefficients from Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 2667-2677.	2.3	121

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19	A Guideline for Life Cycle Assessment of Carbon Capture and Utilization. Frontiers in Energy Research, 2020, 8, .	1.2	111
20	The carbon footprint of the carbon feedstock CO₂. Energy and Environmental Science, 2020, 13, 2979-2992.	15.6	110
21	Simultaneous Optimization of Working Fluid and Process for Organic Rankine Cycles Using PC-SAFT. Industrial & Engineering Chemistry Research, 2014, 53, 8821-8830.	1.8	108
22	Life Cycle Assessment of Power-to-Gas: Syngas vs Methane. ACS Sustainable Chemistry and Engineering, 2016, 4, 4156-4165.	3.2	107
23	Calculating Thermodynamic Properties from Fluctuations at Small Scales. Journal of Physical Chemistry B, 2011, 115, 10911-10918.	1.2	105
24	Diffusion Coefficients from Molecular Dynamics Simulations in Binary and Ternary Mixtures. International Journal of Thermophysics, 2013, 34, 1169-1196.	1.0	102
25	Fully automated indirect hard modeling of mixture spectra. Chemometrics and Intelligent Laboratory Systems, 2008, 91, 181-193.	1.8	101
26	Computer-aided molecular design in the continuous-molecular targeting framework using group-contribution PC-SAFT. Computers and Chemical Engineering, 2015, 81, 278-287.	2.0	97
27	Time-resolved structural evolution during the collapse of responsive hydrogels: The microgel-to-particle transition. Science Advances, 2018, 4, eaao7086.	4.7	90
28	Same or different? Insights on public perception and acceptance of carbon capture and storage or utilization in Germany. Energy Policy, 2019, 125, 235-249.	4.2	88
29	Finite-size effects of diffusion coefficients computed from molecular dynamics: a review of what we have learned so far. Molecular Simulation, 2021, 47, 831-845.	0.9	87
30	Predictive Darken Equation for Maxwell-Stefan Diffusivities in Multicomponent Mixtures. Industrial & Engineering Chemistry Research, 2011, 50, 10350-10358.	1.8	84
31	The optimum is not enough: A near-optimal solution paradigm for energy systems synthesis. Energy, 2015, 82, 446-456.	4.5	81
32	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2012, 51, 10247-10258.	1.8	79
33	Continuous Molecular Targetingâ€“Computer-Aided Molecular Design (CoMTâ€“CAMD) for Simultaneous Process and Solvent Design for CO₂ Capture. Industrial & Engineering Chemistry Research, 2014, 53, 18029-18041.	1.8	79
34	1-stage CoMT-CAMD: An approach for integrated design of ORC process and working fluid using PC-SAFT. Chemical Engineering Science, 2017, 159, 217-230.	1.9	74
35	Nitrogenâ€Based Fuels: A Powerâ€toâ€Fuelâ€toâ€Power Analysis. Angewandte Chemie - International Edition, 2016, 55, 8798-8805.	7.2	73
36	Incremental and simultaneous identification of reaction kinetics: methods and comparison. Chemical Engineering Science, 2004, 59, 2673-2684.	1.9	71

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37	Early-stage evaluation of emerging CO₂utilization technologies at low technology readiness levels. Green Chemistry, 2020, 22, 3842-3859.	4.6	71
38	Fick Diffusion Coefficients of Liquid Mixtures Directly Obtained From Equilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 12921-12929.	1.2	70
39	OCTP: A Tool for On-the-Fly Calculation of Transport Properties of Fluids with the Order-n Algorithm in LAMMPS. Journal of Chemical Information and Modeling, 2019, 59, 1290-1294.	2.5	67
40	Model-based measurement of diffusion using Raman spectroscopy. AICHE Journal, 2003, 49, 323-334.	1.8	63
41	Robust multi-objective optimization for sustainable design of distributed energy supply systems. Computers and Chemical Engineering, 2017, 102, 26-39.	2.0	63
42	General characteristic-based algorithm for off-lattice Boltzmann simulations. Europhysics Letters, 2006, 75, 434-440.	0.7	62
43	Time-series aggregation for synthesis problems by bounding error in the objective function. Energy, 2017, 135, 900-912.	4.5	62
44	Rock â€˜nâ€™ use of CO₂: carbon footprint of carbon capture and utilization by mineralization. Sustainable Energy and Fuels, 2020, 4, 4482-4496.	2.5	62
45	Risk-benefit perceptions and public acceptance of Carbon Capture and Utilization. Environmental Innovation and Societal Transitions, 2020, 35, 292-308.	2.5	61
46	From Unavoidable CO₂ Source to CO₂ Sink? A Cement Industry Based on CO₂ Mineralization. Environmental Science & Technology, 2021, 55, 5212-5223.	4.6	59
47	COSMO-CAMD: A framework for optimization-based computer-aided molecular design using COSMO-RS. Chemical Engineering Science, 2017, 159, 84-92.	1.9	57
48	Energetically-optimal PEM electrolyzer pressure in power-to-gas plants. Applied Energy, 2018, 218, 192-198.	5.1	56
49	Rapid microfluidic screening of CO2 solubility and diffusion in pure and mixed solvents. Lab on A Chip, 2012, 12, 3387.	3.1	55
50	The metabolic potential of plastics as biotechnological carbon sources â€“ Review and targets for the future. Metabolic Engineering, 2022, 71, 77-98.	3.6	55
51	From molecules to dollars: integrating molecular design into thermo-economic process design using consistent thermodynamic modeling. Molecular Systems Design and Engineering, 2017, 2, 301-320.	1.7	54
52	Superstructure-free synthesis and optimization of distributed industrial energy supply systems. Energy, 2012, 45, 424-435.	4.5	53
53	Stochastic Technology Choice Model for Consequential Life Cycle Assessment. Environmental Science & Technology, 2016, 50, 12575-12583.	4.6	53
54	Prediction of SCP and COP for adsorption heat pumps and chillers by combining the large-temperature-jump method and dynamic modeling. Applied Thermal Engineering, 2016, 98, 900-909.	3.0	53

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55	Closing the carbon cycle to maximise climate change mitigation: power-to-methanolvs.power-to-direct air capture. Sustainable Energy and Fuels, 2018, 2, 1153-1169.	2.5	53
56	Environmental potential of carbon dioxide utilization in the polyurethane supply chain. Faraday Discussions, 2015, 183, 291-307.	1.6	51
57	Concentration-dependent diffusion coefficients from a single experiment using model-based Raman spectroscopy. Fluid Phase Equilibria, 2005, 228-229, 357-366.	1.4	50
58	Multicomponent Maxwellâ˜Stefan Diffusivities at Infinite Dilution. Industrial & Engineering Chemistry Research, 2011, 50, 4776-4782.	1.8	50
59	Computer-aided molecular and processes design based on quantum chemistry: current status and future prospects. Current Opinion in Chemical Engineering, 2020, 27, 89-97.	3.8	50
60	How to apply the Kirkwoodâ€“Buff theory to individual species in salt solutions. Chemical Physics Letters, 2013, 582, 154-157.	1.2	49
61	A hybrid approach for the efficient synthesis of renewable energy systems. Applied Energy, 2014, 135, 625-633.	5.1	48
62	Cleaner chlorine production using oxygen depolarized cathodes? A life cycle assessment. Journal of Cleaner Production, 2014, 80, 46-56.	4.6	46
63	Superstructure-free synthesis and optimization of thermal power plants. Energy, 2015, 91, 700-711.	4.5	45
64	Generalized Form for Finite-Size Corrections in Mutual Diffusion Coefficients of Multicomponent Mixtures Obtained from Equilibrium Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2020, 16, 3799-3806.	2.3	45
65	Ternary diffusivities by model-based analysis of Raman spectroscopy measurements. AICHE Journal, 2006, 52, 4004-4015.	1.8	44
66	Life Cycle Assessment for the Design of Chemical Processes, Products, and Supply Chains. Annual Review of Chemical and Biomolecular Engineering, 2020, 11, 203-233.	3.3	44
67	Life cycle assessment of hydrogen production by thermal cracking of methane based on liquid-metal technology. International Journal of Hydrogen Energy, 2016, 41, 23204-23212.	3.8	42
68	Sensitivity coefficient-based uncertainty analysis for multi-functionality in LCA. International Journal of Life Cycle Assessment, 2014, 19, 661-676.	2.2	41
69	Design of low-carbon utility systems: Exploiting time-dependent grid emissions for climate-friendly demand-side management. Applied Energy, 2019, 247, 755-765.	5.1	41
70	Esterification of acrylic acid with methanol by reactive chromatography: Experiments and simulations. Chemical Engineering Science, 2006, 61, 5296-5306.	1.9	39
71	Maxwellâ€“Stefan diffusivities in liquid mixtures: Using molecular dynamics for testing model predictions. Fluid Phase Equilibria, 2011, 301, 110-117.	1.4	39
72	Massive, automated solvent screening for minimum energy demand in hybrid extractionâ€“distillation using COSMO-RS. Chemical Engineering Research and Design, 2016, 115, 433-442.	2.7	39

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73	Towards sustainable elastomers from CO₂: life cycle assessment of carbon capture and utilization for rubbers. Green Chemistry, 2019, 21, 3334-3342.	4.6	37
74	Optimal design of adsorption chillers based on a validated dynamic object-oriented model. Science and Technology for the Built Environment, 2015, 21, 248-257.	0.8	36
75	Optimal experimental design of ill-posed problems: The METER approach. Computers and Chemical Engineering, 2008, 32, 115-124.	2.0	35
76	Maxwellâ€“Stefan Diffusivities in Binary Mixtures of Ionic Liquids with Dimethyl Sulfoxide (DMSO) and H₂O. Journal of Physical Chemistry B, 2011, 115, 8506-8517.	1.2	35
77	Adsorption thermal energy storage for cogeneration in industrial batch processes: Experiment, dynamic modeling and system analysis. Applied Thermal Engineering, 2015, 89, 485-493.	3.0	35
78	RiSES3: Rigorous Synthesis of Energy Supply and Storage Systems via time-series relaxation and aggregation. Computers and Chemical Engineering, 2019, 127, 127-139.	2.0	35
79	Environmental trade-offs of direct air capture technologies in climate change mitigation toward 2100. Nature Communications, 2022, 13, .	5.8	35
80	COSMO-CAMPD: a framework for integrated design of molecules and processes based on COSMO-RS. Molecular Systems Design and Engineering, 2018, 3, 645-657.	1.7	34
81	TRusT: A Two-stage Robustness Trade-off approach for the design of decentralized energy supply systems. Energy, 2017, 118, 590-599.	4.5	33
82	Developments in the pre-combustion CO2 capture pilot plant at the Buggenum IGCC. Energy Procedia, 2011, 4, 1214-1221.	1.8	31
83	Multi-objective superstructure-free synthesis and optimization of thermal power plants. Energy, 2016, 116, 1104-1116.	4.5	31
84	Multicomponent diffusion coefficients from microfluidics using Raman microspectroscopy. Lab on A Chip, 2017, 17, 2768-2776.	3.1	31
85	The impact of filling level resolved: Capillary-assisted evaporation of water for adsorption heat pumps. Applied Thermal Engineering, 2016, 102, 513-519.	3.0	30
86	Rigorous synthesis of energy systems by decomposition via time-series aggregation. Computers and Chemical Engineering, 2018, 112, 70-81.	2.0	30
87	Life-cycle environmental implications of Chinaâ€™s ban on post-consumer plastics import. Resources, Conservation and Recycling, 2020, 156, 104699.	5.3	30
88	Multispeed models in off-lattice Boltzmann simulations. Physical Review E, 2008, 77, 025701.	0.8	28
89	Validation of the CO₂/N₂O Analogy Using Molecular Simulation. Industrial & Engineering Chemistry Research, 2014, 53, 18081-18090.	1.8	28
90	An adaptive discretization MINLP algorithm for optimal synthesis of decentralized energy supply systems. Computers and Chemical Engineering, 2016, 95, 38-48.	2.0	28

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91	Rhâ€Catalyzed Hydrogenation of CO₂ to Formic Acid in DMSOâ€based Reaction Media: Solved and Unsolved Challenges for Process Development. Advanced Synthesis and Catalysis, 2019, 361, 307-316.	2.1	28
92	Prediction of multicomponent mutual diffusion in liquids: Model discrimination using NMR data. Fluid Phase Equilibria, 2009, 278, 27-35.	1.4	27
93	Typical Periods for Two-Stage Synthesis by Time-Series Aggregation with Bounded Error in Objective Function. Frontiers in Energy Research, 2018, 5, .	1.2	27
94	Integrated design of working fluid and organic Rankine cycle utilizing transient exhaust gases of heavy-duty vehicles. Applied Energy, 2019, 255, 113207.	5.1	27
95	Environmental impacts of the future German energy system from integrated energy systems optimization and dynamic life cycle assessment. Computers and Chemical Engineering, 2021, 153, 107406.	2.0	27
96	The role of instrument compliance in normal force measurements of polymer melts. Rheologica Acta, 2006, 45, 393-402.	1.1	26
97	Refrigeration below zero Â°C: Adsorption chillers using water with ethylene glycol as antifreeze. International Journal of Refrigeration, 2017, 77, 39-47.	1.8	26
98	Prediction of Composition-Dependent Self-Diffusion Coefficients in Binary Liquid Mixtures: The Missing Link for Darken-Based Models. Industrial & Engineering Chemistry Research, 2018, 57, 14784-14794.	1.8	26
99	Identification of diffusive transport by means of an incremental approach. Computers and Chemical Engineering, 2004, 28, 585-595.	2.0	25
100	Simultaneous process and working fluid optimisation for Organic Rankine Cycles (ORC) using PC-SAFT. Computer Aided Chemical Engineering, 2012, , 572-576.	0.3	25
101	Comparative LCA of multi-product processes with non-common products: a systematic approach applied to chlorine electrolysis technologies. International Journal of Life Cycle Assessment, 2013, 18, 828-839.	2.2	25
102	CO from CO₂ and fluctuating renewable energy via formic-acid derivatives. Green Chemistry, 2016, 18, 5621-5629.	4.6	25
103	Rx-COSMO-CAMD: Computer-Aided Molecular Design of Reaction Solvents Based on Predictive Kinetics from Quantum Chemistry. Industrial & Engineering Chemistry Research, 2019, 58, 22835-22846.	1.8	25
104	Renewable carbon feedstock for polymers: environmental benefits from synergistic use of biomass and CO₂. Faraday Discussions, 2021, 230, 227-246.	1.6	25
105	Assessing public acceptance of the life cycle of CO2-based fuels: Does information make the difference?. Energy Policy, 2020, 143, 111586.	4.2	25
106	A climate-optimal supply chain for CO2 capture, utilization, and storage by mineralization. Journal of Cleaner Production, 2022, 360, 131750.	4.6	25
107	Industry-Cost-Curve Approach for Modeling the Environmental Impact of Introducing New Technologies in Life Cycle Assessment. Environmental Science & Technology, 2015, 49, 7543-7551.	4.6	24
108	On the assessment of renewable industrial processes: Case study for solar co-production of methanol and power. Applied Energy, 2016, 183, 121-132.	5.1	24

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109	Hybrid refrigeration by CO2 vapour compression cycle and water-based adsorption chiller: An efficient combination of natural working fluids. International Journal of Refrigeration, 2019, 103, 204-214.	1.8	24
110	An Equation of State Based on PC-SAFT for Physical Solvents Composed of Polyethylene Glycol Dimethylethers. Industrial & Engineering Chemistry Research, 2013, 52, 18401-18412.	1.8	23
111	Heat lost or stored: Experimental analysis of adsorption thermal energy storage. Applied Thermal Engineering, 2016, 106, 981-991.	3.0	23
112	Extreme events in time series aggregation: A case study for optimal residential energy supply systems. Applied Energy, 2020, 275, 115223.	5.1	23
113	Towards optimal mixtures of working fluids: Integrated design of processes and mixtures for Organic Rankine Cycles. Renewable and Sustainable Energy Reviews, 2021, 135, 110179.	8.2	23
114	Comment on â€œHow green is blue hydrogen?â€• Energy Science and Engineering, 2022, 10, 1944-1954.	1.9	23
115	Microfluidic diffusion measurements: The optimal H-cell. Chemical Engineering Science, 2012, 72, 45-50.	1.9	21
116	Decarbonizing copper production by power-to-hydrogen: A techno-economic analysis. Journal of Cleaner Production, 2021, 306, 127191.	4.6	21
117	Consequences of the Brenner modification to the Navierâ€“Stokes equations for dynamic light scattering. Physica A: Statistical Mechanics and Its Applications, 2007, 373, 88-96.	1.2	20
118	Integration of process and solvent design towards a novel generation of CO2 absorption capture systems. Energy Procedia, 2011, 4, 282-290.	1.8	20
119	Optimization-based identification and quantification of demand-side management potential for distributed energy supply systems. Energy, 2017, 135, 889-899.	4.5	20
120	When 2nd generation biofuel meets water â€“ The water solubility and phase stability issue. Fuel, 2017, 209, 615-623.	3.4	20
121	Integrated design of ORC process and working fluid using process flowsheeting software and PC-SAFT. Energy Procedia, 2017, 129, 129-136.	1.8	20
122	Dynamic optimisation of adsorber-bed designs ensuring optimal control. Applied Thermal Engineering, 2017, 125, 1565-1576.	3.0	20
123	Chiral separation by combining pertraction and preferential crystallization. Chemical Engineering and Processing: Process Intensification, 2013, 67, 80-88.	1.8	19
124	Comparison of Raman, NIR, and ATR FTIR spectroscopy as analytical tools for in-line monitoring of CO 2 concentration in an amine gas treating process. International Journal of Greenhouse Gas Control, 2016, 47, 17-24.	2.3	19
125	CO2 mitigation costs of catalytic methane decomposition. Energy, 2018, 151, 826-838.	4.5	19
126	Exergy, exergoeconomic, and exergoenvironmental optimization of the geothermal binary cycle power plant at Ampallas, West Sulawesi, Indonesia. Thermal Science and Engineering Progress, 2020, 19, 100625.	1.3	19

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127	Dynamic modelling and validation of pre-combustion CO2 absorption based on a pilot plant at the Buggenum IGCC power station. International Journal of Greenhouse Gas Control, 2015, 36, 13-26.	2.3	18
128	Estimation of the binary interaction parameter k of the PC-SAFT Equation of State based on pure component parameters using a QSPR method. Fluid Phase Equilibria, 2016, 416, 138-149.	1.4	18
129	Toward Optimal Metalâ€“Organic Frameworks for Adsorption Chillers: Insights from the Scaleâ€Up of MILâ€101(Cr) and NH₂â€MILâ€125. Energy Technology, 2020, 8, 1900617.	1.8	18
130	Integrating superstructureâ€based design of molecules, processes, and flowsheets. AICHE Journal, 2020, 66, e16903.	1.8	18
131	COMANDO: A Next-Generation Open-Source Framework for Energy Systems Optimization. Computers and Chemical Engineering, 2021, 152, 107366.	2.0	18
132	Cost-optimal pathways towards net-zero chemicals and plastics based on a circular carbon economy. Computers and Chemical Engineering, 2022, 162, 107798.	2.0	18
133	On the interpretation of ternary diffusion measurements in low-molecular weight fluids by dynamic light scattering. Fluid Phase Equilibria, 2007, 251, 121-127.	1.4	17
134	Coordinating scheduling of production and utility system using a Stackelberg game. Energy, 2019, 175, 1283-1295.	4.5	17
135	Sensitivity-based analysis of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si61.gif" display="inline" overflow="scroll"><mml:mi>k</mml:mi></mml:math>â€“<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si62.gif" display="inline" overflow="scroll"><mml:mi>Îµ</mml:mi></mml:math> model for the turbulent flow between two plates. Chemical Engineering Science, 2008, 63, 4763-4775.	1.9	16
136	Temperature-Dependent Diffusion Coefficients from 1D Raman Spectroscopy. Journal of Solution Chemistry, 2014, 43, 144-157.	0.6	16
137	To Integrate or Not to Integrateâ€”Techno-Economic and Life Cycle Assessment of CO₂ Capture and Conversion to Methyl Formate Using Methanol. ACS Sustainable Chemistry and Engineering, 0, , .	3.2	16
138	A framework for the design & operation of a large-scale wind-powered hydrogen electrolyzer hub. International Journal of Hydrogen Energy, 2022, 47, 8671-8686.	3.8	16
139	Bridging scales with thermodynamics: from nano to macro. Advances in Natural Sciences: Nanoscience and Nanotechnology, 2014, 5, 023002.	0.7	15
140	Model compendium, data, and optimization benchmarks for sector-coupled energy systems. Computers and Chemical Engineering, 2020, 135, 106760.	2.0	15
141	Comparing pathways for electricity-based production of dimethoxymethane as a sustainable fuel. Energy and Environmental Science, 2021, 14, 3686-3699.	15.6	15
142	Life-Cycle Assessment of Sector-Coupled National Energy Systems: Environmental Impacts of Electricity, Heat, and Transportation in Germany Till 2050. Frontiers in Energy Research, 2021, 9, .	1.2	15
143	Direct determination of the concentration dependence of diffusivities using combined model-based Raman and NMR experiments. Fluid Phase Equilibria, 2009, 277, 96-106.	1.4	14
144	Optimal Experimental Design for the Characterization of Liquidâ€“Liquid Equilibria. Industrial & Engineering Chemistry Research, 2014, 53, 19620-19627.	1.8	14

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145	Efficient Determination of Liquidâ€“Liquid Equilibria Using Microfluidics and Raman Microspectroscopy. Industrial & Engineering Chemistry Research, 2017, 56, 13905-13910.	1.8	14
146	Carbon2Polymer â€“ Conceptual Design of a CO₂â€Based Process for the Production of Isocyanates. Chemie-Ingenieur-Technik, 2018, 90, 1497-1503.	0.4	14
147	Quaternary Diffusion Coefficients in Liquids from Microfluidics and Raman Microspectroscopy: Cyclohexane + Toluene + Acetone + Methanol. Journal of Chemical & Engineering Data, 2020, 65, 1273-1288.	1.0	14
148	Beyond Temperature Glide: The Compressor is Key to Realizing Benefits of Zeotropic Mixtures in Heat Pumps. Energy Technology, 2021, 9, 2000955.	1.8	14
149	Computer-aided Molecular Design of ORC Working Fluids using PC-SAFT. Computer Aided Chemical Engineering, 2014, , 357-362.	0.3	13
150	High-pressure vaporâ€“liquid equilibria of the second generation biofuel blends (2-methylfuran+iso-octane) and (2-methyltetrahydrofuran+di-n-butyl ether): Experiments and PCP-SAFT modeling. Fluid Phase Equilibria, 2015, 400, 95-102.	1.4	13
151	Model-free calibration of Raman measurements of reactive systems: Application to monoethanolamine/water/CO2. Fluid Phase Equilibria, 2016, 424, 52-57.	1.4	13
152	Upgrading Waste Heat from 90 to 110â€‰Â°C: The Potential of Adsorption Heat Transformation. Energy Technology, 2021, 9, 2000643.	1.8	13
153	Towards aromatics from biomass: Prospective Life Cycle Assessment of bio-based aniline. Journal of Cleaner Production, 2021, 290, 125818.	4.6	13
154	COSMO-susCAMPD: Sustainable solvents from combining computer-aided molecular and process design with predictive life cycle assessment. Chemical Engineering Science, 2021, 245, 116863.	1.9	13
155	The IR-Large-Temperature-Jump method: Determining heat and mass transfer coefficients for adsorptive heat transformers. Applied Thermal Engineering, 2017, 126, 630-642.	3.0	12
156	Robust analysis of spectra with strong background signals by First-Derivative Indirect Hard Modeling (FD-IHM). Chemometrics and Intelligent Laboratory Systems, 2018, 172, 1-9.	1.8	12
157	A hierarchical approach for solvent selection based on successive model refinement. Computer Aided Chemical Engineering, 2018, 43, 325-330.	0.3	12
158	A Neural Network-Based Framework to Predict Process-Specific Environmental Impacts. Computer Aided Chemical Engineering, 2019, , 1447-1452.	0.3	12
159	DeLoop: Decomposition-based Long-term operational optimization of energy systems with time-coupling constraints. Energy, 2020, 198, 117272.	4.5	12
160	Control of adsorption chillers by a gradient descent method for optimal cycle time allocation. International Journal of Refrigeration, 2015, 56, 52-64.	1.8	11
161	Towards low carbon business park energy systems: A holistic techno-economic optimisation model. Energy, 2017, 125, 747-770.	4.5	11
162	Second-Order Analytical Uncertainty Analysis in Life Cycle Assessment. Environmental Science & Technology, 2017, 51, 13199-13204.	4.6	11

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163	SPREAD â€“ Exploring the decision space in energy systems synthesis. Computers and Chemical Engineering, 2017, 106, 297-308.	2.0	11
164	Multi-objective synthesis of energy systems: Efficient identification of design trade-offs. Computers and Chemical Engineering, 2017, 97, 283-293.	2.0	11
165	Predicting performance of adsorption thermal energy storage: From experiments to validated dynamic models. Applied Thermal Engineering, 2018, 141, 548-557.	3.0	11
166	Only a wet tube is a good tube: understanding capillary-assisted thin-film evaporation of water for adsorption chillers. Applied Thermal Engineering, 2019, 147, 571-578.	3.0	11
167	Optimal (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf design of distributed energy supply systems. Computers and Chemical Engineering, 2019, 121, 317-326.	2.0	11
168	Reaction Mechanisms and Rate Constants of Autoâ€Catalytic Urethane Formation and Cleavage Reactions. ChemistryOpen, 2021, 10, 534-544.	0.9	11
169	Optimal operation of adsorption chillers: First implementation and experimental evaluation of a nonlinear model-predictive-control strategy. Applied Thermal Engineering, 2019, 149, 1503-1521.	3.0	10
170	Toward the Integrated Design of Organic Rankine Cycle Power Plants: A Method for the Simultaneous Optimization of Working Fluid, Thermodynamic Cycle, and Turbine. Journal of Engineering for Gas Turbines and Power, 2019, 141, .	0.5	10
171	Integrated design and control of full sorption chiller systems. Energy, 2019, 185, 409-422.	4.5	10
172	Is the Microgel Collapse a Two-Step Process? Exploiting Cononsolvency to Probe the Collapse Dynamics of Poly-N-isopropylacrylamide (pNIPAM). Journal of Physical Chemistry B, 2021, 125, 1503-1512.	1.2	10
173	Blend for all or pure for few? Well-to-wheel life cycle assessment of blending electricity-based OME_{3â€“5} with fossil diesel. Sustainable Energy and Fuels, 2022, 6, 1959-1973.	2.5	10
174	Software supporting optimal experimental design: A case study of binary diffusion using EFCOSS. Computers and Chemical Engineering, 2009, 33, 838-849.	2.0	9
175	Towards automated characterisation of liquidâ€“liquid equilibria. Fluid Phase Equilibria, 2014, 362, 328-334.	1.4	9
176	Benchmarking commercial adsorbents for drying air in a packed bed. Applied Thermal Engineering, 2019, 160, 113942.	3.0	9
177	Enrichment of methanol inside pNIPAM gels in the cononsolvency-induced collapse. Physical Chemistry Chemical Physics, 2019, 21, 22811-22818.	1.3	9
178	Validated Performance Prediction of Adsorption Chillers: Bridging the Gap from Gramâ€Scale Experiments to Fullâ€Scale Chillers. Energy Technology, 2020, 8, 1901130.	1.8	9
179	Rxâ€COSMOâ€CAMPD: Enhancing Reactions by Integrated Computerâ€Aided Design of Solvents and Processes based on Quantum Chemistry. Chemie-Ingenieur-Technik, 2020, 92, 1489-1500.	0.4	9
180	Flexible here-and-now decisions for two-stage multi-objective optimization: method and application to energy system design selection. Optimization and Engineering, 2021, 22, 821-847.	1.3	9

#	ARTICLE	IF	CITATIONS
181	Life-Cycle and Techno-Economic Assessment of Early-Stage Carbon Capture and Utilization Technologiesâ€"A Discussion of Current Challenges and Best Practices. Frontiers in Climate, 2022, 4, .	1.3	9
182	A Continuous Targeting Approach for Integrated Solvent and Process Design Based on Molecular Thermodynamic Models. Computer Aided Chemical Engineering, 2009, 27, 813-818.	0.3	8
183	Environmental Assessment of CO2 Capture and Utilisation. , 2015, , 45-56.		8
184	A milliliter-scale setup for the efficient characterization of isothermal vapor-liquid equilibria using Raman spectroscopy. Fluid Phase Equilibria, 2017, 446, 36-45.	1.4	8
185	Integrated design of ORC process and working fluid using PC-SAFT and Modelica. Energy Procedia, 2017, 129, 97-104.	1.8	8
186	Integrating working fluid design into the thermo-economic design of ORC processes using PC-SAFT. Energy Procedia, 2017, 129, 121-128.	1.8	8
187	Aquatic toxicity of biofuel candidates on Daphnia magna. Ecotoxicology and Environmental Safety, 2018, 164, 125-130.	2.9	8
188	Converting two wastes to value. Nature Energy, 2019, 4, 440-441.	19.8	8
189	Automated Physical Property Measurements from Calibration to Data Analysis: Microfluidic Platform for Liquidâ€"Liquid Equilibrium Using Raman Microspectroscopy. Journal of Chemical & Engineering Data, 2020, 65, 319-327.	1.0	8
190	Capillary-assisted evaporation of water from finned tubes â€" Impacts of experimental setups and dynamics. Applied Thermal Engineering, 2020, 165, 114620.	3.0	8
191	AutoMoG: Automated data-driven Model Generation of multi-energy systems using piecewise-linear regression. Computers and Chemical Engineering, 2021, 145, 107162.	2.0	8
192	The demand response potential in copper production. Journal of Cleaner Production, 2022, 362, 132221.	4.6	8
193	Simple two-step assessment of novel adsorbents for drying: The trade-off between adsorber size and drying time. Applied Thermal Engineering, 2017, 125, 1075-1082.	3.0	7
194	Optimal design of integrated batch production and utility systems. Computers and Chemical Engineering, 2019, 128, 496-511.	2.0	7
195	AutoMoGâ€‰3D: Automated Data-Driven Modelâ€‰Generation of Multi-Energy Systems Using Hinging Hyperplanes. Frontiers in Energy Research, 2021, 9, .	1.2	7
196	Chapter 5. Diffusion in Liquids: Experiments, Molecular Dynamics, and Engineering Models. , 2015, , 78-104.		7
197	Dielectric constant of mixed solvents based on perturbation theory. Fluid Phase Equilibria, 2022, 555, 113346.	1.4	7
198	SecMOD: An Open-Source Modular Framework Combining Multi-Sector System Optimization and Life-Cycle Assessment. Frontiers in Energy Research, 0, 10, .	1.2	7

#	Article	IF	Citations
199	The optimal diffusion experiment. Chemical Engineering Science, 2016, 152, 392-402.	1.9	6
200	Scheduling coordination of multiple production and utility systems in a multi-leader multi-follower Stackelberg game. Computers and Chemical Engineering, 2021, 150, 107321.	2.0	6
201	CAT-COSMO-CAMPD: Integrated in silico design of catalysts and processes based on quantum chemistry. Computers and Chemical Engineering, 2021, 153, 107438.	2.0	6
202	Integrated Design of Solvents and Processes based on Reaction Kinetics from Quantum Chemical Prediction Methods. Computer Aided Chemical Engineering, 2019, 46, 415-420.	0.3	6
203	Simultaneous mixedâ€integer dynamic scheduling of processes and their energy systems. AICHE Journal, 2022, 68, .	1.8	6
204	The Thermoâ€Economic Potential of ORCâ€Based Pumpedâ€Thermal Electricity Storage: Insights from the Integrated Design of Processes and Working Fluids. Energy Technology, 2022, 10, .	1.8	6
205	Wind data introduce error in time-series reduction for capacity expansion modelling. Energy, 2022, 256, 124467.	4.5	6
206	Stickstoffbasierte Kraftstoffe: eine â€œPowerâ€toâ€Fuelâ€toâ€Powerâ€â€Analyse. Angewandte Chemie, 2016, 128, 8942-8949.	1.6	5
207	Improved Property Predictions by Combination of Predictive Models. Industrial & Engineering Chemistry Research, 2017, 56, 3098-3106.	1.8	5
208	Quaternary isothermal vapor-liquid equilibrium of the model biofuel 2-butanoneÂ+ n-heptaneÂ+ tetrahydrofuranÂ+ cyclohexane using Raman spectroscopic characterization. Fluid Phase Equilibria, 2018, 472, 107-116.	1.4	5
209	Pareto-optimal performance of one-bed adsorption chillers by easy-to-implement heat-flow-based control. Applied Thermal Engineering, 2019, 159, 113590.	3.0	5
210	ORC on tour: Integrated design of dynamic ORC processes and working fluids for waste-heat recovery from heavy-duty vehicles. Computer Aided Chemical Engineering, 2019, 46, 163-168.	0.3	5
211	Synthesis and Optimization of Distributed Energy Supply Systems using Automated Superstructure and Model Generation. Computer Aided Chemical Engineering, 2012, , 1712-1716.	0.3	4
212	Life-Cycle Assessment Principles for the Integrated Product and Process Design of Polymers from CO2. Computer Aided Chemical Engineering, 2015, , 1235-1240.	0.3	4
213	The trade-off between experimental effort and accuracy for determination of PCP-SAFT parameters. Fluid Phase Equilibria, 2016, 428, 182-189.	1.4	4
214	Integrated design of ORC process and working fluid for transient waste-heat recovery from heavy-duty vehicles. Computer Aided Chemical Engineering, 2018, 44, 2443-2448.	0.3	4
215	Environmental Impacts of the Future German Energy System from Integrated Energy Systems Optimization and Life Cycle Assessment. Computer Aided Chemical Engineering, 2020, , 241-246.	0.3	4
216	Integrated In Silico Design of Catalysts and Processes based on Quantum Chemistry. Computer Aided Chemical Engineering, 2020, 48, 889-894.	0.3	4

#	Article	IF	Citations
217	Efficient modeling of adsorption chillers: Avoiding discretization by operator splitting. International Journal of Refrigeration, 2022, 139, 180-191.	1.8	4
218	Waste Heat to Power: Fullâ€Cycle Analysis of a Thermally Regenerative Flow Battery. Energy Technology, 2022, 10, .	1.8	4
219	Optimal experimental design for ill-posed problems. Computer Aided Chemical Engineering, 2006, 21, 173-178.	0.3	3
220	Time-series aggregation for synthesis of distributed energy supply systems by bounding error in operational expenditure. Computer Aided Chemical Engineering, 2016, , 793-798.	0.3	3
221	Integrated process and solvent design using COSMO-RS for the production of CO from CO 2 and H 2. Computer Aided Chemical Engineering, 2017, 40, 1765-1770.	0.3	3
222	Concentration-Dependent Diffusion Coefficients of Binary Gas Mixtures Using a Loschmidt Cell with Holographic Interferometry. International Journal of Thermophysics, 2018, 39, 1.	1.0	3
223	An Uncertainty Assessment Framework for LCA-based Environmental Process Design. Computer Aided Chemical Engineering, 2013, , 937-942.	0.3	3
224	An Adaptive Normal Constraint Method for Bi-Objective Optimal Synthesis of Energy Systems. Computer Aided Chemical Engineering, 2014, , 1279-1284.	0.3	3
225	Closedâ€Loop Adsorptionâ€Based Upgrading of Heat from 90 to 110â€‰Â°C: Experimental Demonstration and Insights for Future Development. Energy Technology, 2022, 10, .	1.8	3
226	Incremental and simultaneous identification of reaction kinetics: methods and comparison. Chemical Engineering Science, 2004, 59, 2673-2673.	1.9	2
227	Purity versus recovery in FricDiff separations for feed-side and sweep-side products. Separation and Purification Technology, 2010, 76, 95-103.	3.9	2
228	One-stage approach for the integrated design of ORC processes and working fluid using PC-SAFT. Computer Aided Chemical Engineering, 2016, 38, 1335-1340.	0.3	2
229	Integrated Synthesis of Batch Plants and Utility Systems. Computer Aided Chemical Engineering, 2017, , 625-630.	0.3	2
230	Concentration-Dependent Diffusion Coefficients of Binary Gas Mixtures Using a Loschmidt Cell with Holographic Interferometry. International Journal of Thermophysics, 2018, 39, 1.	1.0	2
231	Flexibility-expansion planning for enhanced balancing-power market participation of decentralized energy systems. Computer Aided Chemical Engineering, 2021, 50, 1841-1846.	0.3	2
232	Tailor-made solvents by integrated design of molecules and CO2 absorption processes. Computer Aided Chemical Engineering, 2021, 50, 197-202.	0.3	2
233	Optimal Dynamic Operation of Adsorption-based Energy Systems Driven by Fluctuating Renewable Energy. Computer Aided Chemical Engineering, 2015, 37, 2339-2344.	0.3	2
234	Bilevel optimization for joint scheduling of production and energy systems. Optimization and Engineering, 0, , 1.	1.3	2

#	Article	IF	Citations
235	Druids' Knowledge in Chemical Engineering: Analysis of the Illustrated Literature by Goscinny and Uderzo. Chemie-Ingenieur-Technik, 2012, 84, 427-431.	0.4	1
236	CO2 vs Biomass: Identification of Environmentally Beneficial Processes for Platform Chemicals from Renewable Carbon Sources. Computer Aided Chemical Engineering, 2015, 37, 1361-1366.	0.3	1
237	Selecting CO2Sources for CO2Utilization in Europe: Which, Where, and How Much at Which Environmental Costs?. Chemie-Ingenieur-Technik, 2016, 88, 1258-1259.	0.4	1
238	Rigorous synthesis of energy supply systems by time-series aggregation. Computer Aided Chemical Engineering, 2017, , 2413-2418.	0.3	1
239	Energieeffizienz vs. Umweltauswirkungen: Integration von MolekÃ¼l- und Prozessdesign mit prÃdiktiver Ã–kobilanzierung. Chemie-Ingenieur-Technik, 2018, 90, 1163-1163.	0.4	1
240	Rhâ€Catalyzed Hydrogenation of CO 2 to Formic Acid in DMSOâ€Based Reaction Media. Advanced Synthesis and Catalysis, 2018, 361, 219.	2.1	1
241	Rigorous synthesis of energy systems by relaxation and time-series aggregation to typical periods. Computer Aided Chemical Engineering, 2018, , 793-798.	0.3	1
242	Mixed-Integer Dynamic Scheduling Optimization for Demand Side Management. Computer Aided Chemical Engineering, 2020, , 1405-1410.	0.3	1
243	HÃ¼ttengasâ€toâ€X: Life Cycle Assessment zum Potenzial der Sektorenkopplung von Stahl und Chemie. Chemie-Ingenieur-Technik, 2020, 92, 1168-1168.	0.4	1
244	Accelerated mineralisation: general discussion. Faraday Discussions, 2021, 230, 213-226.	1.6	1
245	Molekulare Optimierung von LÃ¶sungsmitteln fÃ¼r die AmeisensÃure-Synthese zur Speicherung von Kohlenstoff und Wasserstoff. Chemie-Ingenieur-Technik, 2012, 84, 1280-1281.	0.4	1
246	Computer-Aided Molecular Design by Combining Genetic Algorithms and COSMO-RS. Computer Aided Chemical Engineering, 2016, 38, 115-120.	0.3	1
247	The Good, the Bad, and Your Real Choices â€“ Decision Support for Energy Systems Synthesis through Near-Optimal Solutions Analysis. Computer Aided Chemical Engineering, 2014, , 25-30.	0.3	1
248	Adaptive Rolling Horizon for operational optimization of multi-energy systems. , 2022, , .		1
249	Optimally designed solvent system for lignocellulosic biomass conversion supported by property predictions. Sustainable Energy and Fuels, 2022, 6, 2734-2744.	2.5	1
250	Ã–kologischer Vergleich mÃ¶glicher Plattformchemikalien aus CO2und Ãœberschussstrom. Chemie-Ingenieur-Technik, 2014, 86, 1429-1429.	0.4	0
251	Thermal Energy Storage Using Adsorption: Is it Really Lossless?. Chemie-Ingenieur-Technik, 2016, 88, 1274-1274.	0.4	0
252	Life Cycle Assessment of C1 Chemicals from Hydrogen and Carbon Dioxide. Chemie-Ingenieur-Technik, 2016, 88, 1343-1344.	0.4	0

#	Article	IF	Citations
253	Integrierte Abscheidung und Umwandlung von CO2 zu CO durch integriertes Design von LÃ¶sungsmittel und Prozess mit COSMO-RS. Chemie-Ingenieur-Technik, 2018, 90, 1158-1158.	0.4	0
254	Automatisiertes In-silico-Design von optimalen LÃ¶sungsmitteln fÃ¼r Reaktionen auf Basis quantenchemischer Methoden. Chemie-Ingenieur-Technik, 2018, 90, 1201-1202.	0.4	0
255	Nicht-invasive Inline-Analyse von Bioprozessen mit Raman-Spektroskopie und Indirect Hard Modeling (IHM). Chemie-Ingenieur-Technik, 2018, 90, 1275-1275.	0.4	0
256	The carbon footprint of a chemical industry based on CO2 utilization. Chemie-Ingenieur-Technik, 2018, 90, 1142-1142.	0.4	0
257	Ensuring (n â^' 1)-reliability in the optimal design of distributed energy supply systems. Computer Aided Chemical Engineering, 2018, 43, 307-312.	0.3	0
258	Die richtige Mischung fÃ¼r Organic Rankine Cycles: Integriertes Design von Prozess und Arbeitsmittelgemisch mit PC-SAFT. Chemie-Ingenieur-Technik, 2018, 90, 1178-1178.	0.4	0
259	Eine Mikrofluidik-Plattform fÃ¼r die automatisierte Bestimmung von FlÃ¼ssig/flÃ¼ssig-Gleichgewichten mittels Raman-Spektroskopie. Chemie-Ingenieur-Technik, 2018, 90, 1322-1322.	0.4	0
260	Environmental Potential of Chemical Recycling of Plastic Packaging Wastes within the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 1152-1152.	0.4	0
261	From peak power prices to seasonal storage: Long-term operational optimization of energy systems by time-series decomposition. Computer Aided Chemical Engineering, 2019, 46, 703-708.	0.3	0
262	Achieving zeroâ€carbon emission chemicals and plastics with limited renewable resources. Chemie-Ingenieur-Technik, 2020, 92, 1169-1169.	0.4	0
263	Welches Experiment fÃ¼r optimale Prozesssimulationen? Optimale Versuchsplanung fÃ¼r lÃ¶sungsmittelbasierte Prozesse. Chemie-Ingenieur-Technik, 2020, 92, 1179-1179.	0.4	0
264	Konsequenzen einer CO 2 â€Bepreisung fÃ¼r die chemische Industrie: Erkenntnisse aus einem Bottomâ€upâ€Modell. Chemie-Ingenieur-Technik, 2020, 92, 1261-1261.	0.4	0
265	The cost of defossilization in energyâ€intensive industries: Technoâ€economic analysis of powerâ€toâ€H 2 in copper production. Chemie-Ingenieur-Technik, 2020, 92, 1264-1264.	0.4	0
266	Optimal physical property data for process simulations by optimal experimental design. Computer Aided Chemical Engineering, 2021, , 851-857.	0.3	0
267	Life cycle and upscaling: general discussion. Faraday Discussions, 2021, 230, 308-330.	1.6	0
268	Emerging technologies: general discussion. Faraday Discussions, 2021, 230, 388-412.	1.6	0
269	Optimal Experiment Design, Ill-Posed Problems. , 2013, , 1579-1583.		0
270	Looking for Alternatives: Optimization of Energy Supply Systems without Superstructure. Lecture Notes in Computer Science, 2014, , 177-188.	1.0	0

#	Article	IF	Citations
271	Coordination of multiple production and utility systems in a multi-leader multi-follower Stackelberg game. Computer Aided Chemical Engineering, 2019, , 697-702.	0.3	0