

Rajamani Krishna

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395
papers

35,504
citations

104
h-index

176
g-index

408
ext. papers

40,346
ext. citations

8.4
avg, IF

7.85
L-index

#	Paper	IF	Citations
395	Hydrocarbon separations in a metal-organic framework with open iron(II) coordination sites. <i>Science</i> , 2012 , 335, 1606-10	33.3	1349
394	The Maxwell-Stefan approach to mass transfer. <i>Chemical Engineering Science</i> , 1997 , 52, 861-911	4.4	1125
393	Pore chemistry and size control in hybrid porous materials for acetylene capture from ethylene. <i>Science</i> , 2016 , 353, 141-4	33.3	783
392	Evaluating metal-organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption. <i>Energy and Environmental Science</i> , 2011 , 4, 3030	35.4	782
391	Microporous metal-organic framework with potential for carbon dioxide capture at ambient conditions. <i>Nature Communications</i> , 2012 , 3, 954	17.4	615
390	Modelling reactive distillation. <i>Chemical Engineering Science</i> , 2000 , 55, 5183-5229	4.4	561
389	Metal-organic frameworks with potential for energy-efficient adsorptive separation of light hydrocarbons. <i>Energy and Environmental Science</i> , 2012 , 5, 9107	35.4	517
388	Separation of hexane isomers in a metal-organic framework with triangular channels. <i>Science</i> , 2013 , 340, 960-4	33.3	490
387	Sulfonate-grafted porous polymer networks for preferential CO ₂ adsorption at low pressure. <i>Journal of the American Chemical Society</i> , 2011 , 133, 18126-9	16.4	479
386	Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. <i>Science</i> , 2018 , 362, 443-446	33.3	478
385	Polyamine-tethered porous polymer networks for carbon dioxide capture from flue gas. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 7480-4	16.4	476
384	Porous Polymer Networks: Synthesis, Porosity, and Applications in Gas Storage/Separation. <i>Chemistry of Materials</i> , 2010 , 22, 5964-5972	9.6	466
383	Enhanced carbon dioxide capture upon incorporation of N,N'-dimethylethylenediamine in the metal-organic framework CuBTTri. <i>Chemical Science</i> , 2011 , 2, 2022	9.4	445
382	Two-dimensional covalent organic frameworks for carbon dioxide capture through channel-wall functionalization. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2986-90	16.4	441
381	Potential of microporous metal-organic frameworks for separation of hydrocarbon mixtures. <i>Energy and Environmental Science</i> , 2016 , 9, 3612-3641	35.4	428
380	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 1102-1118	3.4	420
379	Metal-organic frameworks as adsorbents for hydrogen purification and precombustion carbon dioxide capture. <i>Journal of the American Chemical Society</i> , 2011 , 133, 5664-7	16.4	405

378	Selective binding of O ₂ over N ₂ in a redox-active metal-organic framework with open iron(II) coordination sites. <i>Journal of the American Chemical Society</i> , 2011 , 133, 14814-22	16.4	404
377	Comparative analysis of CFD models of dense gas/solid systems. <i>AIChE Journal</i> , 2001 , 47, 1035-1051	3.6	372
376	UTSA-74: A MOF-74 Isomer with Two Accessible Binding Sites per Metal Center for Highly Selective Gas Separation. <i>Journal of the American Chemical Society</i> , 2016 , 138, 5678-84	16.4	351
375	Ethene/ethane separation by the MOF membrane ZIF-8: Molecular correlation of permeation, adsorption, diffusion. <i>Journal of Membrane Science</i> , 2011 , 369, 284-289	9.6	334
374	Microporous metal-organic framework with dual functionalities for highly efficient removal of acetylene from ethylene/acetylene mixtures. <i>Nature Communications</i> , 2015 , 6, 7328	17.4	326
373	Molecular sieving of ethylene from ethane using a rigid metal-organic framework. <i>Nature Materials</i> , 2018 , 17, 1128-1133	27	326
372	Introduction of π -complexation into porous aromatic framework for highly selective adsorption of ethylene over ethane. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8654-60	16.4	304
371	Interplay of metalloligand and organic ligand to tune micropores within isostructural mixed-metal organic frameworks (M ⁿ MOFs) for their highly selective separation of chiral and achiral small molecules. <i>Journal of the American Chemical Society</i> , 2012 , 134, 8703-10	16.4	296
370	United Atom Force Field for Alkanes in Nanoporous Materials. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 12301-12313	3.4	282
369	In silico screening of metal-organic frameworks in separation applications. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 10593-616	3.6	279
368	An Adsorbate Discriminatory Gate Effect in a Flexible Porous Coordination Polymer for Selective Adsorption of CO ₂ over C ₂ H ₂ . <i>Journal of the American Chemical Society</i> , 2016 , 138, 3022-30	16.4	278
367	Microporous metal-organic frameworks for storage and separation of small hydrocarbons. <i>Chemical Communications</i> , 2012 , 48, 11813-31	5.8	278
366	Tailor-Made Pore Surface Engineering in Covalent Organic Frameworks: Systematic Functionalization for Performance Screening. <i>Journal of the American Chemical Society</i> , 2015 , 137, 7079-82	16.4	264
365	Potential of metal-organic frameworks for separation of xenon and krypton. <i>Accounts of Chemical Research</i> , 2015 , 48, 211-9	24.3	259
364	Modelling of a bubble column slurry reactor for Fischer-Tropsch synthesis. <i>Catalysis Today</i> , 1999 , 52, 279-289	5.3	252
363	Describing the Diffusion of Guest Molecules Inside Porous Structures. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 19756-19781	3.8	244
362	In silico screening of zeolite membranes for CO ₂ capture. <i>Journal of Membrane Science</i> , 2010 , 360, 323-333	9.6	244
361	CFD simulations of mass transfer from Taylor bubbles rising in circular capillaries. <i>Chemical Engineering Science</i> , 2004 , 59, 2535-2545	4.4	234

360	Multicomponent surface diffusion of adsorbed species: a description based on the generalized Maxwell-Stefan equations. <i>Chemical Engineering Science</i> , 1990 , 45, 1779-1791	4.4	223
359	Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. <i>Journal of the American Chemical Society</i> , 2004 , 126, 11377-86	16.4	222
358	Exceptional Hydrophobicity of a Large-Pore Metal-Organic Zeolite. <i>Journal of the American Chemical Society</i> , 2015 , 137, 7217-23	16.4	214
357	An Ideal Molecular Sieve for Acetylene Removal from Ethylene with Record Selectivity and Productivity. <i>Advanced Materials</i> , 2017 , 29, 1704210	24	213
356	Design and scale-up of the Fischer-Tropsch bubble column slurry reactor. <i>Fuel Processing Technology</i> , 2000 , 64, 73-105	7.2	211
355	Hydrodynamics of Taylor Flow in Vertical Capillaries: Flow Regimes, Bubble Rise Velocity, Liquid Slug Length, and Pressure Drop. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 4884-4897	3.9	207
354	Novel MOF-membrane for molecular sieving predicted by IR-diffusion studies and molecular modeling. <i>Advanced Materials</i> , 2010 , 22, 4741-3	24	205
353	Modeling of Diffusion in Zeolites. <i>Reviews in Chemical Engineering</i> , 2000 , 16,	5	197
352	The generalized Maxwell-Stefan model for diffusion in zeolites: sorbate molecules with different saturation loadings. <i>Chemical Engineering Science</i> , 2000 , 55, 2923-2930	4.4	195
351	Diffusion in porous crystalline materials. <i>Chemical Society Reviews</i> , 2012 , 41, 3099-118	58.5	194
350	Improving the efficiency of the configurational-bias Monte Carlo algorithm. <i>Molecular Physics</i> , 1998 , 94, 727-733	1.7	192
349	Pore Space Partition within a Metal-Organic Framework for Highly Efficient CH ₄ /CO Separation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4130-4136	16.4	190
348	A microporous metal-organic framework for highly selective separation of acetylene, ethylene, and ethane from methane at room temperature. <i>Chemistry - A European Journal</i> , 2012 , 18, 613-9	4.8	188
347	A robust doubly interpenetrated metal-organic framework constructed from a novel aromatic tricarboxylate for highly selective separation of small hydrocarbons. <i>Chemical Communications</i> , 2012 , 48, 6493-5	5.8	187
346	Screening Metal-Organic Frameworks by Analysis of Transient Breakthrough of Gas Mixtures in a Fixed Bed Adsorber. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 12941-12950	3.8	184
345	A multicomponent film model incorporating a general matrix method of solution to the Maxwell-Stefan equations. <i>AIChE Journal</i> , 1976 , 22, 383-389	3.6	178
344	Flexible-Robust Metal-Organic Framework for Efficient Removal of Propyne from Propylene. <i>Journal of the American Chemical Society</i> , 2017 , 139, 7733-7736	16.4	177
343	Gas holdup and mass transfer in bubble column reactors operated at elevated pressure. <i>Chemical Engineering Science</i> , 1999 , 54, 2237-2246	4.4	175

342	Entropy effects during sorption of alkanes in zeolites. <i>Chemical Society Reviews</i> , 2002 , 31, 185-94	58.5	174
341	Using molecular simulations for screening of zeolites for separation of CO ₂ /CH ₄ mixtures. <i>Chemical Engineering Journal</i> , 2007 , 133, 121-131	14.7	171
340	Modelling issues in zeolite based separation processes. <i>Separation and Purification Technology</i> , 2003 , 33, 213-254	8.3	170
339	Fundamentals and selection of advanced Fischer-Tropsch reactors. <i>Applied Catalysis A: General</i> , 1999 , 186, 55-70	5.1	169
338	Mixed Metal-Organic Framework with Multiple Binding Sites for Efficient C ₂ H ₂ /CO Separation. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 4396-4400	16.4	169
337	High CO ₂ /N ₂ /O ₂ /CO separation in a chemically robust porous coordination polymer with low binding energy. <i>Chemical Science</i> , 2014 , 5, 660-666	9.4	166
336	Correlation Effects in Diffusion of CH ₄ /CF ₄ Mixtures in MFI Zeolite. A Study Linking MD Simulations with the Maxwell-Stefan Formulation. <i>Langmuir</i> , 2003 , 19, 7977-7988	4	166
335	Characterization of regimes and regime transitions in bubble columns by chaos analysis of pressure signals. <i>Chemical Engineering Science</i> , 1997 , 52, 4447-4459	4.4	165
334	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 8814-8820	3.8	160
333	Problems and pitfalls in the use of the Fick formulation for intraparticle diffusion. <i>Chemical Engineering Science</i> , 1993 , 48, 845-861	4.4	157
332	Microimaging of transient guest profiles to monitor mass transfer in nanoporous materials. <i>Nature Materials</i> , 2014 , 13, 333-43	27	152
331	The Maxwell-Stefan description of mixture diffusion in nanoporous crystalline materials. <i>Microporous and Mesoporous Materials</i> , 2014 , 185, 30-50	5.3	148
330	Insights into diffusion of gases in zeolites gained from molecular dynamics simulations. <i>Microporous and Mesoporous Materials</i> , 2008 , 109, 91-108	5.3	148
329	A computational study of CO ₂ , N ₂ , and CH ₄ adsorption in zeolites. <i>Adsorption</i> , 2007 , 13, 469-476	2.6	145
328	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5599-5600	16.4	145
327	Strategies for multiphase reactor selection. <i>Chemical Engineering Science</i> , 1994 , 49, 4029-4065	4.4	145
326	Gas holdup in slurry bubble columns: Effect of column diameter and slurry concentrations. <i>AIChE Journal</i> , 1997 , 43, 311-316	3.6	144
325	Influence of scale on the hydrodynamics of bubble columns operating in the churn-turbulent regime: experiments vs. Eulerian simulations. <i>Chemical Engineering Science</i> , 1999 , 54, 4903-4911	4.4	143

3 ²⁴	A model for gas holdup in bubble columns incorporating the influence of gas density on flow regime transitions. <i>Chemical Engineering Science</i> , 1991 , 46, 2491-2496	4.4	138
3 ²³	A rod-packing microporous hydrogen-bonded organic framework for highly selective separation of C ₂ H ₂ /CO ₂ at room temperature. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 574-7	16.4	137
3 ²²	Multiple solutions in reactive distillation for methyl tert-butyl ether synthesis. <i>Industrial & Engineering Chemistry Research</i> , 1993 , 32, 1706-1709	3.9	137
3 ²¹	Direct Observation of Xe and Kr Adsorption in a Xe-Selective Microporous Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2015 , 137, 7007-10	16.4	131
3 ²⁰	Mass transfer from Taylor bubbles rising in single capillaries. <i>Chemical Engineering Science</i> , 2005 , 60, 6430-6437	4.4	130
3 ¹⁹	Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and π -complexation. <i>Chemical Communications</i> , 2015 , 51, 2714-7	5.8	129
3 ¹⁸	Adsorption and diffusion of alkanes in CuBTC crystals investigated using infra-red microscopy and molecular simulations. <i>Microporous and Mesoporous Materials</i> , 2009 , 117, 22-32	5.3	129
3 ¹⁷	MASS AND ENERGY TRANSFER IN MULTICOMPONENT SYSTEMS. <i>Chemical Engineering Communications</i> , 1979 , 3, 201-275	2.2	128
3 ¹⁶	Ultrahigh and Selective SO Uptake in Inorganic Anion-Pillared Hybrid Porous Materials. <i>Advanced Materials</i> , 2017 , 29, 1606929	24	127
3 ¹⁵	High separation capacity and selectivity of C ₂ hydrocarbons over methane within a microporous metal-organic framework at room temperature. <i>Chemistry - A European Journal</i> , 2012 , 18, 1901-4	4.8	127
3 ¹⁴	Gas holdup in bubble column reactors operating in the churn-turbulent flow regime. <i>AIChE Journal</i> , 1996 , 42, 2627-2634	3.6	127
3 ¹³	A comparison of the CO ₂ capture characteristics of zeolites and metal-organic frameworks. <i>Separation and Purification Technology</i> , 2012 , 87, 120-126	8.3	126
3 ¹²	Significant Enhancement of C ₂ H ₂ /C ₂ H ₄ Separation by a Photochromic Diarylethene Unit: A Temperature- and Light-Responsive Separation Switch. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 7900-7906	16.4	123
3 ¹¹	Carbon Dioxide Capture from Air Using Amine-Grafted Porous Polymer Networks. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 4057-4061	3.8	123
3 ¹⁰	Rise velocity of a swarm of large gas bubbles in liquids. <i>Chemical Engineering Science</i> , 1999 , 54, 171-183	4.4	122
3 ⁰⁹	Molecular Sieving of Ethane from Ethylene through the Molecular Cross-Section Size Differentiation in Gallate-based Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 16020-16025	16.4	121
3 ⁰⁸	Pore-Space-Partition-Enabled Exceptional Ethane Uptake and Ethane-Selective Ethane-Ethylene Separation. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2222-2227	16.4	120
3 ⁰⁷	A microporous lanthanide-tricarboxylate framework with the potential for purification of natural gas. <i>Chemical Communications</i> , 2012 , 48, 10856-8	5.8	120

306	Eulerian simulations of bubbling behaviour in gas-solid fluidised beds. <i>Computers and Chemical Engineering</i> , 1998 , 22, S299-S306	4	119
305	The Darken Relation for Multicomponent Diffusion in Liquid Mixtures of Linear Alkanes: An Investigation Using Molecular Dynamics (MD) Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 6939-6947	3.9	119
304	Methane storage mechanism in the metal-organic framework Cu ₃ (btc) ₂ : An in situ neutron diffraction study. <i>Microporous and Mesoporous Materials</i> , 2010 , 136, 50-58	5.3	117
303	Induced Fit of C H in a Flexible MOF Through Cooperative Action of Open Metal Sites. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 8515-8519	16.4	116
302	Hydrogen bonding effects in adsorption of water-alcohol mixtures in zeolites and the consequences for the characteristics of the Maxwell-Stefan diffusivities. <i>Langmuir</i> , 2010 , 26, 10854-67	4	115
301	Diffusion of alkane mixtures in zeolites: validating the maxwell-stefan formulation using MD simulations. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 6386-96	3.4	115
300	Segregation effects in adsorption of CO ₂ -containing mixtures and their consequences for separation selectivities in cage-type zeolites. <i>Separation and Purification Technology</i> , 2008 , 61, 414-423	8.3	114
299	Comparison of equilibrium stage and nonequilibrium stage models for reactive distillation. <i>Chemical Engineering Journal</i> , 2000 , 76, 33-47	14.7	113
298	A Chemically Stable Hofmann-Type Metal-Organic Framework with Sandwich-Like Binding Sites for Benchmark Acetylene Capture. <i>Advanced Materials</i> , 2020 , 32, e1908275	24	111
297	Two-Dimensional Covalent Organic Frameworks for Carbon Dioxide Capture through Channel-Wall Functionalization. <i>Angewandte Chemie</i> , 2015 , 127, 3029-3033	3.6	111
296	Size, structure and dynamics of large bubbles in a two-dimensional slurry bubble column. <i>Chemical Engineering Science</i> , 1996 , 51, 4619-4629	4.4	111
295	Three-phase Eulerian simulations of bubble column reactors operating in the churn-turbulent regime: a scale up strategy. <i>Chemical Engineering Science</i> , 2000 , 55, 3275-3286	4.4	110
294	Unified Maxwell-Stefan description of binary mixture diffusion in micro- and meso-porous materials. <i>Chemical Engineering Science</i> , 2009 , 64, 3159-3178	4.4	106
293	Natural gas purification using a porous coordination polymer with water and chemical stability. <i>Inorganic Chemistry</i> , 2015 , 54, 4279-84	5.1	105
292	A microporous six-fold interpenetrated hydrogen-bonded organic framework for highly selective separation of C ₂ H ₄ /C ₂ H ₆ . <i>Chemical Communications</i> , 2014 , 50, 13081-4	5.8	105
291	CO ₂ /CH ₄ , CH ₄ /H ₂ and CO ₂ /CH ₄ /H ₂ separations at high pressures using Mg ₂ (dobdc). <i>Microporous and Mesoporous Materials</i> , 2012 , 151, 481-487	5.3	103
290	Methodologies for evaluation of metal-organic frameworks in separation applications. <i>RSC Advances</i> , 2015 , 5, 52269-52295	3.7	102
289	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. <i>Chemical Engineering Journal</i> , 2002 , 88, 81-94	14.7	101

288	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 7727-7730	2.8	100
287	Enhanced Gas Uptake in a Microporous Metal-Organic Framework a Sorbate Induced-Fit Mechanism. <i>Journal of the American Chemical Society</i> , 2019 , 141, 17703-17712	16.4	94
286	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Short n-Alkanes in Faujasite. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 13481-13491	3.4	93
285	A Rod-Packing Microporous Hydrogen-Bonded Organic Framework for Highly Selective Separation of C ₂ H ₂ /CO ₂ at Room Temperature. <i>Angewandte Chemie</i> , 2015 , 127, 584-587	3.6	92
284	Modeling the occupancy dependence of diffusivities in zeolites. <i>Microporous and Mesoporous Materials</i> , 2004 , 76, 233-246	5.3	92
283	Design of the Reduction of Events with Darbepoetin alfa in Heart Failure (RED-HF): a Phase III, anaemia correction, morbidity-mortality trial. <i>European Journal of Heart Failure</i> , 2009 , 11, 795-801	12.3	88
282	Enhanced CO ₂ sorption and selectivity by functionalization of a NbO-type metal-organic framework with polarized benzothiadiazole moieties. <i>Chemical Communications</i> , 2014 , 50, 12105-8	5.8	86
281	Screening metal-organic frameworks for mixture separations in fixed-bed adsorbers using a combined selectivity/capacity metric. <i>RSC Advances</i> , 2017 , 7, 35724-35737	3.7	86
280	Selective Ethane/Ethylene Separation in a Robust Microporous Hydrogen-Bonded Organic Framework. <i>Journal of the American Chemical Society</i> , 2020 , 142, 633-640	16.4	86
279	Fluorocarbon adsorption in hierarchical porous frameworks. <i>Nature Communications</i> , 2014 , 5, 4368	17.4	85
278	Extraordinary Separation of Acetylene-Containing Mixtures with Microporous Metal-Organic Frameworks with Open O Donor Sites and Tunable Robustness through Control of the Helical Chain Secondary Building Units. <i>Chemistry - A European Journal</i> , 2016 , 22, 5676-83	4.8	85
277	A molecular dynamics investigation of the diffusion characteristics of cavity-type zeolites with 8-ring windows. <i>Microporous and Mesoporous Materials</i> , 2011 , 137, 83-91	5.3	84
276	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwell-Stefan theory. <i>Separation and Purification Technology</i> , 2000 , 21, 111-136	8.3	84
275	A robust Thiazole framework for highly efficient purification of CH ₄ from a CH ₄ /CH ₂ /CH ₂ mixture. <i>Nature Communications</i> , 2020 , 11, 3163	17.4	83
274	A Metal-Organic Framework with Suitable Pore Size and Specific Functional Sites for the Removal of Trace Propyne from Propylene. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 15183-15188	16.4	83
273	A metal-organic framework with suitable pore size and dual functionalities for highly efficient post-combustion CO ₂ capture. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 3128-3134	13	82
272	Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 11867-71	16.4	81
271	Uphill diffusion in multicomponent mixtures. <i>Chemical Society Reviews</i> , 2015 , 44, 2812-36	58.5	80

270	Thermosensitive gating effect and selective gas adsorption in a porous coordination nanocage. <i>Chemical Communications</i> , 2010 , 46, 7352-4	5.8	80
269	Assessing surface permeabilities from transient guest profiles in nanoporous host materials. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 3525-8	16.4	80
268	Hydrodynamics and mass transfer in bubble columns in operating in the churn-turbulent regime. <i>Industrial & Engineering Chemistry Process Design and Development</i> , 1981 , 20, 475-482		78
267	A cationic microporous metal-organic framework for highly selective separation of small hydrocarbons at room temperature. <i>Journal of Materials Chemistry A</i> , 2013 , 1, 9916	13	75
266	Separating xylene isomers by commensurate stacking of p-xylene within channels of MAF-X8. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 7774-8	16.4	75
265	Interpreting Unary, Binary, and Ternary Mixture Permeation Across a SAPO-34 Membrane with Loading-Dependent Maxwell-Stefan Diffusivities. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 5075-5082	3.8	75
264	Kr/Xe Separation over a Chabazite Zeolite Membrane. <i>Journal of the American Chemical Society</i> , 2016 , 138, 9791-4	16.4	75
263	A new metal-organic framework with potential for adsorptive separation of methane from carbon dioxide, acetylene, ethylene, and ethane established by simulated breakthrough experiments. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 2628	13	74
262	Tuning Gate-Opening of a Flexible Metal-Organic Framework for Ternary Gas Sieving Separation. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 22756-22762	16.4	73
261	Investigating the potential of MgMOF-74 membranes for CO ₂ capture. <i>Journal of Membrane Science</i> , 2011 , 377, 249-260	9.6	72
260	Analysis of Diffusion Limitation in the Alkylation of Benzene over H-ZSM-5 by Combining Quantum Chemical Calculations, Molecular Simulations, and a Continuum Approach. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 235-246	3.8	72
259	Modelling sieve tray hydraulics using computational fluid dynamics. <i>Chemical Engineering Journal</i> , 2000 , 77, 143-151	14.7	72
258	The accessibility of nitrogen sites makes a difference in selective CO ₂ adsorption of a family of isostructural metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 19417-19426	13	71
257	A stable metal-organic framework with suitable pore sizes and rich uncoordinated nitrogen atoms on the internal surface of micropores for highly efficient CO ₂ capture. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 7361-7367	13	69
256	Maxwell-Stefan modeling of slowing-down effects in mixed gas permeation across porous membranes. <i>Journal of Membrane Science</i> , 2011 , 383, 289-300	9.6	69
255	Assessing guest diffusivities in porous hosts from transient concentration profiles. <i>Physical Review Letters</i> , 2009 , 102, 065901	7.4	69
254	Efficient separation of ethylene from acetylene/ethylene mixtures by a flexible-robust metal-organic framework. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 18984-18988	13	68
253	Self-diffusivities in multicomponent mixtures in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 1891-1898	3.6	68

252	Investigating cluster formation in adsorption of CO ₂ , CH ₄ , and Ar in zeolites and metal organic frameworks at subcritical temperatures. <i>Langmuir</i> , 2010 , 26, 3981-92	4	67
251	Method for Analyzing Structural Changes of Flexible Metal-Organic Frameworks Induced by Adsorbates. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 19317-19327	3.8	67
250	An Ultramicroporous Metal-Organic Framework for High Sieving Separation of Propylene from Propane. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17795-17801	16.4	67
249	Adsorptive separation of CO ₂ /CH ₄ /CO gas mixtures at high pressures. <i>Microporous and Mesoporous Materials</i> , 2012 , 156, 217-223	5.3	66
248	An investigation of the characteristics of Maxwell-Stefan diffusivities of binary mixtures in silica nanopores. <i>Chemical Engineering Science</i> , 2009 , 64, 870-882	4.4	65
247	Mixture diffusion in zeolites studied by MAS PFG NMR and molecular simulation. <i>Microporous and Mesoporous Materials</i> , 2007 , 105, 124-131	5.3	65
246	CFD Simulations of Sieve Tray Hydrodynamics. <i>Chemical Engineering Research and Design</i> , 1999 , 77, 639-646	5.5	65
245	Separating mixtures by exploiting molecular packing effects in microporous materials. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 39-59	3.6	64
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