Jens Abildskov

List of Publications by Year
in descending order

105	1,928	318942	340414
papers	citations	23 h-index	39 g-index

105	105	105	1705
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Uncertainty estimation in deep learningâ€based property models: Graph neural networks applied to the critical properties. AIChE Journal, 2022, 68, .	1.8	10
2	Quantitative metrics for evaluating reactive cyclic distillation performance. Chemical Engineering and Processing: Process Intensification, 2022, 174, 108843.	1.8	2
3	Molecular tracking: A concept for sideâ€draw distillation column design. AIChE Journal, 2021, 67, .	1.8	2
4	Comparison of Group-Contribution and Machine Learning-based Property Prediction Models with Uncertainty Quantification. Computer Aided Chemical Engineering, 2021, 50, 755-760.	0.3	5
5	Good reporting practice for thermophysical and thermochemical property measurements (IUPAC) Tj ETQq1 1 0.784314 rgBT /Overloc	0.9	24
6	Independent Validation of an In Silico Tool for a Pilot-Scale Pharmaceutical Crystallization Process Development. Processes, 2021, 9, 640.	1.3	0
7	Analysing separation and reaction stage performance in a reactive cyclic distillation process. Chemical Engineering and Processing: Process Intensification, 2021, 167, 108515.	1.8	6
8	Covariance-Based Uncertainty Analysis of Reference Equations of State. Journal of Chemical & Engineering Data, 2020, 65, 503-522.	1.0	4
9	A mass and energy balance stage model for cyclic distillation. AIChE Journal, 2020, 66, e16259.	1.8	9
10	On the thermodynamics of biocatalytic reactions with application of group-contribution correlation and prediction. Fluid Phase Equilibria, 2020, 518, 112623.	1.4	2
11	ChromaTech: A discontinuous Galerkin spectral element simulator for preparative liquid chromatography. Computers and Chemical Engineering, 2020, 141, 107012.	2.0	13
12	Computer-aided molecular product-process design under property uncertainties â€“ A Monte Carlo based optimization strategy. Computers and Chemical Engineering, 2019, 122, 247-257.	2.0	12
13	Uncertainty in the prediction of the thermophysical behavior of new halogenated working fluids. Fluid Phase Equilibria, 2019, 485, 220-233.	1.4	7
14	Economic analysis of a horizontal diabatic separation system. Chemical Engineering Research and Design, 2019, 147, 709-720.	2.7	1
15	CAMD for entrainer screening of extractive distillation process based on new thermodynamic criteria. Chemical Engineering Research and Design, 2019, 147, 721-733.	2.7	19
16	6. Graphical tools for designing intensified distillation processes: Methods and applications. , 2019, , 145-179.		3
17	Raw material quality assessment approaches comparison in pectin production. Biotechnology Progress, 2019, 35, e2762.	1.3	5
18	Systematic Optimization-Based Integrated Chemical Productâ€“Process Design Framework. Industrial & Engineering Chemistry Research, 2018, 57, 677-688.	1.8	28

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19	High-order approximation of chromatographic models using a nodal discontinuous Galerkin approach. Computers and Chemical Engineering, 2018, 109, 68-76.	2.0	14
20	Integrated Process Design and Control of Cyclic Distillation Columns. IFAC-PapersOnLine, 2018, 51, 542-547.	0.5	13
21	Analysis and evaluation of a heat integrated horizontal distillation system. Computer Aided Chemical Engineering, 2018, , 217-222.	0.3	1
22	Reverse Engineering of Working Fluid Selection for Industrial Heat Pump Based on Monte Carlo Sampling and Uncertainty Analysis. Industrial & Engineering Chemistry Research, 2018, 57, 13463-13477.	1.8	12
23	Uncertainty assessment of equations of state with application to an organic Rankine cycle. Molecular Physics, 2017, 115, 1225-1244.	0.8	24
24	Adding Value to Bioethanol through a Purification Process Revamp. Industrial & Engineering Chemistry Research, 2017, 56, 5692-5704.	1.8	7
25	Reliable Correlation for Liquidâ€“Liquid Equilibria outside the Critical Region. Journal of Chemical & Engineering Data, 2017, 62, 2842-2854.	1.0	3
26	Parameter estimation and analysis of an automotive heavy-duty SCR catalyst model. Chemical Engineering Science, 2017, 161, 167-177.	1.9	21
27	Reply to â€œComment on â€˜Reliable Correlation for Liquidâ€“Liquid Equilibria outside the Critical Regionâ€™â€• Journal of Chemical & Engineering Data, 2017, 62, 4043-4044.	1.0	0
28	Driving Force Based Design of Cyclic Distillation. Industrial & Engineering Chemistry Research, 2017, 56, 10833-10844.	1.8	14
29	Integrated working fluid-thermodynamic cycle design of organic Rankine cycle power systems for waste heat recovery. Applied Energy, 2017, 203, 442-453.	5.1	46
30	Prediction of properties of new halogenated olefins using two group contribution approaches. Fluid Phase Equilibria, 2017, 433, 79-96.	1.4	31
31	Optimal operation and stabilising control of the concentric heat-integrated distillation column (HIDiC). Computers and Chemical Engineering, 2017, 96, 196-211.	2.0	21
32	Methodology for Analysing the NOx-NH 3 Trade-off for the Heavy-duty Automotive SCR Catalyst. IFAC-PapersOnLine, 2017, 50, 5998-6003.	0.5	2
33	Supervisory Model Predictive Control of the Heat Integrated Distillation Column. IFAC-PapersOnLine, 2017, 50, 7375-7380.	0.5	8
34	Integrated computer-aided framework for chemical product and process application design and optimization for waste heat recovery. Computer Aided Chemical Engineering, 2017, , 1777-1782.	0.3	2
35	Data Validation and Modelling of Thermodynamic Properties of Systems with Active Pharmaceutical Ingredients (APIs) in Complex Media for Skin Absorption Processes. Computer Aided Chemical Engineering, 2017, 40, 247-252.	0.3	1
36	Computational chemical product design problems under property uncertainties. Computer Aided Chemical Engineering, 2017, , 973-978.	0.3	2

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37	Global sensitivity analysis of computer-aided molecular design problem for the development of novel working fluids for power cycles. Computer Aided Chemical Engineering, 2016, 38, 283-288.	0.3	6
38	Group-contribution based property estimation and uncertainty analysis for flammability-related properties. Journal of Hazardous Materials, 2016, 318, 783-793.	6.5	36
39	Cyclic distillation technology - a mini-review. Journal of Chemical Technology and Biotechnology, 2016, 91, 1215-1223.	1.6	25
40	Optimal Operation and Stabilising Control of the Concentric Heat-Integrated Distillation Column. IFAC-PapersOnLine, 2016, 49, 747-752.	0.5	1
41	Estimation of Kinetic Parameters in an Automotive SCR Catalyst Model. Topics in Catalysis, 2016, 59, 945-951.	1.3	3
42	Working fluid selection for organic Rankine cycles â€“ Impact of uncertainty of fluid properties. Energy, 2016, 109, 987-997.	4.5	52
43	New Realization of Periodic Cycled Separation. Industrial & Engineering Chemistry Research, 2016, 55, 1720-1730.	1.8	17
44	A Comprehensive Methodology for Development, Parameter Estimation, and Uncertainty Analysis of Group Contribution Based Property Modelsâ€”An Application to the Heat of Combustion. Journal of Chemical & Engineering Data, 2016, 61, 602-613.	1.0	57
45	Modeling and analysis of conventional and heatâ€integrated distillation columns. AICHE Journal, 2015, 61, 4251-4263.	1.8	18
46	A Framework for Modular Modeling of the Diesel Engine Exhaust Gas Cleaning System. Computer Aided Chemical Engineering, 2015, 37, 455-460.	0.3	5
47	Outlier treatment for improving parameter estimation of group contribution based models for upper flammability limit. Computer Aided Chemical Engineering, 2015, , 503-508.	0.3	3
48	Densities of Pure Ionic Liquids and Mixtures: Modeling and Data Analysis. Journal of Solution Chemistry, 2015, 44, 558-592.	0.6	6
49	Representation and Validation of Liquid Densities for Pure Compounds and Mixtures. Journal of Chemical & Engineering Data, 2015, 60, 3545-3553.	1.0	7
50	Responses of azeotropes and relative volatilities to pressure variations. Chemical Engineering Research and Design, 2015, 99, 97-110.	2.7	4
51	Vapour liquid equilibria of monocaprylin plus palmitic acid or methyl stearate at P = (1.20 and 2.50) kPa by using DSC technique. Journal of Chemical Thermodynamics, 2015, 91, 108-115.	1.0	19
52	Modelling of cyclopentane promoted gas hydrate systems for carbon dioxide capture processes. Fluid Phase Equilibria, 2014, 375, 89-103.	1.4	18
53	Modelling of tetrahydrofuran promoted gas hydrate systems for carbon dioxide capture processes. Fluid Phase Equilibria, 2014, 375, 45-65.	1.4	20
54	Measuring and modelling of the combined thermodynamic promoting effect of tetrahydrofuran and cyclopentane on carbon dioxide hydrates. Fluid Phase Equilibria, 2014, 381, 20-27.	1.4	45

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55	Pressure Control in Distillation Columns: A Model-Based Analysis. Industrial & Engineering Chemistry Research, 2014, 53, 14776-14787.	1.8	7
56	Thermodynamic promotion of carbon dioxideâ€“clathrate hydrate formation by tetrahydrofuran, cyclopentane and their mixtures. International Journal of Greenhouse Gas Control, 2013, 17, 397-410.	2.3	46
57	Application of the cubic-plus-association (CPA) equation of state to model the fluid phase behaviour of binary mixtures of water and tetrahydrofuran. Fluid Phase Equilibria, 2013, 356, 209-222.	1.4	11
58	A Modeling Framework for Conventional and Heat Integrated Distillation Columns. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2013, 46, 373-378.	0.4	2
59	Dynamic effects of diabatization in distillation columns. Computer Aided Chemical Engineering, 2013, , 1015-1020.	0.3	4
60	The Solvent Selection framework. Computer Aided Chemical Engineering, 2012, 30, 762-766.	0.3	14
61	Protein Dynamics in Organic Media at Varying Water Activity Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2012, 116, 2575-2585.	1.2	68
62	Group-contribution+ (GC+) based estimation of properties of pure components: Improved property estimation and uncertainty analysis. Fluid Phase Equilibria, 2012, 321, 25-43.	1.4	249
63	Phase equilibrium modeling of gas hydrate systems for CO2 capture. Journal of Chemical Thermodynamics, 2012, 48, 13-27.	1.0	50
64	Sensitivity of Process Design due to Uncertainties in Property Estimates. Computer Aided Chemical Engineering, 2012, , 200-204.	0.3	2
65	Pair correlation function integrals: Computation and use. Journal of Chemical Physics, 2011, 135, 084113.	1.2	13
66	Molecular Thermodynamic Modeling and Design of Microencapsulation Systems for Drug Delivery. Journal of Chemical & Engineering Data, 2011, 56, 1229-1237.	1.0	7
67	Total and direct correlation function integrals from molecular simulation of binary systems. Fluid Phase Equilibria, 2011, 302, 32-42.	1.4	16
68	Solubilities of gases in ionic liquids using a corresponding-states approach to Kirkwood-Buff solution theory. Fluid Phase Equilibria, 2011, 302, 93-102.	1.4	11
69	Densities and isothermal compressibilities of ionic liquidsâ€"Modeling and application. Fluid Phase Equilibria, 2010, 295, 215-229.	1.4	38
70	Phase behavior of mixtures of ionic liquids and organic solvents. Journal of Supercritical Fluids, 2010, 55, 833-845.	1.6	14
71	Molecular Thermodynamic Modeling of Mixed Solvent Solubility. Industrial & Engineering Chemistry Research, 2010, 49, 11620-11632.	1.8	23
72	Accurate Kirkwoodâ€“Buff integrals from molecular simulations. Molecular Simulation, 2010, 36, 1243-1252.	0.9	24

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73	Method for predicting solubilities of solids in mixed solvents. AICHE Journal, 2009, 55, 1256-1264.	1.8	13
74	Correlation of phase equilibria and liquid densities for gases with ionic liquids. Fluid Phase Equilibria, 2009, 286, 95-106.	1.4	25
75	Computer-aided polymer design using group contribution plus property models. Computers and Chemical Engineering, 2009, 33, 1004-1013.	2.0	37
76	Multiscale Modelling for Computer Aided Polymer Design. Computer Aided Chemical Engineering, 2009, 27, 213-218.	0.3	2
77	Total correlation function integrals and isothermal compressibilities from molecular simulations. Fluid Phase Equilibria, 2008, 273, 1-10.	1.4	11
78	Model-Based Calculation of Solid Solubility for Solvent Selectionâ€"A Review. Industrial & Engineering Chemistry Research, 2008, 47, 5234-5242.	1.8	78
79	A hierarchal approach based on reverse design algorithm for simultaneous design and analysis of product and processes.. Computer Aided Chemical Engineering, 2007, 24, 461-466.	0.3	0
80	Generation of thermodynamic data for organic liquid mixtures from molecular simulations. Molecular Simulation, 2007, 33, 449-457.	0.9	16
81	A computer aided framework for prediction of properties of organic systems. Computer Aided Chemical Engineering, 2007, 24, 141-146.	0.3	3
82	Simultaneous polymer property modeling using grid technology for structured products. Computer Aided Chemical Engineering, 2007, , 321-326.	0.3	1
83	A method for prediction of UNIFAC group interaction parameters. AICHE Journal, 2007, 53, 1620-1632.	1.8	23
84	Computer-aided framework for pure component properties and phase equilibria prediction for organic systems. Fluid Phase Equilibria, 2007, 261, 199-204.	1.4	18
85	Polymer property modeling using grid technology for design of structured products. Fluid Phase Equilibria, 2007, 261, 58-63.	1.4	17
86	Lumped parameter model for prediction of initial breakthrough profiles for the chromatographic capture of antibodies from a complex feedstock. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2007, 848, 131-141.	1.2	18
87	State conditions transferability of vaporâ€"liquid equilibria via fluctuation solution theory with correlation function integrals from molecular dynamics simulation. Fluid Phase Equilibria, 2007, 260, 169-176.	1.4	17
88	Thermodynamic models from fluctuation solution theory analysis of molecular simulations. Fluid Phase Equilibria, 2007, 261, 185-190.	1.4	10
89	Evaluation of Binary Solvent Mixtures for Efficient Monoacylglycerol Production by Continuous Enzymatic Glycerolysis. Journal of Agricultural and Food Chemistry, 2006, 54, 7113-7119.	2.4	61
90	Computer Aided Polymer Design Using Group Contribution Techniques. Computer Aided Chemical Engineering, 2006, , 257-299.	0.3	0

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91	Prediction of solubilities of complex medium-sized chemicals. Solutes in pure solvents, mixed solvents and cosolvent mixtures. Computer Aided Chemical Engineering, 2005, 20, 217-222.	0.3	0
92	Thermodynamic method for obtaining the solubilities of complex medium-sized chemicals in pure and mixed solvents. Fluid Phase Equilibria, 2005, 228-229, 395-400.	1.4	15
93	Models for Liquid Phase Activity Coefficients - UNIFAC. Computer Aided Chemical Engineering, 2004, 19, 59-74.	0.3	4
94	Chapter 14: Application of Property Models in Chemical Product Design. Computer Aided Chemical Engineering, 2004, , 339-369.	0.3	2
95	The use of VMD data/model to test different thermodynamic models for vapourâ€“liquid equilibrium. Journal of Membrane Science, 2004, 239, 227-241.	4.1	20
96	Prediction of Solubilities of Complex Medium-sized Chemicals. II. Solutes in Mixed Solvents. Molecular Simulation, 2004, 30, 367-378.	0.9	15
97	Prediction of gas solubilities in elastomeric polymers for the design of thermopane windows. Fluid Phase Equilibria, 2003, 211, 17-33.	1.4	15
98	Predicting the Solubilities of Complex Chemicals I. Solutes in Different Solvents. Industrial & Engineering Chemistry Research, 2003, 42, 5622-5634.	1.8	53
99	Estimation of Mixture Properties from First- and Second-Order Group Contributions with the UNIFAC Model. Industrial & Engineering Chemistry Research, 2002, 41, 3260-3273.	1.8	51
100	UNIFAC Parameters for Four New Groups. Industrial & Engineering Chemistry Research, 2002, 41, 2047-2057.	1.8	35
101	The CAPEC Databaseâ€. Journal of Chemical & Engineering Data, 2001, 46, 1041-1044.	1.0	48
102	Integrated Computer-Aided Methods and Tools as Educational Modules. , 0, , 773-798.		0
103	Divided Wall Distillation Column Design using Molecular Tracking. AICHE Journal, 0, , .	1.8	2
104	Flue Gas Cleaning by Periodic Absorption. AICHE Journal, 0, , .	1.8	2
105	Modeling Drainage in Periodic Separation. Industrial & Engineering Chemistry Research, 0, , .	1.8	1