Rajamani Krishna

List of Publications by Year in Descending Order

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	Collaborative pore partition and pore surface fluorination within a metal‐organic framework for high-performance C2H2/CO2 separation. *Chemical Engineering Journal*, **2022**, 432, 134433	14.7	6
394	Comprehensive Pore Tuning in an Ultrastable Fluorinated Anion Cross-Linked Cage-Like MOF for Simultaneous Benchmark Propyne Recovery and Propylene Purification.. *Angewandte Chemie - International Edition*, **2022**,	16.4	3
393	Highlighting the Anti-Synergy between Adsorption and Diffusion in Cation-Exchanged Faujasite Zeolites.. *ACS Omega*, **2022**, 7, 13050-13056	3.9	1
392	Using the spreading pressure to inter-relate the characteristics of unary, binary and ternary mixture permeation across microporous membranes. *Journal of Membrane Science*, **2021**, 120049	9.6	3
391	Separation of propylene from propane and nitrogen by Ag(I)-doped nanoporous carbons obtained from hydrothermally treated lignin. *Diamond and Related Materials*, **2021**, 121, 108750	3.5	0
390	Highly selective gas separation by two isostructural boron cluster pillared MOFs. *Separation and Purification Technology*, **2021**, 120220	8.3	1
389	Synthesis of Cu(I) doped mesoporous carbon for selective capture of ethylene from reaction products of oxidative coupling of methane (OCM). *Microporous and Mesoporous Materials*, **2021**, 328, 111488	5.3	0
388	Efficient Purification of Ethylene from C Hydrocarbons with an CH/CH-Selective Metal-Organic Framework. *ACS Applied Materials & Interfaces*, **2021**, 13, 962-969	9.5	22
387	A stable metal‐organic framework with well-matched pore cavity for efficient acetylene separation. *AICHE Journal*, **2021**, 67, e17152	3.6	4
386	Synergistically enhance confined diffusion by continuum intersecting channels in zeolites. *Science Advances*, **2021**, 7,	14.3	11
385	A Rod-Packing Hydrogen-Bonded Organic Framework with Suitable Pore Confinement for Benchmark Ethane/Ethylene Separation. *Angewandte Chemie - International Edition*, **2021**, 60, 10304-10310	16.4	41
384	A Rod-Packing Hydrogen-Bonded Organic Framework with Suitable Pore Confinement for Benchmark Ethane/Ethylene Separation. *Angewandte Chemie*, **2021**, 133, 10392-10398	3.6	14
383	Thermal resistance effect on anomalous diffusion of molecules under confinement. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	4
382	Realization of Ethylene Production from Its Quaternary Mixture through Metal-Organic Framework Materials. *ACS Applied Materials & Interfaces*, **2021**, 13, 22514-22520	9.5	8
381	Optimal Pore Chemistry in an Ultramicroporous Metal‐Organic Framework for Benchmark Inverse CO2/C2H2 Separation. *Angewandte Chemie*, **2021**, 133, 17335-17341	3.6	5
380	Robust metal‐organic framework with multiple traps for trace Xe/Kr separation. *Science Bulletin*, **2021**, 66, 1073-1079	10.6	18
379	How Reliable Is the Ideal Adsorbed Solution Theory for the Estimation of Mixture Separation Selectivities in Microporous Crystalline Adsorbents?. *ACS Omega*, **2021**, 6, 15499-15513	3.9	4

378	Optimal Pore Chemistry in an Ultramicroporous Metal-Organic Framework for Benchmark Inverse CO /C H Separation. *Angewandte Chemie - International Edition*, **2021**, 60, 17198-17204	16.4	27
377	Propane-Trapping Ultramicroporous Metal-Organic Framework in the Low-Pressure Area toward the Purification of Propylene. *ACS Applied Materials & Interfaces*, **2021**, 13, 35990-35996	9.5	7
376	A robust heterometallic ultramicroporous MOF with ultrahigh selectivity for propyne/propylene separation. *Journal of Materials Chemistry A*, **2021**, 9, 2850-2856	13	11
375	High Adsorption Capacity and Selectivity of SO over CO in a Metal-Organic Framework. *Inorganic Chemistry*, **2021**, 60, 4-8	5.1	7
374	Ultrafine tuning of the pore size in zeolite A for efficient propyne removal from propylene. *Chinese Journal of Chemical Engineering*, **2021**, 37, 217-217	3.2	1
373	Constructing a robust gigantic drum-like hydrophobic [Co24U6] nanocage in a metal□organic framework for high-performance SO2 removal in humid conditions. *Journal of Materials Chemistry A* , **2021**, 9, 4075-4081	13	4
372	Robust 4d-5f Bimetal-Organic Framework for Efficient Removal of Trace SO from SO/CO and SO/CO/N Mixtures. *Inorganic Chemistry*, **2021**, 60, 1310-1314	5.1	5
371	A Robust Cage-Based Metal-Organic Framework Showing Ultrahigh SO Uptake for Efficient Removal of Trace SO from SO/CO and SO/CO/N Mixtures. *Inorganic Chemistry*, **2021**, 60, 3447-3451	5.1	6
370	Interpenetration Symmetry Control Within Ultramicroporous Robust Boron Cluster Hybrid MOFs for Benchmark Purification of Acetylene from Carbon Dioxide. *Angewandte Chemie*, **2021**, 133, 23047	3.6	4
369	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	16.4	17
368	A robust metal-organic framework showing two distinct pores for effective separation of xenon and krypton. *Microporous and Mesoporous Materials*, **2021**, 326, 111350	5.3	1
367	Efficient propyne/propadiene separation by microporous crystalline physiadsorbents. *Nature Communications*, **2021**, 12, 5768	17.4	9
366	Metal-Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation.. *Journal of the American Chemical Society*, **2021**,	16.4	25
365	Using Molecular Simulations to Unravel the Benefits of Characterizing Mixture Permeation in Microporous Membranes in Terms of the Spreading Pressure. *ACS Omega*, **2020**, 5, 32769-32780	3.9	3
364	Simultaneous interlayer and intralayer space control in two-dimensional metal-organic frameworks for acetylene/ethylene separation. *Nature Communications*, **2020**, 11, 6259	17.4	23
363	A Chemically Stable Hofmann-Type Metal-Organic Framework with Sandwich-Like Binding Sites for Benchmark Acetylene Capture. *Advanced Materials*, **2020**, 32, e1908275	24	111
362	Dependence of zeolite topology on alkane diffusion inside diverse channels. *AICHE Journal*, **2020**, 66, e16269	3.6	6
361	A robust Th-azole framework for highly efficient purification of CH from a CH/CH/CH mixture. *Nature Communications*, **2020**, 11, 3163	17.4	83

360	Using transient breakthrough experiments for screening of adsorbents for separation of C2H4/CO2 mixtures. *Separation and Purification Technology*, **2020**, 241, 116706	8.3	16
359	Separation of ethane-ethylene and propane-propylene by Ag(I) doped and sulfurized microporous carbon. *Microporous and Mesoporous Materials*, **2020**, 299, 110099	5.3	21
358	Rational Design of Microporous MOFs with Anionic Boron Cluster Functionality and Cooperative Dihydrogen Binding Sites for Highly Selective Capture of Acetylene. *Angewandte Chemie*, **2020**, 132, 17817-17822	3.6	11
357	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	16.4	44
356	Highlighting Thermodynamic Coupling Effects in the Immersion Precipitation Process for Formation of Polymeric Membranes. *ACS Omega*, **2020**, 5, 2819-2828	3.9	1
355	Mixed Metal□Organic Framework with Multiple Binding Sites for Efficient C2H2/CO2 Separation. *Angewandte Chemie*, **2020**, 132, 4426-4430	3.6	32
354	Pore-Space-Partition-Enabled Exceptional Ethane Uptake and Ethane-Selective Ethane-Ethylene Separation. *Journal of the American Chemical Society*, **2020**, 142, 2222-2227	16.4	120
353	Understanding How Ligand Functionalization Influences CO and N Adsorption in a Sodalite Metal-Organic Framework. *Chemistry of Materials*, **2020**, 32,	9.6	7
352	An Ultramicroporous Metal-Organic Framework for High Sieving Separation of Propylene from Propane. *Journal of the American Chemical Society*, **2020**, 142, 17795-17801	16.4	67
351	A multifunctional double walled zirconium metal□organic framework: high performance for CO2 adsorption and separation and detecting explosives in the aqueous phase. *Journal of Materials Chemistry A*, **2020**, 8, 17106-17112	13	11
350	Mixed Metal-Organic Framework with Multiple Binding Sites for Efficient C H /CO Separation. *Angewandte Chemie - International Edition*, **2020**, 59, 4396-4400	16.4	169
349	Microporous Metal-Organic Framework with a Completely Reversed Adsorption Relationship for C Hydrocarbons at Room Temperature. *ACS Applied Materials & Interfaces*, **2020**, 12, 6105-6111	9.5	41
348	Selective Ethane/Ethylene Separation in a Robust Microporous Hydrogen-Bonded Organic Framework. *Journal of the American Chemical Society*, **2020**, 142, 633-640	16.4	86
347	Metrics for Evaluation and Screening of Metal-Organic Frameworks for Applications in Mixture Separations. *ACS Omega*, **2020**, 5, 16987-17004	3.9	15
346	Boosting Selective Adsorption of Xe over Kr by Double-Accessible Open-Metal Site in Metal-Organic Framework: Experimental and Theoretical Research. *Inorganic Chemistry*, **2020**, 59, 11793-11800	5.1	23
345	Water/Alcohol Mixture Adsorption in Hydrophobic Materials: Enhanced Water Ingress Caused by Hydrogen Bonding. *ACS Omega*, **2020**, 5, 28393-28402	3.9	4
344	Tuning Gate-Opening of a Flexible Metal-Organic Framework for Ternary Gas Sieving Separation. *Angewandte Chemie - International Edition*, **2020**, 59, 22756-22762	16.4	73
343	Tuning Gate-Opening of a Flexible Metal□Organic Framework for Ternary Gas Sieving Separation. *Angewandte Chemie*, **2020**, 132, 22944-22950	3.6	21

342	Using Molecular Simulations for Elucidation of Thermodynamic Nonidealities in Adsorption of CO-Containing Mixtures in NaX Zeolite. *ACS Omega*, **2020**, 5, 20535-20542	3.9	5
341	Constructing redox-active microporous hydrogen-bonded organic framework by imide-functionalization: Photochromism, electrochromism, and selective adsorption of C2H2 over CO2. *Chemical Engineering Journal*, **2020**, 383, 123117	14.7	22
340	Elucidation of Selectivity Reversals for Binary Mixture Adsorption in Microporous Adsorbents. *ACS Omega*, **2020**, 5, 9031-9040	3.9	10
339	Enhancing C2H2/C2H4 separation by incorporating low-content sodium in covalent organic frameworks. *Inorganic Chemistry Frontiers*, **2019**, 6, 2921-2926	6.8	17
338	Highlighting Thermodynamic Coupling Effects in Alcohol/Water Pervaporation across Polymeric Membranes. *ACS Omega*, **2019**, 4, 15255-15264	3.9	5
337	A metal□rganic framework with suitable pore size and dual functionalities for highly efficient post-combustion CO2 capture. *Journal of Materials Chemistry A*, **2019**, 7, 3128-3134	13	82
336	Elucidating Traffic Junction Effects in MFI Zeolite Using Kinetic Monte Carlo Simulations. *ACS Omega*, **2019**, 4, 10761-10766	3.9	2
335	Highlighting non-idealities in C2H4/CO2 mixture adsorption in 5A zeolite. *Separation and Purification Technology*, **2019**, 227, 115730	8.3	15
334	Thermodynamic Insights into the Characteristics of Unary and Mixture Permeances in Microporous Membranes. *ACS Omega*, **2019**, 4, 9512-9521	3.9	7
333	Dual Strategic Approach to Prepare Defluorinated Triazole-Embedded Covalent Triazine Frameworks with High Gas Uptake Performance. *Chemistry of Materials*, **2019**, 31, 3929-3940	9.6	22
332	Robust Microporous Metal□rganic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. *Angewandte Chemie*, **2019**, 131, 10315-10320	3.6	12
331	Induced Fit of C2H2 in a Flexible MOF Through Cooperative Action of Open Metal Sites. *Angewandte Chemie*, **2019**, 131, 8603	3.6	
330	Robust Microporous Metal-Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. *Angewandte Chemie - International Edition*, **2019**, 58, 10209-10214	16.4	45
329	Induced Fit of C H in a Flexible MOF Through Cooperative Action of Open Metal Sites. *Angewandte Chemie - International Edition*, **2019**, 58, 8515-8519	16.4	116
328	Water-Stable Europium 1,3,6,8-Tetrakis(4-carboxylphenyl)pyrene Framework for Efficient CH/CO Separation. *Inorganic Chemistry*, **2019**, 58, 5089-5095	5.1	44
327	Pore Space Partition within a Metal-Organic Framework for Highly Efficient CH/CO Separation. *Journal of the American Chemical Society*, **2019**, 141, 4130-4136	16.4	190
326	Highlighting the Influence of Thermodynamic Coupling on Kinetic Separations with Microporous Crystalline Materials. *ACS Omega*, **2019**, 4, 3409-3419	3.9	8
325	Thermodynamically Consistent Methodology for Estimation of Diffusivities of Mixtures of Guest Molecules in Microporous Materials. *ACS Omega*, **2019**, 4, 13520-13529	3.9	5

324	Maxwell-Stefan modelling of mixture desorption kinetics in microporous crystalline materials. *Separation and Purification Technology*, **2019**, 229, 115790	8.3	2
323	Enhanced Gas Uptake in a Microporous Metal-Organic Framework a Sorbate Induced-Fit Mechanism. *Journal of the American Chemical Society*, **2019**, 141, 17703-17712	16.4	94
322	Microporous Metal-Organic Framework with Dual Functionalities for Efficient Separation of Acetylene from Light Hydrocarbon Mixtures. *ACS Sustainable Chemistry and Engineering*, **2019**, 7,	8.3	39
321	Elucidation and characterization of entropy effects in mixture separations with micro-porous crystalline adsorbents. *Separation and Purification Technology*, **2019**, 215, 227-241	8.3	10
320	Diffusing uphill with James Clerk Maxwell and Josef Stefan. *Chemical Engineering Science*, **2019**, 195, 851-880	4.4	17
319	Newly designed 1,2,3-triazole functionalized covalent triazine frameworks with exceptionally high uptake capacity for both CO2 and H2. *Journal of Materials Chemistry A*, **2019**, 7, 1055-1068	13	34
318	Preparation of benzodiimidazole-containing covalent triazine frameworks for enhanced selective CO2 capture and separation. *Microporous and Mesoporous Materials*, **2019**, 276, 213-222	5.3	13
317	Dynamic Adsorption of CO/N on Cation-Exchanged Chabazite SSZ-13: A Breakthrough Analysis. *ACS Applied Materials & Interfaces*, **2018**, 10, 14287-14291	9.5	11
316	Adjusting the proportions of extra-framework K+ and Cs+ cations to construct a molecular gate on ZK-5 for CO2 removal. *Microporous and Mesoporous Materials*, **2018**, 268, 50-57	5.3	13
315	The Maxwell–Stefan description of mixture permeation across nanoporous graphene membranes. *Chemical Engineering Research and Design*, **2018**, 133, 316-325	5.5	11
314	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	14.7	41
313	Beyond Crystal Engineering: Significant Enhancement of CH/CO Separation by Constructing Composite Material. *Inorganic Chemistry*, **2018**, 57, 3679-3682	5.1	31
312	Highlighting the origins and consequences of thermodynamic non-idealities in mixture separations using zeolites and metal-organic frameworks. *Microporous and Mesoporous Materials*, **2018**, 267, 274-292	5.3	21
311	Using Molecular Dynamics simulations for elucidation of molecular traffic in ordered crystalline microporous materials. *Microporous and Mesoporous Materials*, **2018**, 258, 151-169	5.3	14
310	A Maxwell-Stefan-Glueckauf description of transient mixture uptake in microporous adsorbents. *Separation and Purification Technology*, **2018**, 191, 392-399	8.3	9
309	Nickel-4'-(3,5-dicarboxyphenyl)-2,2',6',2?-terpyridine Framework: Efficient Separation of Ethylene from Acetylene/Ethylene Mixtures with a High Productivity. *Inorganic Chemistry*, **2018**, 57, 9489-9494	5.1	22
308	Enhancing Gas Sorption and Separation Performance via Bisbenzimidazole Functionalization of Highly Porous Covalent Triazine Frameworks. *ACS Applied Materials & Interfaces*, **2018**, 10, 26678-26686	9.5	36
307	Investigating the non-idealities in adsorption of CO2-bearing mixtures in cation-exchanged zeolites. *Separation and Purification Technology*, **2018**, 206, 208-217	8.3	24

306	Methodologies for screening and selection of crystalline microporous materials in mixture separations. *Separation and Purification Technology*, **2018**, 194, 281-300	8.3	58
305	Alkane/alkene mixture diffusion in silicalite-1 studied by MAS PFG NMR. *Microporous and Mesoporous Materials*, **2018**, 257, 128-134	5.3	19
304	MIL-100Cr with open Cr sites for a record NO capture. *Chemical Communications*, **2018**, 54, 14061-14064	5.8	19
303	Occupancy Dependency of Maxwell-Stefan Diffusivities in Ordered Crystalline Microporous Materials. *ACS Omega*, **2018**, 3, 15743-15753	3.9	10
302	Enhancing CO Adsorption and Separation Properties of Aluminophosphate Zeolites by Isomorphous Heteroatom Substitutions. *ACS Applied Materials & Interfaces*, **2018**, 10, 43570-43577	9.5	20
301	A Metal-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	16.4	83
300	A Metal□Organic Framework with Suitable Pore Size and Specific Functional Sites for the Removal of Trace Propyne from Propylene. *Angewandte Chemie*, **2018**, 130, 15403-15408	3.6	30
299	Molecular Sieving of Ethane from Ethylene through the Molecular Cross-Section Size Differentiation in Gallate-based Metal□Organic Frameworks. *Angewandte Chemie*, **2018**, 130, 16252-16257	3.6	47
298	Molecular Sieving of Ethane from Ethylene through the Molecular Cross-Section Size Differentiation in Gallate-based Metal-Organic Frameworks. *Angewandte Chemie - International Edition*, **2018**, 57, 16020-16025	16.4	121
297	Molecular sieving of ethylene from ethane using a rigid metal-organic framework. *Nature Materials*, **2018**, 17, 1128-1133	27	326
296	Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. *Science*, **2018**, 362, 443-446	33.3	478
295	Exploring the Effect of Ligand-Originated MOF Isomerism and Methoxy Group Functionalization on Selective Acetylene/Methane and Carbon Dioxide/Methane Adsorption Properties in Two NbO-Type MOFs. *ACS Applied Materials & Interfaces*, **2018**, 10, 20559-20568	9.5	40
294	Screening metal-organic frameworks for separation of pentane isomers. *Physical Chemistry Chemical Physics*, **2017**, 19, 8380-8387	3.6	14
293	A New Isomeric Porous Coordination Framework Showing Single-Crystal to Single-Crystal Structural Transformation and Preferential Adsorption of 1,3-Butadiene from C4 Hydrocarbons. *Crystal Growth and Design*, **2017**, 17, 2166-2171	3.5	22
292	Highlighting diffusional coupling effects in zeolite catalyzed reactions by combining the Maxwell□Stefan and Langmuir□Hinshelwood formulations. *Reaction Chemistry and Engineering*, **2017**, 2, 324-336	4.9	6
291	Significant Enhancement of C2H2/C2H4 Separation by a Photochromic Diarylethene Unit: A Temperature- and Light-Responsive Separation Switch. *Angewandte Chemie*, **2017**, 129, 8008-8014	3.6	22
290	Significant Enhancement of C H /C H Separation by a Photochromic Diarylethene Unit: A Temperature- and Light-Responsive Separation Switch. *Angewandte Chemie - International Edition*, **2017**, 56, 7900-7906	16.4	123
289	Ultrahigh and Selective SO Uptake in Inorganic Anion-Pillared Hybrid Porous Materials. *Advanced Materials*, **2017**, 29, 1606929	24	127

288	Flexible-Robust Metal-Organic Framework for Efficient Removal of Propyne from Propylene. *Journal of the American Chemical Society*, **2017**, 139, 7733-7736	16.4	177
287	Highlighting multiplicity in the Gilliland solution to the Maxwell-Stefan equations describing diffusion distillation. *Chemical Engineering Science*, **2017**, 164, 63-70	4.4	4
286	Pre-design and synthesis of a five-fold interpenetrated pcu-type porous coordination polymer and its CO2/CO separation. *CrystEngComm*, **2017**, 19, 6927-6931	3.3	6
285	Highly selective adsorption of p-xylene over other C aromatic hydrocarbons by Co-CUK-1: a combined experimental and theoretical assessment. *Dalton Transactions*, **2017**, 46, 16096-16101	4.3	14
284	Resolving steady-state multiplicities for diffusion with surface chemical reaction by invoking the Prigogine principle of minimum entropy production. *Chemical Engineering Research and Design*, **2017**, 128, 231-239	5.5	1
283	Two Analogous Polyhedron-Based MOFs with High Density of Lewis Basic Sites and Open Metal Sites: Significant CO Capture and Gas Selectivity Performance. *ACS Applied Materials & Interfaces*, **2017**, 9, 32820-32828	9.5	38
282	Screening metal□rganic frameworks for mixture separations in fixed-bed adsorbers using a combined selectivity/capacity metric. *RSC Advances*, **2017**, 7, 35724-35737	3.7	86
281	Efficient separation of ethylene from acetylene/ethylene mixtures by a flexible-robust metal□rganic framework. *Journal of Materials Chemistry A*, **2017**, 5, 18984-18988	13	68
280	Commensurate-incommensurate adsorption and diffusion in ordered crystalline microporous materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 20320-20337	3.6	15
279	An Ideal Molecular Sieve for Acetylene Removal from Ethylene with Record Selectivity and Productivity. *Advanced Materials*, **2017**, 29, 1704210	24	213
278	Fine-tuning optimal porous coordination polymers using functional alkyl groups for CH4 purification. *Journal of Materials Chemistry A*, **2017**, 5, 17874-17880	13	23
277	Using the Maxwell-Stefan formulation for highlighting the influence of interspecies (1□2) friction on binary mixture permeation across microporous and polymeric membranes. *Journal of Membrane Science*, **2017**, 540, 261-276	9.6	25
276	Flow Enhancement of Shear-Thinning Liquids in Capillaries Subjected to Longitudinal Vibrations. *Chemie-Ingenieur-Technik*, **2017**, 89, 1360-1366	0.8	3
275	Potential of microporous metal□rganic frameworks for separation of hydrocarbon mixtures. *Energy and Environmental Science*, **2016**, 9, 3612-3641	35.4	428
274	Highlighting coupling effects in ionic diffusion. *Chemical Engineering Research and Design*, **2016**, 114, 1-12	5.5	4
273	Describing mixture permeation across polymeric membranes by a combination of Maxwell-Stefan and Flory-Huggins models. *Polymer*, **2016**, 103, 124-131	3.9	19
272	Describing diffusion in fluid mixtures at elevated pressures by combining the Maxwell□Stefan formulation with an equation of state. *Chemical Engineering Science*, **2016**, 153, 174-187	4.4	16
271	A versatile synthesis of metal□rganic framework-derived porous carbons for CO2 capture and gas separation. *Journal of Materials Chemistry A*, **2016**, 4, 19095-19106	13	38

270	Redox-Active Metal-Organic Composites for Highly Selective Oxygen Separation Applications. *Advanced Materials*, **2016**, 28, 3572-7	24	37
269	Tracing the origins of transient overshoots for binary mixture diffusion in microporous crystalline materials. *Physical Chemistry Chemical Physics*, **2016**, 18, 15482-95	3.6	27
268	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, 3022-30	16.4	278
267	Light Hydrocarbon Adsorption Mechanisms in Two Calcium-Based Microporous Metal Organic Frameworks. *Chemistry of Materials*, **2016**, 28, 1636-1646	9.6	61
266	Adsorptive separation of C2/C3/C4-hydrocarbons on a flexible Cu-MOF: The influence of temperature, chain length and bonding character. *Microporous and Mesoporous Materials*, **2016**, 224, 392-399	5.3	15
265	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	13	63
264	High acetylene/ethylene separation in a microporous zinc(II) metal-organic framework with low binding energy. *Chemical Communications*, **2016**, 52, 1166-9	5.8	57
263	Flexible Metal□Organic Frameworks with Discriminatory Gate-Opening Effect for the Separation of Acetylene from Ethylene/Acetylene Mixtures. *European Journal of Inorganic Chemistry*, **2016**, 2016, 4457-4462	2.3	32
262	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. *Chemistry - A European Journal*, **2016**, 22, 5676-83	4.8	85
261	Bimodal Functionality in a Porous Covalent Triazine Framework by Rational Integration of an Electron-Rich and -Deficient Pore Surface. *Chemistry - A European Journal*, **2016**, 22, 4931-7	4.8	30
260	Investigating the Validity of the Knudsen Diffusivity Prescription for Mesoporous and Macroporous Materials. *Industrial & Engineering Chemistry Research*, **2016**, 55, 4749-4759	3.9	18
259	Diffusing uphill with James Clerk Maxwell and Josef Stefan. *Current Opinion in Chemical Engineering* , **2016**, 12, 106-119	5.4	17
258	Highlighting Diffusional Coupling Effects in Ternary Liquid Extraction and Comparisons with Distillation. *Industrial & Engineering Chemistry Research*, **2016**, 55, 1053-1063	3.9	8
257	Pore chemistry and size control in hybrid porous materials for acetylene capture from ethylene. *Science*, **2016**, 353, 141-4	33.3	783
256	Harnessing Lewis acidic open metal sites of metal-organic frameworks: the foremost route to achieve highly selective benzene sorption over cyclohexane. *Chemical Communications*, **2016**, 52, 8215-8	5.8	62
255	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, 5678-84	16.4	351
254	Two heterovalent copper□organic frameworks with multiple secondary building units: high performance for gas adsorption and separation and I2 sorption and release. *Journal of Materials Chemistry A*, **2016**, 4, 15081-15087	13	40
253	A Porous Zirconium-Based Metal-Organic Framework with the Potential for the Separation of Butene Isomers. *Chemistry - A European Journal*, **2016**, 22, 14988-14997	4.8	46

252	Kr/Xe Separation over a Chabazite Zeolite Membrane. *Journal of the American Chemical Society*, **2016**, 138, 9791-4	16.4	75
251	Nitrogen-rich microporous carbons for highly selective separation of light hydrocarbons. *Journal of Materials Chemistry A*, **2016**, 4, 13957-13966	13	43
250	Separation of polar compounds using a flexible metal-organic framework. *Chemical Communications*, **2015**, 51, 8421-4	5.8	32
249	Uphill diffusion in multicomponent mixtures. *Chemical Society Reviews*, **2015**, 44, 2812-36	58.5	80
248	Separation of benzene from mixtures with water, methanol, ethanol, and acetone: highlighting hydrogen bonding and molecular clustering influences in CuBTC. *Physical Chemistry Chemical Physics*, **2015**, 17, 20114-24	3.6	13
247	Hydroquinone and Quinone-Grafted Porous Carbons for Highly Selective CO2 Capture from Flue Gases and Natural Gas Upgrading. *Environmental Science & Technology*, **2015**, 49, 9364-73	10.3	39
246	Exploiting Framework Flexibility of a Metal-Organic Framework for Selective Adsorption of Styrene over Ethylbenzene. *Inorganic Chemistry*, **2015**, 54, 4403-8	5.1	44
245	Natural gas purification using a porous coordination polymer with water and chemical stability. *Inorganic Chemistry*, **2015**, 54, 4279-84	5.1	105
244	Exceptional Hydrophobicity of a Large-Pore Metal-Organic Zeolite. *Journal of the American Chemical Society*, **2015**, 137, 7217-23	16.4	214
243	The accessibility of nitrogen sites makes a difference in selective CO2 adsorption of a family of isostructural metal□organic frameworks. *Journal of Materials Chemistry A*, **2015**, 3, 19417-19426	13	71
242	A □electron deficient diaminotriazine functionalized MOF for selective sorption of benzene over cyclohexane. *Chemical Communications*, **2015**, 51, 15386-9	5.8	56
241	Entropic separations of mixtures of aromatics by selective face-to-face molecular stacking in one-dimensional channels of metal-organic frameworks and zeolites. *ChemPhysChem*, **2015**, 16, 532-5	3.2	15
240	Potential of metal-organic frameworks for separation of xenon and krypton. *Accounts of Chemical Research*, **2015**, 48, 211-9	24.3	259
239	Evaluation of procedures for estimation of the isosteric heat of adsorption in microporous materials. *Chemical Engineering Science*, **2015**, 123, 191-196	4.4	22
238	Separating mixtures by exploiting molecular packing effects in microporous materials. *Physical Chemistry Chemical Physics*, **2015**, 17, 39-59	3.6	64
237	A rod-packing microporous hydrogen-bonded organic framework for highly selective separation of C2H2/CO2 at room temperature. *Angewandte Chemie - International Edition*, **2015**, 54, 574-7	16.4	137
236	Adsorptive Separation of Acetylene from Light Hydrocarbons by Mesoporous Iron Trimesate MIL-100(Fe). *Chemistry - A European Journal*, **2015**, 21, 18431-8	4.8	45
235	Entropic separation of styrene/ethylbenzene mixtures by exploitation of subtle differences in molecular configurations in ordered crystalline nanoporous adsorbents. *Langmuir*, **2015**, 31, 3771-8	4	40

234	Direct Observation of Xe and Kr Adsorption in a Xe-Selective Microporous Metal-Organic Framework. *Journal of the American Chemical Society*, **2015**, 137, 7007-10	16.4	131
233	Microporous metal-organic framework with dual functionalities for highly efficient removal of acetylene from ethylene/acetylene mixtures. *Nature Communications*, **2015**, 6, 7328	17.4	326
232	Tailor-Made Pore Surface Engineering in Covalent Organic Frameworks: Systematic Functionalization for Performance Screening. *Journal of the American Chemical Society*, **2015**, 137, 7079-82	16.4	264
231	Methodologies for evaluation of metal□organic frameworks in separation applications. *RSC Advances*, **2015**, 5, 52269-52295	3.7	102
230	Polyfuran-Derived Microporous Carbons for Enhanced Adsorption of CO□and CH□*Langmuir*, **2015**, 31, 9845-52	4	27
229	Serpentine diffusion trajectories and the Ouzo effect in partially miscible ternary liquid mixtures. *Physical Chemistry Chemical Physics*, **2015**, 17, 27428-36	3.6	18
228	Nitrogen-doped porous carbons for highly selective CO2 capture from flue gases and natural gas upgrading. *Materials Today Communications*, **2015**, 4, 156-165	2.5	28
227	A combined theoretical and experimental analysis on transient breakthroughs of C2H6/C2H4 in fixed beds packed with ZIF-7. *Microporous and Mesoporous Materials*, **2015**, 208, 55-65	5.3	48
226	Utilizing transient breakthroughs for evaluating the potential of Kureha carbon for CO2 capture. *Chemical Engineering Journal*, **2015**, 269, 135-147	14.7	20
225	Selective Adsorption of Water from Mixtures with 1-Alcohols by Exploitation of Molecular Packing Effects in CuBTC. *Journal of Physical Chemistry C*, **2015**, 119, 3658-3666	3.8	23
224	A stable metal□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	13	69
223	Two-Dimensional Covalent Organic Frameworks for Carbon Dioxide Capture through Channel-Wall Functionalization. *Angewandte Chemie*, **2015**, 127, 3029-3033	3.6	111
222	A Rod-Packing Microporous Hydrogen-Bonded Organic Framework for Highly Selective Separation of C2H2/CO2 at Room Temperature. *Angewandte Chemie*, **2015**, 127, 584-587	3.6	92
221	Two-dimensional covalent organic frameworks for carbon dioxide capture through channel-wall functionalization. *Angewandte Chemie - International Edition*, **2015**, 54, 2986-90	16.4	441
220	Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and □complexation. *Chemical Communications*, **2015**, 51, 2714-7	5.8	129
219	Reprint of: Transient breakthroughs of CO 2 /CH 4 and C 3 H 6 /C 3 H 8 mixtures in fixed beds packed with Ni-MOF-74. *Chemical Engineering Science*, **2015**, 124, 109-117	4.4	24
218	A microporous metal-organic framework with rare lvt topology for highly selective C2H2/C2H4 separation at room temperature. *Chemical Communications*, **2015**, 51, 5610-3	5.8	54
217	The Maxwell□tefan description of mixture diffusion in nanoporous crystalline materials. *Microporous and Mesoporous Materials*, **2014**, 185, 30-50	5.3	148

216	High CO2/N2/O2/CO separation in a chemically robust porous coordination polymer with low binding energy. *Chemical Science*, **2014**, 5, 660-666	9.4	166
215	Microimaging of transient guest profiles to monitor mass transfer in nanoporous materials. *Nature Materials*, **2014**, 13, 333-43	27	152
214	A new metal□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	13	74
213	Transient breakthroughs of CO2/CH4 and C3H6/C3H8 mixtures in fixed beds packed with Ni-MOF-74. *Chemical Engineering Science*, **2014**, 117, 407-415	4.4	41
212	A new MOF-5 homologue for selective separation of methane from C2 hydrocarbons at room temperature. *APL Materials*, **2014**, 2, 124102	5.7	27
211	Separating Xylene Isomers by Commensurate Stacking of p-Xylene within Channels of MAF-X8. *Angewandte Chemie*, **2014**, 126, 7908-7912	3.6	10
210	A microporous six-fold interpenetrated hydrogen-bonded organic framework for highly selective separation of C2H4/C2H6. *Chemical Communications*, **2014**, 50, 13081-4	5.8	105
209	Enhanced CO2 sorption and selectivity by functionalization of a NbO-type metal-organic framework with polarized benzothiadiazole moieties. *Chemical Communications*, **2014**, 50, 12105-8	5.8	86
208	The adsorption and simulated separation of light hydrocarbons in isoreticular metal-organic frameworks based on dendritic ligands with different aliphatic side chains. *Chemistry - A European Journal*, **2014**, 20, 9073-80	4.8	23
207	Highly selective separation of small hydrocarbons and carbon dioxide in a metal□organic framework with open copper(II) coordination sites. *RSC Advances*, **2014**, 4, 23058	3.7	31
206	Utilizing the Gate-Opening Mechanism in ZIF-7 for Adsorption Discrimination between N2O and CO2. *Journal of Physical Chemistry C*, **2014**, 118, 17831-17837	3.8	40
205	Uncommon Synergy between Adsorption and Diffusion of Hexane Isomer Mixtures in MFI Zeolite Induced by Configurational Entropy Effects. *Journal of Physical Chemistry C*, **2014**, 118, 2660-2665	3.8	32
204	Fluorocarbon adsorption in hierarchical porous frameworks. *Nature Communications*, **2014**, 5, 4368	17.4	85
203	A Sm□gs□bord of Separation Strategies Using Microporous Crystalline Materials□This lecture was delivered at CHEMCON 2013, held in Mumbai, India during 27□0 December 2013.View all notes. *Indian Chemical Engineer*, **2014**, 56, 147-174	1	1
202	Experiments and simulations on separating a CO2/CH4 mixture using K-KFI at low and high pressures. *Microporous and Mesoporous Materials*, **2014**, 184, 21-27	5.3	30
201	Introduction of □complexation into porous aromatic framework for highly selective adsorption of ethylene over ethane. *Journal of the American Chemical Society*, **2014**, 136, 8654-60	16.4	304
200	Strong influence of the H2 binding energy on the Maxwell□tefan diffusivity in NU-100, UiO-68, and IRMOF-16. *Microporous and Mesoporous Materials*, **2014**, 185, 190-196	5.3	7
199	Separating xylene isomers by commensurate stacking of p-xylene within channels of MAF-X8. *Angewandte Chemie - International Edition*, **2014**, 53, 7774-8	16.4	75

198	Highly selective water adsorption in a lanthanum metal-organic framework. *Chemistry - A European Journal*, **2014**, 20, 7922-5	4.8	48
197	Separation of hexane isomers in a metal-organic framework with triangular channels. *Science*, **2013**, 340, 960-4	33.3	490
196	Investigating the influence of diffusional coupling on mixture permeation across porous membranes. *Journal of Membrane Science*, **2013**, 430, 113-128	9.6	42
195	A cationic microporous metal□organic framework for highly selective separation of small hydrocarbons at room temperature. *Journal of Materials Chemistry A*, **2013**, 1, 9916	13	75
194	Low-energy regeneration and high productivity in a lanthanide-hexacarboxylate framework for high-pressure CO2-CH4-H2 separation. *Chemical Communications*, **2013**, 49, 6773-5	5.8	61
193	A microporous metal□organic framework assembled from an aromatic tetracarboxylate for H2 purification. *Journal of Materials Chemistry A*, **2013**, 1, 2543	13	59
192	Metal□Organic Framework with Functional Amide Groups for Highly Selective Gas Separation. *Crystal Growth and Design*, **2013**, 13, 2670-2674	3.5	61
191	Carbon Dioxide Capture from Air Using Amine-Grafted Porous Polymer Networks. *Journal of Physical Chemistry C*, **2013**, 117, 4057-4061	3.8	123
190	Influence of adsorption thermodynamics on guest diffusivities in nanoporous crystalline materials. *Physical Chemistry Chemical Physics*, **2013**, 15, 7994-8016	3.6	61
189	Expanded organic building units for the construction of highly porous metal-organic frameworks. *Chemistry - A European Journal*, **2013**, 19, 14886-94	4.8	60
188	A comparison of the CO2 capture characteristics of zeolites and metal□organic frameworks. *Separation and Purification Technology*, **2012**, 87, 120-126	8.3	126
187	Hindering effects in diffusion of CO2/CH4 mixtures in ZIF-8 crystals. *Journal of Membrane Science*, **2012**, 397-398, 87-91	9.6	58
186	CO2/CH4, CH4/H2 and CO2/CH4/H2 separations at high pressures using Mg2(dobdc). *Microporous and Mesoporous Materials*, **2012**, 151, 481-487	5.3	103
185	Adsorptive separation of CO2/CH4/CO gas mixtures at high pressures. *Microporous and Mesoporous Materials*, **2012**, 156, 217-223	5.3	66
184	Reprint of: CO2/CH4, CH4/H2 and CO2/CH4/H2 separations at high pressures using Mg2(dobdc). *Microporous and Mesoporous Materials*, **2012**, 157, 94-100	5.3	34
183	A microporous metal-organic framework for highly selective separation of acetylene, ethylene, and ethane from methane at room temperature. *Chemistry - A European Journal*, **2012**, 18, 613-9	4.8	188
182	High separation capacity and selectivity of C2 hydrocarbons over methane within a microporous metal-organic framework at room temperature. *Chemistry - A European Journal*, **2012**, 18, 1901-4	4.8	127
181	Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers. *Angewandte Chemie - International Edition*, **2012**, 51, 11867-71	16.4	81

180	Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. *Angewandte Chemie*, **2012**, 124, 12037-12041	3.6	13
179	A robust doubly interpenetrated metal-organic framework constructed from a novel aromatic tricarboxylate for highly selective separation of small hydrocarbons. *Chemical Communications*, **2012**, 48, 6493-5	5.8	187
178	A microporous lanthanide-tricarboxylate framework with the potential for purification of natural gas. *Chemical Communications*, **2012**, 48, 10856-8	5.8	120
177	Cu-TDPAT, an rht-Type Dual-Functional Metal□Organic Framework Offering Significant Potential for Use in H2 and Natural Gas Purification Processes Operating at High Pressures. *Journal of Physical Chemistry C*, **2012**, 116, 16609-16618	3.8	64
176	Microporous metal-organic framework with potential for carbon dioxide capture at ambient conditions. *Nature Communications*, **2012**, 3, 954	17.4	615
175	Microporous metal-organic frameworks for storage and separation of small hydrocarbons. *Chemical Communications*, **2012**, 48, 11813-31	5.8	278
174	Investigating the Relative Influences of Molecular Dimensions and Binding Energies on Diffusivities of Guest Species Inside Nanoporous Crystalline Materials. *Journal of Physical Chemistry C*, **2012**, 116, 23556-23568	3.8	56
173	Metal□rganic frameworks with potential for energy-efficient adsorptive separation of light hydrocarbons. *Energy and Environmental Science*, **2012**, 5, 9107	35.4	517
172	Interplay of metalloligand and organic ligand to tune micropores within isostructural mixed-metal organic frameworks (M'MOFs) for their highly selective separation of chiral and achiral small molecules. *Journal of the American Chemical Society*, **2012**, 134, 8703-10	16.4	296
171	Diffusion in porous crystalline materials. *Chemical Society Reviews*, **2012**, 41, 3099-118	58.5	194
170	Hydrocarbon separations in a metal-organic framework with open iron(II) coordination sites. *Science*, **2012**, 335, 1606-10	33.3	1349
169	Polyamine-Tethered Porous Polymer Networks for Carbon Dioxide Capture from Flue Gas. *Angewandte Chemie*, **2012**, 124, 7598-7602	3.6	53
168	Polyamine-tethered porous polymer networks for carbon dioxide capture from flue gas. *Angewandte Chemie - International Edition*, **2012**, 51, 7480-4	16.4	476
167	Investigating the validity of the Bosanquet formula for estimation of diffusivities in mesopores. *Chemical Engineering Science*, **2012**, 69, 684-688	4.4	30
166	In silico screening of metal-organic frameworks in separation applications. *Physical Chemistry Chemical Physics*, **2011**, 13, 10593-616	3.6	279
165	Enhanced carbon dioxide capture upon incorporation of N,N?-dimethylethylenediamine in the metal□rganic framework CuBTTri. *Chemical Science*, **2011**, 2, 2022	9.4	445
164	Screening Metal□rganic Frameworks by Analysis of Transient Breakthrough of Gas Mixtures in a Fixed Bed Adsorber. *Journal of Physical Chemistry C*, **2011**, 115, 12941-12950	3.8	184
163	Investigating the Validity of the Knudsen Prescription for Diffusivities in a Mesoporous Covalent Organic Framework. *Industrial & Engineering Chemistry Research*, **2011**, 50, 7083-7087	3.9	19

162	Metal-organic frameworks as adsorbents for hydrogen purification and precombustion carbon dioxide capture. *Journal of the American Chemical Society*, **2011**, 133, 5664-7	16.4	405
161	Sulfonate-grafted porous polymer networks for preferential CO2 adsorption at low pressure. *Journal of the American Chemical Society*, **2011**, 133, 18126-9	16.4	479
160	Evaluating metal□organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption. *Energy and Environmental Science*, **2011**, 4, 3030	35.4	782
159	Maxwell□Stefan modeling of slowing-down effects in mixed gas permeation across porous membranes. *Journal of Membrane Science*, **2011**, 383, 289-300	9.6	69
158	Selective binding of O2 over N2 in a redox-active metal-organic framework with open iron(II) coordination sites. *Journal of the American Chemical Society*, **2011**, 133, 14814-22	16.4	404
157	Investigating the potential of MgMOF-74 membranes for CO2 capture. *Journal of Membrane Science*, **2011**, 377, 249-260	9.6	72
156	A molecular dynamics investigation of the diffusion characteristics of cavity-type zeolites with 8-ring windows. *Microporous and Mesoporous Materials*, **2011**, 137, 83-91	5.3	84
155	A molecular dynamics investigation of the unusual concentration dependencies of Fick diffusivities in silica mesopores. *Microporous and Mesoporous Materials*, **2011**, 138, 228-234	5.3	23
154	Molecular dynamics investigation of the self-diffusion of binary mixture diffusion in the metal-organic framework Zn(tbip) accounting for framework flexibility. *Microporous and Mesoporous Materials*, **2011**, 143, 125-131	5.3	10
153	In-Depth Study of Mass Transfer in Nanoporous Materials by Micro-Imaging. *Chemie-Ingenieur-Technik*, **2011**, 83, 2211-2218	0.8	10
152	A simplified procedure for estimation of mixture permeances from unary permeation data. *Journal of Membrane Science*, **2011**, 367, 204-210	9.6	12
151	A rationalization of the Type IV loading dependence in the K□ger□Pfeifer classification of self-diffusivities. *Microporous and Mesoporous Materials*, **2011**, 142, 745-748	5.3	9
150	Ethene/ethane separation by the MOF membrane ZIF-8: Molecular correlation of permeation, adsorption, diffusion. *Journal of Membrane Science*, **2011**, 369, 284-289	9.6	334
149	Influence of adsorption on the diffusion selectivity for mixture permeation across mesoporous membranes. *Journal of Membrane Science*, **2011**, 369, 545-549	9.6	30
148	Entropy-based separation of linear chain molecules by exploiting differences in the saturation capacities in cage-type zeolites. *Separation and Purification Technology*, **2011**, 76, 325-330	8.3	24
147	Distance and angular holonomic constraints in molecular simulations. *Journal of Chemical Physics*, **2010**, 133, 034114	3.9	14
146	Porous Polymer Networks: Synthesis, Porosity, and Applications in Gas Storage/Separation. *Chemistry of Materials*, **2010**, 22, 5964-5972	9.6	466
145	Hydrogen bonding effects in adsorption of water-alcohol mixtures in zeolites and the consequences for the characteristics of the Maxwell-Stefan diffusivities. *Langmuir*, **2010**, 26, 10854-67	4	115

144	Describing Mixture Diffusion in Microporous Materials under Conditions of Pore Saturation. *Journal of Physical Chemistry C*, **2010**, 114, 11557-11563	3.8	22
143	Highlighting a variety of unusual characteristics of adsorption and diffusion in microporous materials induced by clustering of guest molecules. *Langmuir*, **2010**, 26, 8450-63	4	50
142	Comment on "Modeling Adsorption and Self-Diffusion of Methane in LTA Zeolites: The Influence of Framework Flexibility". *Journal of Physical Chemistry C*, **2010**, 114, 18017-18021	3.8	33
141	Mutual Slowing-Down Effects in Mixture Diffusion in Zeolites. *Journal of Physical Chemistry C*, **2010**, 114, 13154-13156	3.8	28
140	Investigating cluster formation in adsorption of CO2, CH4, and Ar in zeolites and metal organic frameworks at subcritical temperatures. *Langmuir*, **2010**, 26, 3981-92	4	67
139	Thermosensitive gating effect and selective gas adsorption in a porous coordination nanocage. *Chemical Communications*, **2010**, 46, 7352-4	5.8	80
138	Comment on comparative molecular simulation study of CO2/N2 and CH4/N2 separation in zeolites and metal-organic frameworks. *Langmuir*, **2010**, 26, 2975-8	4	39
137	Highlighting pitfalls in the Maxwell–Stefan modeling of water–alcohol mixture permeation across pervaporation membranes. *Journal of Membrane Science*, **2010**, 360, 476-482	9.6	36
136	Investigating the reasons for the significant influence of lattice flexibility on self-diffusivity of ethane in Zn(tbip). *Microporous and Mesoporous Materials*, **2010**, 130, 92-96	5.3	36
135	Novel MOF-membrane for molecular sieving predicted by IR-diffusion studies and molecular modeling. *Advanced Materials*, **2010**, 22, 4741-3	24	205
134	In silico screening of zeolite membranes for CO2 capture. *Journal of Membrane Science*, **2010**, 360, 323-333	9.6	244
133	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	5.3	117
132	Reactor simulation of benzene ethylation and ethane dehydrogenation catalyzed by ZSM-5: A multiscale approach. *Chemical Engineering Science*, **2010**, 65, 2472-2480	4.4	30
131	Assessing guest diffusivities in porous hosts from transient concentration profiles. *Physical Review Letters*, **2009**, 102, 065901	7.4	69
130	Design of the Reduction of Events with Darbepoetin alfa in Heart Failure (RED-HF): a Phase III, anaemia correction, morbidity-mortality trial. *European Journal of Heart Failure*, **2009**, 11, 795-801	12.3	88
129	Assessing surface permeabilities from transient guest profiles in nanoporous host materials. *Angewandte Chemie - International Edition*, **2009**, 48, 3525-8	16.4	80
128	Adsorption and diffusion of alkanes in CuBTC crystals investigated using infra-red microscopy and molecular simulations. *Microporous and Mesoporous Materials*, **2009**, 117, 22-32	5.3	129
127	A Molecular Dynamics investigation of the influence of framework flexibility on self-diffusivity of ethane in Zn(tbip) frameworks. *Microporous and Mesoporous Materials*, **2009**, 125, 97-100	5.3	45

126	Diffusion of n-butane/iso-butane mixtures in silicalite-1 investigated using infrared (IR) microscopy. *Microporous and Mesoporous Materials*, **2009**, 125, 11-16	5.3	24
125	A molecular dynamics investigation of a variety of influences of temperature on diffusion in zeolites. *Microporous and Mesoporous Materials*, **2009**, 125, 126-134	5.3	34
124	An investigation of the characteristics of Maxwell–Stefan diffusivities of binary mixtures in silica nanopores. *Chemical Engineering Science*, **2009**, 64, 870-882	4.4	65
123	Unified Maxwell–Stefan description of binary mixture diffusion in micro- and meso-porous materials. *Chemical Engineering Science*, **2009**, 64, 3159-3178	4.4	106
122	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	3.8	72
121	Method for Analyzing Structural Changes of Flexible Metal–Organic Frameworks Induced by Adsorbates. *Journal of Physical Chemistry C*, **2009**, 113, 19317-19327	3.8	67
120	Describing the Diffusion of Guest Molecules Inside Porous Structures. *Journal of Physical Chemistry C*, **2009**, 113, 19756-19781	3.8	244
119	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2009**, 113, 8814-8820	3.8	160
118	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	8.3	114
117	Liquid Dispersion in Large Diameter Bubble Columns, with and without Internals. *Canadian Journal of Chemical Engineering*, **2008**, 81, 360-366	2.3	37
116	2D Slurry Bubble Column Hydrodynamic Phenomena Clarified with a 3D Gas–Liquid Model. *Canadian Journal of Chemical Engineering*, **2008**, 81, 456-464	2.3	2
115	Intensification of Slurry Bubble Columns by Vibration Excitement. *Canadian Journal of Chemical Engineering*, **2008**, 81, 655-659	2.3	5
114	Using CFD to Describe the Hydrodynamics of Internal Air-lift Reactors. *Canadian Journal of Chemical Engineering*, **2008**, 81, 660-668	2.3	15
113	Insights into diffusion of gases in zeolites gained from molecular dynamics simulations. *Microporous and Mesoporous Materials*, **2008**, 109, 91-108	5.3	148
112	Investigation of slowing-down and speeding-up effects in binary mixture permeation across SAPO-34 and MFI membranes. *Separation and Purification Technology*, **2008**, 60, 230-236	8.3	39
111	Separating n-alkane mixtures by exploiting differences in the adsorption capacity within cages of CHA, AFX and ERI zeolites. *Separation and Purification Technology*, **2008**, 60, 315-320	8.3	22
110	Diffusion of hydrocarbon mixtures in MFI zeolite: Influence of intersection blocking. *Chemical Engineering Journal*, **2008**, 140, 614-620	14.7	48
109	1H NMR signal broadening in spectra of alkane molecules adsorbed on MFI-type zeolites. *Solid State Nuclear Magnetic Resonance*, **2008**, 33, 65-71	3.1	12

108	Diffusion of alkane mixtures in MFI zeolite. *Microporous and Mesoporous Materials*, **2008**, 107, 296-298	5.3	17
107	Interpreting Unary, Binary, and Ternary Mixture Permeation Across a SAPO-34 Membrane with Loading-Dependent Maxwell□Stefan Diffusivities. *Journal of Physical Chemistry C*, **2007**, 111, 5075-5082	3.8	75
106	Using molecular simulations for screening of zeolites for separation of CO2/CH4 mixtures. *Chemical Engineering Journal*, **2007**, 133, 121-131	14.7	171
105	Mixture diffusion in zeolites studied by MAS PFG NMR and molecular simulation. *Microporous and Mesoporous Materials*, **2007**, 105, 124-131	5.3	65
104	A computational study of CO2, N2, and CH4 adsorption in zeolites. *Adsorption*, **2007**, 13, 469-476	2.6	145
103	A Simulation Study of Alkanes in Linde Type A Zeolites. *Adsorption Science and Technology*, **2007**, 25, 417-427	3.6	22
102	Influence of isotherm inflection on the loading dependence of the diffusivities of n-hexane and n-heptane in MFI zeolite. Quasi-elastic neutron scattering experiments supplemented by molecular simulations. *Journal of Physical Chemistry B*, **2006**, 110, 2195-201	3.4	49
101	Scale Up of Slurry Bubble Reactors. *Oil and Gas Science and Technology*, **2006**, 61, 443-458	1.9	27
100	Relation between pore sizes of protein crystals and anisotropic solute diffusivities. *Journal of the American Chemical Society*, **2005**, 127, 875-9	16.4	51
99	Quantification of binary diffusion in protein crystals. *Journal of Physical Chemistry B*, **2005**, 109, 10561-6	3.4	23
98	Diffusion of alkane mixtures in zeolites: validating the maxwell-stefan formulation using MD simulations. *Journal of Physical Chemistry B*, **2005**, 109, 6386-96	3.4	115
97	Hydrodynamics of Taylor Flow in Vertical Capillaries:□Flow Regimes, Bubble Rise Velocity, Liquid Slug Length, and Pressure Drop. *Industrial & Engineering Chemistry Research*, **2005**, 44, 4884-4897	3.9	207
96	Adsorption of xanthene dyes by lysozyme crystals. *Langmuir*, **2005**, 21, 1475-80	4	29
95	The Darken Relation for Multicomponent Diffusion in Liquid Mixtures of Linear Alkanes: An Investigation Using Molecular Dynamics (MD) Simulations. *Industrial & Engineering Chemistry Research*, **2005**, 44, 6939-6947	3.9	119
94	Entropy effects in adsorption and diffusion of alkane isomers in mordenite: An investigation using CBMC and MD simulations. *Microporous and Mesoporous Materials*, **2005**, 84, 179-191	5.3	55
93	A moving bed reactor concept for alkane isomerization. *Chemical Engineering Journal*, **2005**, 109, 107-113	14.7	12
92	Exploiting the Bjerknes force in bubble column reactors. *Chemical Engineering Science*, **2005**, 60, 5962-5970	4.4	18
91	Mass transfer from Taylor bubbles rising in single capillaries. *Chemical Engineering Science*, **2005**, 60, 6430-6437	4.4	130

90	Analytic solution of the Maxwell–Stefan equations for multicomponent permeation across a zeolite membrane. *Chemical Engineering Journal*, **2004**, 97, 37-45	14.7	59
89	Modeling the occupancy dependence of diffusivities in zeolites. *Microporous and Mesoporous Materials*, **2004**, 76, 233-246	5.3	92
88	Effectiveness factor for zeolite catalysed isomerization reactions. *Chemical Engineering Journal*, **2004**, 99, 105-116	14.7	8
87	CFD simulations of mass transfer from Taylor bubbles rising in circular capillaries. *Chemical Engineering Science*, **2004**, 59, 2535-2545	4.4	234
86	On the Inflection in the Concentration Dependence of the Maxwell–Stefan Diffusivity of CF4 in MFI Zeolite. *Journal of Physical Chemistry B*, **2004**, 108, 14820-14822	3.4	25
85	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Short n-Alkanes in Faujasite. *Journal of Physical Chemistry B*, **2004**, 108, 13481-13491	3.4	93
84	United Atom Force Field for Alkanes in Nanoporous Materials. *Journal of Physical Chemistry B*, **2004**, 108, 12301-12313	3.4	282
83	Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. *Journal of the American Chemical Society*, **2004**, 126, 11377-86	16.4	222
82	Simulating Adsorption of Alkanes in Zeolites **2003**,		1
81	A Strategy for Scaling Up the Fischer–Tropsch Bubble Column Slurry Reactor. *Topics in Catalysis*, **2003**, 26, 21-28	2.3	15
80	Modelling issues in zeolite based separation processes. *Separation and Purification Technology*, **2003**, 33, 213-254	8.3	170
79	Correlation Effects in Diffusion of CH4/CF4Mixtures in MFI Zeolite. A Study Linking MD Simulations with the Maxwell–Stefan Formulation. *Langmuir*, **2003**, 19, 7977-7988	4	166
78	Influence of interphase mass transfer on the composition trajectories and crossing of boundaries in ternary azeotropic distillation. *Separation and Purification Technology*, **2002**, 29, 1-13	8.3	16
77	Verification of the Maxwell–Stefan theory for tracer diffusion in zeolites. *Chemical Engineering Journal*, **2002**, 85, 7-15	14.7	31
76	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. *Chemical Engineering Journal*, **2002**, 88, 81-94	14.7	101
75	Verification of the Maxwell–Stefan theory for diffusion of three-component mixtures in zeolites. *Chemical Engineering Journal*, **2002**, 87, 1-9	14.7	26
74	Entropy effects during sorption of alkanes in zeolites. *Chemical Society Reviews*, **2002**, 31, 185-94	58.5	174
73	Self-diffusivities in multicomponent mixtures in zeolites. *Physical Chemistry Chemical Physics*, **2002**, 4, 1891-1898	3.6	68

72	Verification of the Maxwell–Stefan theory for mixture diffusion in zeolites by comparison with MD simulations. *Chemical Engineering Journal*, **2001**, 84, 207-214	14.7	9
71	Comparative analysis of CFD models of dense gas–solid systems. *AICHE Journal*, **2001**, 47, 1035-1051	3.6	372
70	Using CFD for scaling up gas–solid bubbling fluidised bed reactors with Geldart A powders. *Chemical Engineering Journal*, **2001**, 82, 247-257	14.7	49
69	Monte Carlo simulations in zeolites. *Current Opinion in Solid State and Materials Science*, **2001**, 5, 455-461	12	34
68	Separation of linear, mono-methyl and di-methyl alkanes in the 5–7 carbon atom range by exploiting configurational entropy effects during sorption on silicalite-1. *Physical Chemistry Chemical Physics*, **2001**, 3, 4390-4398	3.6	56
67	Molecular simulations of adsorption and siting of light alkanes in silicalite-1. *Physical Chemistry Chemical Physics*, **2001**, 3, 453-462	3.6	63
66	Kinetic Monte Carlo simulations of transport diffusivities of binary mixtures in zeolites. *Physical Chemistry Chemical Physics*, **2001**, 3, 3185-3191	3.6	36
65	Gas hold-up in bubble columns: Operation with concentrated slurries versus high viscosity liquid. *Canadian Journal of Chemical Engineering*, **2000**, 78, 442-448	2.3	21
64	Modelling reactive distillation. *Chemical Engineering Science*, **2000**, 55, 5183-5229	4.4	561
63	Modelling sieve tray hydraulics using computational fluid dynamics. *Chemical Engineering Journal*, **2000**, 77, 143-151	14.7	72
62	Liquid phase dispersion in bubble columns operating in the churn-turbulent flow regime. *Chemical Engineering Journal*, **2000**, 78, 43-51	14.7	51
61	The generalized Maxwell–Stefan model for diffusion in zeolites:: sorbate molecules with different saturation loadings. *Chemical Engineering Science*, **2000**, 55, 2923-2930	4.4	195
60	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	4.4	110
59	Design and scale-up of the Fischer–Tropsch bubble column slurry reactor. *Fuel Processing Technology*, **2000**, 64, 73-105	7.2	211
58	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwell–Stefan theory. *Separation and Purification Technology*, **2000**, 21, 111-136	8.3	84
57	A Scale-Up Strategy for a Commercial Scale Bubble Column Slurry Reactor for Fischer-Tropsch Synthesis. *Oil and Gas Science and Technology*, **2000**, 55, 359-393	1.9	60
56	Comparison of equilibrium stage and nonequilibrium stage models for reactive distillation. *Chemical Engineering Journal*, **2000**, 76, 33-47	14.7	113
55	Modeling of Diffusion in Zeolites. *Reviews in Chemical Engineering*, **2000**, 16,	5	197

54	Monte Carlo simulations of self- and transport-diffusivities of 2-methylhexane in silicalite. *Physical Chemistry Chemical Physics*, **2000**, 2, 2389-2394	3.6	55
53	Permeation of Hexane Isomers across ZSM-5 Zeolite Membranes. *Industrial & Engineering Chemistry Research*, **2000**, 39, 2618-2622	3.9	38
52	Fundamentals and selection of advanced Fischer□ropsch reactors. *Applied Catalysis A: General*, **1999**, 186, 55-70	5.1	169
51	Modelling of a bubble column slurry reactor for Fischer□ropsch synthesis. *Catalysis Today*, **1999**, 52, 279-289	5.3	252
50	Gas holdup and mass transfer in bubble column reactors operated at elevated pressure. *Chemical Engineering Science*, **1999**, 54, 2237-2246	4.4	175
49	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	4.4	143
48	Rise velocity of a swarm of large gas bubbles in liquids. *Chemical Engineering Science*, **1999**, 54, 171-183	4.4	122
47	Multicomponent reaction engineering model for Fe-catalyzed Fischer□ropsch synthesis in commercial scale slurry bubble column reactors. *Chemical Engineering Science*, **1999**, 54, 5013-5019	4.4	58
46	CFD Simulations of Sieve Tray Hydrodynamics. *Chemical Engineering Research and Design*, **1999**, 77, 639-646	3.5	65
45	Molecular Simulations of Adsorption Isotherms for Linear and Branched Alkanes and Their Mixtures in Silicalite. *Journal of Physical Chemistry B*, **1999**, 103, 1102-1118	3.4	420
44	Effect of gas density on large-bubble holdup in bubble column reactors. *AICHE Journal*, **1998**, 44, 2333-2336	3.6	32
43	Eulerian simulations of bubbling behaviour in gas-solid fluidised beds. *Computers and Chemical Engineering*, **1998**, 22, S299-S306	4	119
42	Sorption-Induced Diffusion-Selective Separation of Hydrocarbon Isomers Using Silicalite. *Journal of Physical Chemistry A*, **1998**, 102, 7727-7730	2.8	100
41	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. *Journal of the American Chemical Society*, **1998**, 120, 5599-5600	16.4	145
40	Improving the efficiency of the configurational-bias Monte Carlo algorithm. *Molecular Physics*, **1998**, 94, 727-733	1.7	192
39	Gas holdup in slurry bubble columns: Effect of column diameter and slurry concentrations. *AICHE Journal*, **1997**, 43, 311-316	3.6	144
38	The Maxwell-Stefan approach to mass transfer. *Chemical Engineering Science*, **1997**, 52, 861-911	4.4	1125
37	Characterization of regimes and regime transitions in bubble columns by chaos analysis of pressure signals. *Chemical Engineering Science*, **1997**, 52, 4447-4459	4.4	165

36	Size, structure and dynamics of large bubbles in a two-dimensional slurry bubble column. *Chemical Engineering Science*, **1996**, 51, 4619-4629	4.4	111
35	Gas holdup in bubble column reactors operating in the churn-turbulent flow regime. *AICHE Journal*, **1996**, 42, 2627-2634	3.6	127
34	Influence of increased gas density on hydrodynamics of bubble-column reactors. *AICHE Journal*, **1994**, 40, 112-119	3.6	53
33	Strategies for multiphase reactor selection. *Chemical Engineering Science*, **1994**, 49, 4029-4065	4.4	145
32	Multiple solutions in reactive distillation for methyl tert-butyl ether synthesis. *Industrial & Engineering Chemistry Research*, **1993**, 32, 1706-1709	3.9	137
31	Influence of gas density on the stability of homogeneous flow in bubble columns. *Industrial & Engineering Chemistry Research*, **1993**, 32, 747-750	3.9	13
30	Problems and pitfalls in the use of the fick formulation for intraparticle diffusion. *Chemical Engineering Science*, **1993**, 48, 845-861	4.4	157
29	Film model for mass transfer in non-ideal multicomponent fluid mixtures. *The Chemical Engineering Journal*, **1993**, 52, 19-29		2
28	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	4.4	138
27	Multicomponent surface diffusion of adsorbed species: a description based on the generalized Maxwell Stefan equations. *Chemical Engineering Science*, **1990**, 45, 1779-1791	4.4	223
26	Liquid-liquid equilibrium in the toluene-methyl ethyl ketone-water system. *Fluid Phase Equilibria*, **1989**, 50, 339-346	2.5	2
25	Use of an axial-dispersion model for kinetic description of hydrocracking. *Chemical Engineering Science*, **1989**, 44, 703-712	4.4	37
24	Use of additives to enhance the selectivity of liquid surfactant membranes. *Journal of Membrane Science*, **1989**, 40, 329-342	9.6	5
23	Mass-transfer efficiency of sieve tray extraction columns. *Industrial & Engineering Chemistry Research*, **1989**, 28, 642-644	3.9	7
22	Comments on "Simulation and optimization of an industrial ammonia reactor". *Industrial & Engineering Chemistry Research*, **1989**, 28, 1266-1266	3.9	2
21	Rapid hydrocarbon type separation of vacuum residues. *Fresenius Zeitschrift Fü Analytische Chemie*, **1988**, 332, 358-361		1
20	SEPARATION-IRREVERSIBLE THERMO A UNIFIED THEORY OF SEPARATION PROCESSES BASED ON. *Chemical Engineering Communications*, **1987**, 59, 33-64	2.2	21
19	Effect of emulsion breakage on selectivity in the separation of hydrocarbon mixtures using aqueous surfactant membranes. *Journal of Membrane Science*, **1987**, 34, 141-154	9.6	12

18	Effect of surfactant type on selectivity for the separation of 1-methylnaphthalene from dodecane using liquid membranes. *Journal of Membrane Science*, **1987**, 32, 19-30	9.6	9
17	Simple gas chromatographic determination of the distribution of normal alkanes in the kerosene fraction of petroleum. *Analyst, The*, **1987**, 112, 49	5	4
16	A simplified procedure for the solution of the dusty gas model equations for steady-state transport in non-reacting systems. *The Chemical Engineering Journal*, **1987**, 35, 75-81		39
15	Diffusion in multicomponent electrolyte systems. *The Chemical Engineering Journal*, **1987**, 35, 19-24		29
14	Physical significance of the mass transfer coefficient. *The Chemical Engineering Journal*, **1987**, 35, 67-68		1
13	Condensation of vapor mixtures. 2. Comparison with experiment. *Industrial & Engineering Chemistry Process Design and Development*, **1986**, 25, 98-101		8
12	Condensation of vapor mixtures. 1. Nonequilibrium models and design procedures. *Industrial & Engineering Chemistry Process Design and Development*, **1986**, 25, 83-97		15
11	Comments on "Effect of vapor efflux from a spherical particle on heat transfer from a hot gas". *Industrial & Engineering Chemistry Fundamentals*, **1984**, 23, 377-379		3
10	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		78
9	MASS AND ENERGY TRANSFER IN MULTICOMPONENT SYSTEMS. *Chemical Engineering Communications*, **1979**, 3, 201-275	2.2	128
8	A SIMPLIFIED FILM MODEL DESCRIPTION OF MULTICOMPONENT INTERPHASE MASS TRANSFER. *Chemical Engineering Communications*, **1979**, 3, 29-39	2.2	11
7	A note on the film and penetration models for multicomponent mass transfer. *Chemical Engineering Science*, **1978**, 33, 765-767	4.4	14
6	Penetration depths in multicomponent mass transfer. *Chemical Engineering Science*, **1978**, 33, 1495-1497	4.4	5
5	Multicomponent Gaseous Diffusion in Porous Media in the Transition Region. A Matrix Method for Calculation of Steady-State Transport Rates. *Industrial & Engineering Chemistry Fundamentals*, **1977**, 16, 228-232		10
4	A film model analysis of non-equimolar distillation of multicomponent mixtures. *Chemical Engineering Science*, **1977**, 32, 1197-1203	4.4	16
3	Condensation of a binary vapour mixture in the presence of an inert gas. *Chemical Engineering Science*, **1977**, 32, 741-745	4.4	31
2	A generalized film model for mass transfer in non-ideal fluid mixtures. *Chemical Engineering Science* , **1977**, 32, 659-667	4.4	45
1	A multicomponent film model incorporating a general matrix method of solution to the Maxwell-Stefan equations. *AICHE Journal*, **1976**, 22, 383-389	3.6	178