Rajamani Krishna

List of Publications by Year
in descending order

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399	45,013	950 115	2506 196
papers	citations	h-index	g-index

408	408	408	19528
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydrocarbon Separations in a Metal-Organic Framework with Open Iron(II) Coordination Sites. Science, 2012, 335, 1606-1610.	6.0	1,635
2	The Maxwell-Stefan approach to mass transfer. Chemical Engineering Science, 1997, 52, 861-911.	1.9	1,310
3	Pore chemistry and size control in hybrid porous materials for acetylene capture from ethylene. Science, 2016, 353, 141-144.	6.0	1,088
4	Evaluating metalâ€“organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption. Energy and Environmental Science, 2011, 4, 3030.	15.6	901
5	Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. Science, 2018, 362, 443-446.	6.0	763
6	Microporous metal-organic framework with potential for carbon dioxide capture at ambient conditions. Nature Communications, 2012, 3, 954.	5.8	716
7	Modelling reactive distillation. Chemical Engineering Science, 2000, 55, 5183-5229.	1.9	643
8	Metalâ€“organic frameworks with potential for energy-efficient adsorptive separation of light hydrocarbons. Energy and Environmental Science, 2012, 5, 9107.	15.6	604
9	Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels. Science, 2013, 340, 960-964.	6.0	589
10	Twoâ€Dimensional Covalent Organic Frameworks for Carbon Dioxide Capture through Channelâ€Wall Functionalization. Angewandte Chemie - International Edition, 2015, 54, 2986-2990.	7.2	572
11	Molecular sieving of ethylene from ethane using a rigid metalâ€“organic framework. Nature Materials, 2018, 17, 1128-1133.	13.3	532
12	Potential of microporous metalâ€“organic frameworks for separation of hydrocarbon mixtures. Energy and Environmental Science, 2016, 9, 3612-3641.	15.6	530
13	Sulfonate-Grafted Porous Polymer Networks for Preferential CO₂ Adsorption at Low Pressure. Journal of the American Chemical Society, 2011, 133, 18126-18129.	6.6	522
14	Polyamineâ€Tethered Porous Polymer Networks for Carbon Dioxide Capture from Flue Gas. Angewandte Chemie - International Edition, 2012, 51, 7480-7484.	7.2	518
15	Porous Polymer Networks: Synthesis, Porosity, and Applications in Gas Storage/Separation. Chemistry of Materials, 2010, 22, 5964-5972.	3.2	512
16	Enhanced carbon dioxide capture upon incorporation of N,Nâ€²-dimethylethylenediamine in the metalâ€“organic framework CuBTTri. Chemical Science, 2011, 2, 2022.	3.7	491
17	UTSA-74: A MOF-74 Isomer with Two Accessible Binding Sites per Metal Center for Highly Selective Gas Separation. Journal of the American Chemical Society, 2016, 138, 5678-5684.	6.6	489
18	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. Journal of Physical Chemistry B, 1999, 103, 1102-1118.	1.2	472

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19	Selective Binding of O₂ over N₂ in a Redoxâ€“Active Metalâ€“Organic Framework with Open Iron(II) Coordination Sites. Journal of the American Chemical Society, 2011, 133, 14814-14822.	6.6	470
20	Metalâ^'Organic Frameworks as Adsorbents for Hydrogen Purification and Precombustion Carbon Dioxide Capture. Journal of the American Chemical Society, 2011, 133, 5664-5667.	6.6	465
21	Comparative analysis of CFD models of dense gasâ€“solid systems. AICHE Journal, 2001, 47, 1035-1051.	1.8	432
22	Microporous metalâ€“organic framework with dual functionalities for highly efficient removal of acetylene from ethylene/acetylene mixtures. Nature Communications, 2015, 6, 7328.	5.8	404
23	Ethene/ethane separation by the MOF membrane ZIF-8: Molecular correlation of permeation, adsorption, diffusion. Journal of Membrane Science, 2011, 369, 284-289.	4.1	386
24	Introduction of Ï€-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. Journal of the American Chemical Society, 2014, 136, 8654-8660.	6.6	383
25	An Adsorbate Discriminatory Gate Effect in a Flexible Porous Coordination Polymer for Selective Adsorption of CO₂ over C₂H₂. Journal of the American Chemical Society, 2016, 138, 3022-3030.	6.6	359
26	Tailor-Made Pore Surface Engineering in Covalent Organic Frameworks: Systematic Functionalization for Performance Screening. Journal of the American Chemical Society, 2015, 137, 7079-7082.	6.6	351
27	Pore Space Partition within a Metalâ€“Organic Framework for Highly Efficient C₂H₂/CO₂ Separation. Journal of the American Chemical Society, 2019, 141, 4130-4136.	6.6	338
28	Potential of Metalâ€“Organic Frameworks for Separation of Xenon and Krypton. Accounts of Chemical Research, 2015, 48, 211-219.	7.6	330
29	Interplay of Metalloligand and Organic Ligand to Tune Micropores within Isostructural Mixed-Metal Organic Frameworks (Mâ€²MOFs) for Their Highly Selective Separation of Chiral and Achiral Small Molecules. Journal of the American Chemical Society, 2012, 134, 8703-8710.	6.6	326
30	CFD simulations of mass transfer from Taylor bubbles rising in circular capillaries. Chemical Engineering Science, 2004, 59, 2535-2545.	1.9	323
31	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	1.2	314
32	Mixed Metalâ€“Organic Framework with Multiple Binding Sites for Efficient C₂H₂/CO₂Separation. Angewandte Chemie - International Edition, 2020, 59, 4396-4400.	7.2	313
33	An Ideal Molecular Sieve for Acetylene Removal from Ethylene with Record Selectivity and Productivity. Advanced Materials, 2017, 29, 1704210.	11.1	310
34	In silico screening of metalâ€“organic frameworks in separation applications. Physical Chemistry Chemical Physics, 2011, 13, 10593.	1.3	300
35	Microporous metalâ€“organic frameworks for storage and separation of small hydrocarbons. Chemical Communications, 2012, 48, 11813.	2.2	297
36	A Rodâ€Packing Microporous Hydrogenâ€Bonded Organic Framework for Highly Selective Separation of C₂H₂/CO₂ at Room Temperature. Angewandte Chemie - International Edition, 2015, 54, 574-577.	7.2	289

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37	In silico screening of zeolite membranes for CO2 capture. Journal of Membrane Science, 2010, 360, 323-333.	4.1	280
38	Modelling of a bubble column slurry reactor for Fischerâ€“Tropsch synthesis. Catalysis Today, 1999, 52, 279-289.	2.2	273
39	Exceptional Hydrophobicity of a Large-Pore Metalâ€“Organic Zeolite. Journal of the American Chemical Society, 2015, 137, 7217-7223.	6.6	270
40	Describing the Diffusion of Guest Molecules Inside Porous Structures. Journal of Physical Chemistry C, 2009, 113, 19756-19781.	1.5	263
41	Understanding the Role of Sodium during Adsorption:Â A Force Field for Alkanes in Sodium-Exchanged Faujasites. Journal of the American Chemical Society, 2004, 126, 11377-11386.	6.6	255
42	Hydrodynamics of Taylor Flow in Vertical Capillaries:Â Flow Regimes, Bubble Rise Velocity, Liquid Slug Length, and Pressure Drop. Industrial & Engineering Chemistry Research, 2005, 44, 4884-4897.	1.8	250
43	Flexibleâ€“Robust Metalâ€“Organic Framework for Efficient Removal of Propyne from Propylene. Journal of the American Chemical Society, 2017, 139, 7733-7736.	6.6	242
44	A multicomponent film model incorporating a general matrix method of solution to the Maxwell-Stefan equations. AICHE Journal, 1976, 22, 383-389.	1.8	240
45	Multicomponent surface diffusion of adsorbed species: a description based on the generalized Maxwellâ€”Stefan equations. Chemical Engineering Science, 1990, 45, 1779-1791.	1.9	240
46	Diffusion in porous crystalline materials. Chemical Society Reviews, 2012, 41, 3099.	18.7	239
47	A Chemically Stable Hofmannâ€Type Metalâ€'Organic Framework with Sandwichâ€Like Binding Sites for Benchmark Acetylene Capture. Advanced Materials, 2020, 32, e1908275.	11.1	236
48	Design and scale-up of the Fischerâ€“Tropsch bubble column slurry reactor. Fuel Processing Technology, 2000, 64, 73-105.	3.7	230
49	Modeling of Diffusion in Zeolites. Reviews in Chemical Engineering, 2000, 16, .	2.3	228
50	A robust doubly interpenetrated metalâ€“organic framework constructed from a novel aromatic tricarboxylate for highly selective separation of small hydrocarbons. Chemical Communications, 2012, 48, 6493.	2.2	224
51	Novel MOFâ€Membrane for Molecular Sieving Predicted by IRâ€Diffusion Studies and Molecular Modeling. Advanced Materials, 2010, 22, 4741-4743.	11.1	222
52	The generalized Maxwellâ€“Stefan model for diffusion in zeolites:. Chemical Engineering Science, 2000, 55, 2923-2930.	1.9	216
53	Improving the efficiency of the configurational-bias Monte Carlo algorithm. Molecular Physics, 1998, 94, 727-733.	0.8	212
54	Induced Fit of C₂H₂ in a Flexible MOF Through Cooperative Action of Open Metal Sites. Angewandte Chemie - International Edition, 2019, 58, 8515-8519.	7.2	208

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55	A Microporous Metalâ€“Organic Framework for Highly Selective Separation of Acetylene, Ethylene, and Ethane from Methane at Room Temperature. Chemistry - A European Journal, 2012, 18, 613-619.	1.7	204
56	Molecular Sieving of Ethane from Ethylene through the Molecular Crossâ€Section Size Differentiation in Gallateâ€based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2018, 57, 16020-16025.	7.2	202
57	Mass transfer from Taylor bubbles rising in single capillaries. Chemical Engineering Science, 2005, 60, 6430-6437.	1.9	199
58	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. Journal of Physical Chemistry C, 2009, 113, 8814-8820.	1.5	199
59	Pore-Space-Partition-Enabled Exceptional Ethane Uptake and Ethane-Selective Ethaneâ€“Ethylene Separation. Journal of the American Chemical Society, 2020, 142, 2222-2227.	6.6	199
60	Gas holdup and mass transfer in bubble column reactors operated at elevated pressure. Chemical Engineering Science, 1999, 54, 2237-2246.	1.9	198
61	Screening Metalâ€“Organic Frameworks by Analysis of Transient Breakthrough of Gas Mixtures in a Fixed Bed Adsorber. Journal of Physical Chemistry C, 2011, 115, 12941-12950.	1.5	197
62	Fundamentals and selection of advanced Fischerâ€“Tropsch reactors. Applied Catalysis A: General, 1999, 186, 55-70.	2.2	196
63	Entropy effects during sorption of alkanes in zeolites. Chemical Society Reviews, 2002, 31, 185-194.	18.7	193
64	A robust Th-azole framework for highly efficient purification of C2H4 from a C2H4/C2H2/C2H6 mixture. Nature Communications, 2020, 11, 3163.	5.8	192
65	Modelling issues in zeolite based separation processes. Separation and Purification Technology, 2003, 33, 213-254.	3.9	191
66	Characterization of regimes and regime transitions in bubble columns by chaos analysis of pressure signals. Chemical Engineering Science, 1997, 52, 4447-4459.	1.9	188
67	Microimaging of transient guest profiles to monitor mass transfer in nanoporous materials. Nature Materials, 2014, 13, 333-343.	13.3	187
68	Using molecular simulations for screening of zeolites for separation of CO2/CH4 mixtures. Chemical Engineering Journal, 2007, 133, 121-131.	6.6	186
69	An Ultramicroporous Metalâ€“Organic Framework for High Sieving Separation of Propylene from Propane. Journal of the American Chemical Society, 2020, 142, 17795-17801.	6.6	186
70	Ultrahigh and Selective SO₂ Uptake in Inorganic Anionâ€Pillared Hybrid Porous Materials. Advanced Materials, 2017, 29, 1606929.	11.1	183
71	Selective Ethane/Ethylene Separation in a Robust Microporous Hydrogen-Bonded Organic Framework. Journal of the American Chemical Society, 2020, 142, 633-640.	6.6	183
72	High CO₂/N₂/O₂/CO separation in a chemically robust porous coordination polymer with low binding energy. Chemical Science, 2014, 5, 660-666.	3.7	181

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73	Direct Observation of Xe and Kr Adsorption in a Xe-Selective Microporous Metalâ€“Organic Framework. Journal of the American Chemical Society, 2015, 137, 7007-7010.	6.6	179
74	Correlation Effects in Diffusion of CH4/CF4Mixtures in MFI Zeolite. A Study Linking MD Simulations with the Maxwellâ^'Stefan Formulation. Langmuir, 2003, 19, 7977-7988.	1.6	177
75	The Maxwellâ€“Stefan description of mixture diffusion in nanoporous crystalline materials. Microporous and Mesoporous Materials, 2014, 185, 30-50.	2.2	176
76	Problems and pitfalls in the use of the fick formulation for intraparticle diffusion. Chemical Engineering Science, 1993, 48, 845-861.	1.9	173
77	Tuning Gateâ€Opening of a Flexible Metalâ€“Organic Framework for Ternary Gas Sieving Separation. Angewandte Chemie - International Edition, 2020, 59, 22756-22762.	7.2	173
78	Metalâ€“Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. Journal of the American Chemical Society, 2022, 144, 1681-1689.	6.6	172
79	Strategies for multiphase reactor selection. Chemical Engineering Science, 1994, 49, 4029-4065.	1.9	165
80	Gas holdup in slurry bubble columns: Effect of column diameter and slurry concentrations. AICHE Journal, 1997, 43, 311-316.	1.8	165
81	Insights into diffusion of gases in zeolites gained from molecular dynamics simulations. Microporous and Mesoporous Materials, 2008, 109, 91-108.	2.2	164
82	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. Journal of the American Chemical Society, 1998, 120, 5599-5600.	6.6	163
83	Influence of scale on the hydrodynamics of bubble columns operating in the churn-turbulent regime: experiments vs. Eulerian simulations. Chemical Engineering Science, 1999, 54, 4903-4911.	1.9	161
84	A computational study of CO2, N2, and CH4 adsorption in zeolites. Adsorption, 2007, 13, 469-476.	1.4	159
85	The Darken Relation for Multicomponent Diffusion in Liquid Mixtures of Linear Alkanes:â€‰ An Investigation Using Molecular Dynamics (MD) Simulations. Industrial & Engineering Chemistry Research, 2005, 44, 6939-6947.	1.8	155
86	Carbon Dioxide Capture from Air Using Amine-Grafted Porous Polymer Networks. Journal of Physical Chemistry C, 2013, 117, 4057-4061.	1.5	153
87	A model for gas holdup in bubble columns incorporating the influence of gas density on flow regime transitions. Chemical Engineering Science, 1991, 46, 2491-2496.	1.9	152
88	Enhanced Gas Uptake in a Microporous Metalâ€“Organic Framework via a Sorbate Induced-Fit Mechanism. Journal of the American Chemical Society, 2019, 141, 17703-17712.	6.6	152
89	MASS AND ENERGY TRANSFER IN MULTICOMPONENT SYSTEMS. Chemical Engineering Communications, 1979, 3, 201-275.	1.5	151
90	Gas holdup in bubble column reactors operating in the churn-turbulent flow regime. AICHE Journal, 1996, 42, 2627-2634.	1.8	151

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91	Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and Ï€-complexation. Chemical Communications, 2015, 51, 2714-2717.	2.2	151
92	Multiple solutions in reactive distillation for methyl tert-butyl ether synthesis. Industrial & Engineering Chemistry Research, 1993, 32, 1706-1709.	1.8	148
93	A comparison of the CO2 capture characteristics of zeolites and metalâ€“organic frameworks. Separation and Purification Technology, 2012, 87, 120-126.	3.9	147
94	A microporous six-fold interpenetrated hydrogen-bonded organic framework for highly selective separation of C₂H₄/C₂H₆. Chemical Communications, 2014, 50, 13081-13084.	2.2	147
95	Significant Enhancement of C₂H₂/C₂H₄ Separation by a Photochromic Diarylethene Unit: A Temperatureâ€and Lightâ€Responsive Separation Switch. Angewandte Chemie - International Edition, 2017, 56, 7900-7906.	7.2	145
96	Rise velocity of a swarm of large gas bubbles in liquids. Chemical Engineering Science, 1999, 54, 171-183.	1.9	142
97	High Separation Capacity and Selectivity of C₂ Hydrocarbons over Methane within a Microporous Metalâ€“Organic Framework at Room Temperature. Chemistry - A European Journal, 2012, 18, 1901-1904.	1.7	142
98	Methodologies for evaluation of metalâ€“organic frameworks in separation applications. RSC Advances, 2015, 5, 52269-52295.	1.7	139
99	Screening metalâ€“organic frameworks for mixture separations in fixed-bed adsorbers using a combined selectivity/capacity metric. RSC Advances, 2017, 7, 35724-35737.	1.7	137
100	Adsorption and diffusion of alkanes in CuBTC crystals investigated using infra-red microscopy and molecular simulations. Microporous and Mesoporous Materials, 2009, 117, 22-32.	2.2	135
101	A microporous lanthanide-tricarboxylate framework with the potential for purification of natural gas. Chemical Communications, 2012, 48, 10856.	2.2	134
102	Eulerian simulations of bubbling behaviour in gas-solid fluidised beds. Computers and Chemical Engineering, 1998, 22, S299-S306.	2.0	133
103	Natural Gas Purification Using a Porous Coordination Polymer with Water and Chemical Stability. Inorganic Chemistry, 2015, 54, 4279-4284.	1.9	133
104	Methane storage mechanism in the metal-organic framework Cu3(btc)2: An in situ neutron diffraction study. Microporous and Mesoporous Materials, 2010, 136, 50-58.	2.2	132
105	Diffusion of Alkane Mixtures in Zeolites:â€‰ Validating the Maxwellâ€“Stefan Formulation Using MD Simulations. Journal of Physical Chemistry B, 2005, 109, 6386-6396.	1.2	129
106	Segregation effects in adsorption of CO2-containing mixtures and their consequences for separation selectivities in cage-type zeolites. Separation and Purification Technology, 2008, 61, 414-423.	3.9	129
107	Twoâ€Dimensional Covalent Organic Frameworks for Carbon Dioxide Capture through Channelâ€Wall Functionalization. Angewandte Chemie, 2015, 127, 3029-3033.	1.6	129
108	Size, structure and dynamics of â€œlargeâ€•bubbles in a two-dimensional slurry bubble column. Chemical Engineering Science, 1996, 51, 4619-4629.	1.9	127

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109	Hydrogen Bonding Effects in Adsorption of Waterâ"Alcohol Mixtures in Zeolites and the Consequences for the Characteristics of the Maxwellâ"Stefan Diffusivities. Langmuir, 2010, 26, 10854-10867.	1.6	127
110	Comparison of equilibrium stage and nonequilibrium stage models for reactive distillation. Chemical Engineering Journal, 2000, 76, 33-47.	6.6	125
111	A Metalâ€"Organic Framework with Suitable Pore Size and Specific Functional Sites for the Removal of Trace Propyne from Propylene. Angewandte Chemie - International Edition, 2018, 57, 15183-15188.	7.2	124
112	A metalâ€"organic framework with suitable pore size and dual functionalities for highly efficient post-combustion CO₂ capture. Journal of Materials Chemistry A, 2019, 7, 3128-3134.	5.2	124
113	CO2/CH4, CH4/H2 and CO2/CH4/H2 separations at high pressures using Mg2(dobdc). Microporous and Mesoporous Materials, 2012, 151, 481-487.	2.2	123
114	Three-phase Eulerian simulations of bubble column reactors operating in the churn-turbulent regime: a scale up strategy. Chemical Engineering Science, 2000, 55, 3275-3286.	1.9	122
115	Unified Maxwellâ€"Stefan description of binary mixture diffusion in micro- and meso-porous materials. Chemical Engineering Science, 2009, 64, 3159-3178.	1.9	119
116	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. Journal of Physical Chemistry A, 1998, 102, 7727-7730.	1.1	118
117	Extraordinary Separation of Acetyleneâ€Containing Mixtures with Microporous Metalâ€"Organic Frameworks with Open O Donor Sites and Tunable Robustness through Control of the Helical Chain Secondary Building Units. Chemistry - A European Journal, 2016, 22, 5676-5683.	1.7	113
118	Rational Design of Microporous MOFs with Anionic Boron Cluster Functionality and Cooperative Dihydrogen Binding Sites for Highly Selective Capture of Acetylene. Angewandte Chemie - International Edition, 2020, 59, 17664-17669.	7.2	110
119	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. Chemical Engineering Journal, 2002, 88, 81-94.	6.6	109
120	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Shortn-Alkanes in Faujasite. Journal of Physical Chemistry B, 2004, 108, 13481-13491.	1.2	108
121	Design of the Reduction of Events with Darbepoetin alfa in Heart Failure (REDâ€HF): a Phase III, anaemia correction, morbidityâ€"mortality trial. European Journal of Heart Failure, 2009, 11, 795-801.	2.9	107
122	Uphill diffusion in multicomponent mixtures. Chemical Society Reviews, 2015, 44, 2812-2836.	18.7	106
123	Fluorocarbon adsorption in hierarchical porous frameworks. Nature Communications, 2014, 5, 4368.	5.8	104
124	A Rodâ€Packing Hydrogenâ€Bonded Organic Framework with Suitable Pore Confinement for Benchmark Ethane/Ethylene Separation. Angewandte Chemie - International Edition, 2021, 60, 10304-10310.	7.2	104
125	Enhanced CO₂sorption and selectivity by functionalization of a NbO-type metalâ€"organic framework with polarized benzothiadiazole moieties. Chemical Communications, 2014, 50, 12105-12108.	2.2	103
126	Kr/Xe Separation over a Chabazite Zeolite Membrane. Journal of the American Chemical Society, 2016, 138, 9791-9794.	6.6	103

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127	Interpenetration Symmetry Control Within Ultramicroporous Robust Boron Cluster Hybrid MOFs for Benchmark Purification of Acetylene from Carbon Dioxide. Angewandte Chemie - International Edition, 2021, 60, 22865-22870.	7.2	103
128	Modeling the occupancy dependence of diffusivities in zeolites. Microporous and Mesoporous Materials, 2004, 76, 233-246.	2.2	100
129	A Metalâ€“Organic Framework with Suitable Pore Size and Specific Functional Sites for the Removal of Trace Propyne from Propylene. Angewandte Chemie, 2018, 130, 15403-15408.	1.6	98
130	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwellâ€“Stefan theory. Separation and Purification Technology, 2000, 21, 111-136.	3.9	95
131	Separating Xylene Isomers by Commensurate Stacking of pâ€Xylene within Channels of MAFâ€X8. Angewandte Chemie - International Edition, 2014, 53, 7774-7778.	7.2	93
132	Optimal Pore Chemistry in an Ultramicroporous Metalâ€“Organic Framework for Benchmark Inverse CO₂/C₂H₂ Separation. Angewandte Chemie - International Edition, 2021, 60, 17198-17204.	7.2	93
133	Thermosensitive gating effect and selective gas adsorption in a porous coordination nanocage. Chemical Communications, 2010, 46, 7352.	2.2	91
134	A molecular dynamics investigation of the diffusion characteristics of cavity-type zeolites with 8-ring windows. Microporous and Mesoporous Materials, 2011, 137, 83-91.	2.2	91
135	A new metalâ€“organic framework with potential for adsorptive separation of methane from carbon dioxide, acetylene, ethylene, and ethane established by simulated breakthrough experiments. Journal of Materials Chemistry A, 2014, 2, 2628.	5.2	91
136	Methodologies for screening and selection of crystalline microporous materials in mixture separations. Separation and Purification Technology, 2018, 194, 281-300.	3.9	91
137	Hydrodynamics and mass transfer in bubble columns in operating in the churn-turbulent regime. Industrial & Engineering Chemistry Process Design and Development, 1981, 20, 475-482.	0.6	89
138	Computerâ€Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. Angewandte Chemie - International Edition, 2012, 51, 11867-11871.	7.2	89
139	Efficient separation of ethylene from acetylene/ethylene mixtures by a flexible-robust metalâ€“organic framework. Journal of Materials Chemistry A, 2017, 5, 18984-18988.	5.2	88
140	Light Hydrocarbon Adsorption Mechanisms in Two Calcium-Based Microporous Metal Organic Frameworks. Chemistry of Materials, 2016, 28, 1636-1646.	3.2	87
141	Guest-dependent pressure induced gate-opening effect enables effective separation of propene and propane in a flexible MOF. Chemical Engineering Journal, 2018, 346, 489-496.	6.6	87
142	A stable metalâ€“organic framework with suitable pore sizes and rich uncoordinated nitrogen atoms on the internal surface of micropores for highly efficient CO₂ capture. Journal of Materials Chemistry A, 2015, 3, 7361-7367.	5.2	86
143	Investigating the potential of MgMOF-74 membranes for CO2 capture. Journal of Membrane Science, 2011, 377, 249-260.	4.1	85
144	Simultaneous interlayer and intralayer space control in two-dimensional metalâ˜’organic frameworks for acetylene/ethylene separation. Nature Communications, 2020, 11, 6259.	5.8	85

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145	Modelling sieve tray hydraulics using computational fluid dynamics. Chemical Engineering Journal, 2000, 77, 143-151.	6.6	83
146	A cationic microporous metalâ€“organic framework for highly selective separation of small hydrocarbons at room temperature. Journal of Materials Chemistry A, 2013, 1, 9916.	5.2	83
147	Assessing Surface Permeabilities from Transient Guest Profiles in Nanoporous Host Materials. Angewandte Chemie - International Edition, 2009, 48, 3525-3528.	7.2	82
148	Exploiting the gate opening effect in a flexible MOF for selective adsorption of propyne from C1/C2/C3 hydrocarbons. Journal of Materials Chemistry A, 2016, 4, 751-755.	5.2	81
149	Interpreting Unary, Binary, and Ternary Mixture Permeation Across a SAPO-34 Membrane with Loading-Dependent Maxwellâ˜Stefan Diffusivities. Journal of Physical Chemistry C, 2007, 111, 5075-5082.	1.5	80
150	Adsorptive separation of CO2/CH4/CO gas mixtures at high pressures. Microporous and Mesoporous Materials, 2012, 156, 217-223.	2.2	80
151	The accessibility of nitrogen sites makes a difference in selective CO2 adsorption of a family of isostructural metalâ€“organic frameworks. Journal of Materials Chemistry A, 2015, 3, 19417-19426.	5.2	80
152	Analysis of Diffusion Limitation in the Alkylation of Benzene over H-ZSM-5 by Combining Quantum Chemical Calculations, Molecular Simulations, and a Continuum Approach. Journal of Physical Chemistry C, 2009, 113, 235-246.	1.5	78
153	Maxwellâ€“Stefan modeling of slowing-down effects in mixed gas permeation across porous membranes. Journal of Membrane Science, 2011, 383, 289-300.	4.1	78
154	An investigation of the characteristics of Maxwellâ€“Stefan diffusivities of binary mixtures in silica nanopores. Chemical Engineering Science, 2009, 64, 870-882.	1.9	77
155	Mixture diffusion in zeolites studied by MAS PFG NMR and molecular simulation. Microporous and Mesoporous Materials, 2007, 105, 124-131.	2.2	76
156	Assessing Guest Diffusivities in Porous Hosts from Transient Concentration Profiles. Physical Review Letters, 2009, 102, 065901.	2.9	76
157	Harnessing Lewis acidic open metal sites of metalâ€“organic frameworks: the foremost route to achieve highly selective benzene sorption over cyclohexane. Chemical Communications, 2016, 52, 8215-8218.	2.2	76
158	Separating mixtures by exploiting molecular packing effects in microporous materials. Physical Chemistry Chemical Physics, 2015, 17, 39-59.	1.3	75
159	Investigating Cluster Formation in Adsorption of CO₂, CH₄, and Ar in Zeolites and Metal Organic Frameworks at Subcritical Temperatures. Langmuir, 2010, 26, 3981-3992.	1.6	74
160	Self-diffusivities in multicomponent mixtures in zeolites. Physical Chemistry Chemical Physics, 2002, 4, 1891-1898.	1.3	73
161	CFD Simulations of Sieve Tray Hydrodynamics. Chemical Engineering Research and Design, 1999, 77, 639-646.	2.7	72
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