Randall Q Snurr

List of Publications by Year
in descending order

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336 papers	45,244 citations	2215 99 h-index	2033 205 g-index
354 all docs	354 docs citations	354 times ranked	24861 citing authors

#	Article	IF	Citations
1	Ultrahigh Porosity in Metal-Organic Frameworks. Science, 2010, 329, 424-428.	12.6	3,306
2	De novo synthesis of a metalâ€“organic framework material featuring ultrahigh surface area and gas storage capacities. Nature Chemistry, 2010, 2, 944-948.	13.6	1,535
3	Metalâ€“Organic Framework Materials with Ultrahigh Surface Areas: Is the Sky the Limit?. Journal of the American Chemical Society, 2012, 134, 15016-15021.	13.7	1,497
4	A facile synthesis of UiO-66, UiO-67 and their derivatives. Chemical Communications, 2013, 49, 9449.	4.1	1,340
5	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. Molecular Simulation, 2016, 42, 81-101.	2.0	1,266
6	Large-scale screening of hypothetical metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 83-89.	13.6	1,098
7	Review and Analysis of Molecular Simulations of Methane, Hydrogen, and Acetylene Storage in Metalâ€“Organic Frameworks. Chemical Reviews, 2012, 112, 703-723.	47.7	1,085
8	Development and Evaluation of Porous Materials for Carbon Dioxide Separation and Capture. Angewandte Chemie - International Edition, 2011, 50, 11586-11596.	13.8	1,025
9	Applicability of the BET Method for Determining Surface Areas of Microporous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2007, 129, 8552-8556.	13.7	885
10	Vapor-Phase Metalation by Atomic Layer Deposition in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 10294-10297.	13.7	821
11	Screening of Metalâ€“Organic Frameworks for Carbon Dioxide Capture from Flue Gas Using a Combined Experimental and Modeling Approach. Journal of the American Chemical Society, 2009, 131, 18198-18199.	13.7	816
12	Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516.	27.5	790
13	Metalâ€“organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. Chemical Society Reviews, 2017, 46, 3357-3385.	38.1	707
14	Design of New Materials for Methane Storage. Langmuir, 2004, 20, 2683-2689.	3.5	663
15	Using molecular simulation to characterise metalâ€“organic frameworks for adsorption applications. Chemical Society Reviews, 2009, 38, 1237.	38.1	613
16	Effects of Surface Area, Free Volume, and Heat of Adsorption on Hydrogen Uptake in Metalâ€“Organic Frameworks. Journal of Physical Chemistry B, 2006, 110, 9565-9570.	2.6	558
17	Separation of CO₂ from CH₄ Using Mixed-Ligand Metalâ€“Organic Frameworks. Langmuir, 2008, 24, 8592-8598.	3.5	557
18	Computation-Ready, Experimental Metalâ€“Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. Chemistry of Materials, 2014, 26, 6185-6192.	6.7	524

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19	Enhanced CO₂ Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. Chemistry of Materials, 2009, 21, 1425-1430.	6.7	523
20	Light-Harvesting and Ultrafast Energy Migration in Porphyrin-Based Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 862-869.	13.7	510
21	Calculating Geometric Surface Areas as a Characterization Tool for Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2007, 111, 15350-15356.	3.1	498
22	Understanding Inflections and Steps in Carbon Dioxide Adsorption Isotherms in Metal-Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 406-407.	13.7	485
23	Perfluoroalkane Functionalization of NU-1000 via Solvent-Assisted Ligand Incorporation: Synthesis and CO₂ Adsorption Studies. Journal of the American Chemical Society, 2013, 135, 16801-16804.	13.7	473
24	High Propene/Propane Selectivity in Isostructural Metalâ€“Organic Frameworks with High Densities of Open Metal Sites. Angewandte Chemie - International Edition, 2012, 51, 1857-1860.	13.8	392
25	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metalâ€“Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data, 2019, 64, 5985-5998.	1.9	372
26	Enhancement of CO2/N2 selectivity in a metal-organic framework by cavity modification. Journal of Materials Chemistry, 2009, 19, 2131.	6.7	370
27	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. The Journal of Physical Chemistry, 1993, 97, 13742-13752.	2.9	366
28	Object-oriented Programming Paradigms for Molecular Modeling. Molecular Simulation, 2003, 29, 29-46.	2.0	360
29	Carborane-based metalâ€“organic frameworks as highly selective sorbents for CO2 over methane. Chemical Communications, 2008, , 4135.	4.1	349
30	High-throughput computational screening of metalâ€“organic frameworks. Chemical Society Reviews, 2014, 43, 5735-5749.	38.1	336
31	Structureâ€“property relationships of porous materials for carbon dioxide separation and capture. Energy and Environmental Science, 2012, 5, 9849.	30.8	334
32	Ultrahigh Surface Area Zirconium MOFs and Insights into the Applicability of the BET Theory. Journal of the American Chemical Society, 2015, 137, 3585-3591.	13.7	329
33	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	30.8	314
34	Highly Selective Carbon Dioxide Uptake by [Cu(bpy-n)₂(SiF₆)] (bpy-1 =) Tj ETQq0 0 0 rgBT /Overlock 1 3663-3666.	13.7	303
35	Exceptional Negative Thermal Expansion in Isoreticular Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2007, 46, 4496-4499.	13.8	289
36	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. CheM, 2016, 1, 154-169.	11.7	286

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37	Synthesis, Properties, and Gas Separation Studies of a Robust Diimide-Based Microporous Organic Polymer. Chemistry of Materials, 2009, 21, 3033-3035.	6.7	272
38	Nanoporous Carbohydrate Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 406-417.	13.7	271
39	CD-MOF: A Versatile Separation Medium. Journal of the American Chemical Society, 2016, 138, 2292-2301.	13.7	269
40	Kinetic Separation of Propene and Propane in Metalâ˜Organic Frameworks: Controlling Diffusion Rates in Plate-Shaped Crystals via Tuning of Pore Apertures and Crystallite Aspect Ratios. Journal of the American Chemical Society, 2011, 133, 5228-5231.	13.7	263
41	Evaluation of the BET Method for Determining Surface Areas of MOFs and Zeolites that Contain Ultra-Micropores. Langmuir, 2010, 26, 5475-5483.	3.5	257
42	Incorporation of an A1/A2-Difunctionalized Pillar[5]arene into a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2012, 134, 17436-17439.	13.7	254
43	An Extended Charge Equilibration Method. Journal of Physical Chemistry Letters, 2012, 3, 2506-2511.	4.6	253
44	Prospects for nanoporous metal-organic materials in advanced separations processes. AICHE Journal, 2004, 50, 1090-1095.	3.6	249
45	Thermodynamic analysis of Xe/Kr selectivity in over 137â€‰000 hypothetical metalâ€“organic frameworks. Chemical Science, 2012, 3, 2217.	7.4	248
46	Evaluating topologically diverse metalâ€“organic frameworks for cryo-adsorbed hydrogen storage. Energy and Environmental Science, 2016, 9, 3279-3289.	30.8	231
47	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. Science Advances, 2016, 2, e1600909.	10.3	231
48	Water adsorption in UiO-66: the importance of defects. Chemical Communications, 2014, 50, 11329-11331.	4.1	227
49	Molecular Modeling and Experimental Studies of the Thermodynamic and Transport Properties of Pyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 2821-2832.	2.6	226
50	Monomolecular cracking of n-hexane on Y, MOR, and ZSM-5 zeolites. Applied Catalysis A: General, 1999, 179, 71-86.	4.3	219
51	Gram-scale, high-yield synthesis of a robust metalâ€“organic framework for storing methane and other gases. Energy and Environmental Science, 2013, 6, 1158.	30.8	219
52	Screening of bio-compatible metalâ€“organic frameworks as potential drug carriers using Monte Carlo simulations. Journal of Materials Chemistry B, 2014, 2, 766-774.	5.8	215
53	Heats of Adsorption for Seven Gases in Three Metalâ˜Organic Frameworks: Systematic Comparison of Experiment and Simulation. Langmuir, 2009, 25, 7383-7388.	3.5	212
54	Framework-Topology-Dependent Catalytic Activity of Zirconium-Based (Porphinato)zinc(II) MOFs. Journal of the American Chemical Society, 2016, 138, 14449-14457.	13.7	210

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55	Nanosizing a Metalâ€“Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. ACS Nano, 2016, 10, 9174-9182.	14.6	202
56	Application of Consistency Criteria To Calculate BET Areas of Micro- And Mesoporous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 215-224.	13.7	201
57	Designing Higher Surface Area Metalâ€“Organic Frameworks: Are Triple Bonds Better Than Phenyls?. Journal of the American Chemical Society, 2012, 134, 9860-9863.	13.7	198
58	Computational Design of Metalâ€“Organic Frameworks Based on Stable Zirconium Building Units for Storage and Delivery of Methane. Chemistry of Materials, 2014, 26, 5632-5639.	6.7	191
59	Design Requirements for Metal-Organic Frameworks as Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 18794-18803.	3.1	190
60	Energy-based descriptors to rapidly predict hydrogen storage in metalâ€“organic frameworks. Molecular Systems Design and Engineering, 2019, 4, 162-174.	3.4	179
61	Topologically Guided, Automated Construction of Metalâ€“Organic Frameworks and Their Evaluation for Energy-Related Applications. Crystal Growth and Design, 2017, 17, 5801-5810.	3.0	176
62	Large-Scale Quantitative Structureâ€“Property Relationship (QSPR) Analysis of Methane Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	3.1	174
63	A combined experimental and quantum chemical study of CO2 adsorption in the metalâ€“organic framework CPO-27 with different metals. Chemical Science, 2013, 4, 3544.	7.4	172
64	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
65	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	10.0	170
66	Recent developments in the molecular modeling of diffusion in nanoporous materials. Molecular Simulation, 2007, 33, 305-325.	2.0	166
67	Assessment of Isoreticular Metalâ€'Organic Frameworks for Adsorption Separations:Â A Molecular Simulation Study of Methane/n-Butane Mixtures. Journal of Physical Chemistry B, 2004, 108, 15703-15708.	2.6	165
68	Molecular Simulations and NMR Measurements of Binary Diffusion in Zeolites. Journal of Physical Chemistry B, 1997, 101, 6469-6473.	2.6	154
69	Waterâ€Stable Zirconiumâ€Based Metalâ€“Organic Framework Material with Highâ€Surface Area and Gasâ€Storage Capacities. Chemistry - A European Journal, 2014, 20, 12389-12393.	3.3	150
70	Ultraporous, Water Stable, and Breathing Zirconium-Based Metalâ€“Organic Frameworks with ftw Topology. Journal of the American Chemical Society, 2015, 137, 13183-13190.	13.7	149
71	Computational screening of metal-organic frameworks for xenon/krypton separation. AICHE Journal, 2011, 57, 1759-1766.	3.6	147
72	The roles of acid strength and pore diffusion in the enhanced cracking activity of steamed Y zeolites. Applied Catalysis A: General, 1999, 177, 161-175.	4.3	144

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73	Chemical reduction of a diimide based porous polymer for selective uptake of carbon dioxide versus methane. Chemical Communications, 2010, 46, 1056.	4.1	144
74	Towards rapid computational screening of metal-organic frameworks for carbon dioxide capture: Calculation of framework charges via charge equilibration. Chemical Engineering Journal, 2011, 171, 775-781.	12.7	141
75	Simultaneously high gravimetric and volumetric methane uptake characteristics of the metalâ€“organic framework NU-111. Chemical Communications, 2013, 49, 2992.	4.1	137
76	Adsorption of CH4â^'CF4 Mixtures in Silicalite:â€‰ Simulation, Experiment, and Theory. Langmuir, 1997, 13, 6795-6804.	3.5	136
77	Computer-aided discovery of a metalâ€“organic framework with superior oxygen uptake. Nature Communications, 2018, 9, 1378.	12.8	136
78	Separation of gas mixtures using Co(ii) carborane-based porous coordination polymers. Chemical Communications, 2010, 46, 3478.	4.1	135
79	Control over Catenation in Pillared Paddlewheel Metalâ€“Organic Framework Materials via Solvent-Assisted Linker Exchange. Chemistry of Materials, 2013, 25, 739-744.	6.7	135
80	Optimal isosteric heat of adsorption for hydrogen storage and delivery using metalâ€“organic frameworks. Microporous and Mesoporous Materials, 2010, 132, 300-303.	4.4	130
81	High-Throughput Screening of Metalâ€“Organic Frameworks for Hydrogen Storage at Cryogenic Temperature. Journal of Physical Chemistry C, 2016, 120, 27328-27341.	3.1	130
82	Molecular simulation of adsorption sites of light gases in the metal-organic framework IRMOF-1. Fluid Phase Equilibria, 2007, 261, 152-161.	2.5	129
83	Enhancement of CO2/CH4 selectivity in metal-organic frameworks containing lithium cations. Microporous and Mesoporous Materials, 2011, 141, 231-235.	4.4	128
84	Molecular modelling of adsorption in novel nanoporous metalâ€“organic materials. Molecular Physics, 2004, 102, 211-221.	1.7	126
85	High-Throughput Screening of Metalâ€“Organic Frameworks for CO₂ Capture in the Presence of Water. Langmuir, 2016, 32, 10368-10376.	3.5	124
86	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	3.0	123
87	Separation and Molecular-Level Segregation of Complex Alkane Mixtures in Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 10884-10885.	13.7	116
88	Carborane-Based Metalâ€“Organic Framework with High Methane and Hydrogen Storage Capacities. Chemistry of Materials, 2013, 25, 3539-3543.	6.7	115
89	A Redox-Active Bistable Molecular Switch Mounted inside a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 14242-14245.	13.7	114
90	Carbohydrate-Mediated Purification of Petrochemicals. Journal of the American Chemical Society, 2015, 137, 5706-5719.	13.7	112

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91	Metal Alkoxide Functionalization in Metalâ˜Organic Frameworks for Enhanced Ambient-Temperature Hydrogen Storage. Journal of Physical Chemistry C, 2011, 115, 2066-2075.	3.1	111
92	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Shortn-Alkanes in Faujasite. Journal of Physical Chemistry B, 2004, 108, 13481-13491.	2.6	108
93	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. Journal of Physical Chemistry C, 2014, 118, 6941-6951.	3.1	108
94	Ultrastable Mesoporous Hydrogen-Bonded Organic Framework-Based Fiber Composites toward Mustard Gas Detoxification. Cell Reports Physical Science, 2020, 1, 100024.	5.6	107
95	Zirconium-Based Metalâ€“Organic Frameworks for the Removal of Protein-Bound Uremic Toxin from Human Serum Albumin. Journal of the American Chemical Society, 2019, 141, 2568-2576.	13.7	105
96	Structureâ€“Activity Relationships That Identify Metalâ€“Organic Framework Catalysts for Methane Activation. ACS Catalysis, 2019, 9, 3576-3587.	11.2	105
97	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2017, 9, 33419-33428.	8.0	104
98	Applications of molecular modeling in heterogeneous catalysis research. Applied Catalysis A: General, 2000, 200, 23-46.	4.3	103
99	Diffusion of binary mixtures of CF4 and n-alkanes in faujasite. Separation and Purification Technology, 2000, 20, 1-13.	7.9	103
100	Large-Scale Refinement of Metalâ˜Organic Framework Structures Using Density Functional Theory. Chemistry of Materials, 2017, 29, 2521-2528.	6.7	103
101	Water stabilization of Zr₆-based metalâ€“organic frameworks via solvent-assisted ligand incorporation. Chemical Science, 2015, 6, 5172-5176.	7.4	102
102	High volumetric uptake of ammonia using Cu-MOF-74/Cu-CPO-27. Dalton Transactions, 2016, 45, 4150-4153.	3.3	102
103	High xenon/krypton selectivity in a metal-organic framework with small pores and strong adsorption sites. Microporous and Mesoporous Materials, 2013, 169, 176-179.	4.4	101
104	G-quadruplex organic frameworks. Nature Chemistry, 2017, 9, 466-472.	13.6	99
105	Molecular mechanisms of liquid slip. Journal of Fluid Mechanics, 2008, 600, 257-269.	3.4	96
106	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. The Journal of Physical Chemistry, 1994, 98, 11948-11961.	2.9	93
107	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. Journal of Materials Chemistry A, 2016, 4, 529-536.	10.3	93
108	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. Journal of Physical Chemistry C, 2013, 117, 20116-20126.	3.1	92

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109	Characterization of Acidic OH Groups in Zeolites of Different Types:Â An Interpretation of NH3-TPD Results in the Light of Confinement Effects. Journal of Physical Chemistry B, 2002, 106, 3882-3889.	2.6	89
110	A hierarchical atomistic/lattice simulation approach for the prediction of adsorption thermodynamics of benzene in silicalite. The Journal of Physical Chemistry, 1994, 98, 5111-5119.	2.9	87
111	Identifying promising metalâ€“organic frameworks for heterogeneous catalysis via highâ€throughput periodic density functional theory. Journal of Computational Chemistry, 2019, 40, 1305-1318.	3.3	87
112	Mesoporous Thin Films of â€œMolecular Squaresâ€•as Sensors for Volatile Organic Compounds. Langmuir, 2000, 16, 3964-3970.	3.5	86
113	One-dimensional zeolites as hydrocarbon traps. Microporous and Mesoporous Materials, 2002, 56, 55-64.	4.4	85
114	Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 3143-3152.	3.1	85
115	Creating Optimal Pockets in a Clathrochelate-Based Metalâ€“Organic Framework for Gas Adsorption and Separation: Experimental and Computational Studies. Journal of the American Chemical Society, 2022, 144, 3737-3745.	13.7	85
116	Water adsorption in hydrophobic nanopores: Monte Carlo simulations of water in silicalite. Microporous and Mesoporous Materials, 2006, 90, 293-298.	4.4	84
117	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. Journal of Physical Chemistry C, 2014, 118, 5383-5389.	3.1	84
118	A thermodynamic tank model for studying the effect of higher hydrocarbons on natural gas storage in metalâ€“organic frameworks. Energy and Environmental Science, 2015, 8, 1501-1510.	30.8	84
119	Electrochemically addressable trisradical rotaxanes organized within a metalâ€“organic framework. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11161-11168.	7.1	83
120	A new perspective on the order-nalgorithm for computing correlation functions. Molecular Simulation, 2009, 35, 1084-1097.	2.0	82
121	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. Journal of Physical Chemistry C, 2010, 114, 10527-10534.	3.1	82
122	High-Throughput Computational Screening of Multivariate Metalâ€“Organic Frameworks (MTV-MOFs) for CO₂ Capture. Journal of Physical Chemistry Letters, 2017, 8, 6135-6141.	4.6	82
123	How Reproducible are Surface Areas Calculated from the BET Equation?. Advanced Materials, 2022, 34, .	21.0	82
124	Is catenation beneficial for hydrogen storage in metalâ€“organic frameworks?. Chemical Communications, 2008, , 4132.	4.1	80
125	Fine-Tuning a Robust Metalâ€“Organic Framework toward Enhanced Clean Energy Gas Storage. Journal of the American Chemical Society, 2021, 143, 18838-18843.	13.7	79
126	Effects of Molecular Siting and Adsorbent Heterogeneity on the Ideality of Adsorption Equilibria. Langmuir, 2004, 20, 2489-2497.	3.5	78

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127	Isoreticular Series of (3,24)-Connected Metalâ€“Organic Frameworks: Facile Synthesis and High Methane Uptake Properties. Chemistry of Materials, 2014, 26, 1912-1917.	6.7	76
128	Optimization of Two-Stage Pressure/Vacuum Swing Adsorption with Variable Dehydration Level for Postcombustion Carbon Capture. Industrial & Engineering Chemistry Research, 2016, 55, 3338-3350.	3.7	75
129	Adsorption of Liquid-Phase Alkane Mixtures in Silicalite:Â Simulations and Experiment. Langmuir, 2004, 20, 150-156.	3.5	74
130	Enhanced Hydrogen Uptake and the Electronic Structure of Lithium-Doped Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 9278-9284.	3.1	74
131	Development of a General Evaluation Metric for Rapid Screening of Adsorbent Materials for Postcombustion CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 11529-11539.	6.7	74
132	Predicting membrane flux of CH4 and CF4 mixtures in Faujasite from molecular simulations. AICHE Journal, 2001, 47, 2032-2041.	3.6	73
133	Grand Canonical Monte Carlo Simulations of Nonrigid Molecules:Â Siting and Segregation in Silicalite Zeolite. Langmuir, 2000, 16, 3910-3919.	3.5	72
134	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. Adsorption, 2021, 27, 683-760.	3.0	72
135	Method for Analyzing Structural Changes of Flexible Metalâ^'Organic Frameworks Induced by Adsorbates. Journal of Physical Chemistry C, 2009, 113, 19317-19327.	3.1	71
136	Strategies for Characterization of Large-Pore Metal-Organic Frameworks by Combined Experimental and Computational Methods. Chemistry of Materials, 2009, 21, 4768-4777.	6.7	68
137	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. Chemical Science, 2015, 6, 384-389.	7.4	68
138	Monte Carlo simulation of n-alkane adsorption isotherms in carbon slit pores. Journal of Chemical Physics, 2007, 126, 134708.	3.0	67
139	Tuning the Redox Activity of Metalâ€“Organic Frameworks for Enhanced, Selective O₂ Binding: Design Rules and Ambient Temperature O₂ Chemisorption in a Cobaltâ€“Triazolate Framework. Journal of the American Chemical Society, 2020, 142, 4317-4328.	13.7	67
140	Nanoconfinement and mass transport in metalâ€“organic frameworks. Chemical Society Reviews, 2021, 50, 11530-11558.	38.1	67
141	Molecular Traffic Control in a Nanoscale System. Physical Review Letters, 2000, 84, 2893-2896.	7.8	66
142	Siting and Segregation Effects of Simple Molecules in Zeolites MFI, MOR, and BOG. Journal of Physical Chemistry B, 1998, 102, 6720-6731.	2.6	65
143	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. Chemistry of Materials, 2017, 29, 6315-6328.	6.7	65
144	Computational Study of Water Adsorption in the Hydrophobic Metalâ€“Organic Framework ZIF-8: Adsorption Mechanism and Acceleration of the Simulations. Journal of Physical Chemistry C, 2017, 121, 24000-24010.	3.1	62

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145	Molecular modelling and machine learning for high-throughput screening of metal-organic frameworks for hydrogen storage. Molecular Simulation, 2019, 45, 1069-1081.	2.0	62
146	Molecular Simulations of Methane Adsorption in Silicalite. Molecular Simulation, 1991, 8, 73-92.	2.0	61
147	110th Anniversary: Surrogate Models Based on Artificial Neural Networks To Simulate and Optimize Pressure Swing Adsorption Cycles for CO₂ Capture. Industrial & Engineering Chemistry Research, 2019, 58, 18241-18252.	3.7	61
148	Stepwise adsorption in a mesoporous metalâ€“organic framework: experimental and computational analysis. Chemical Communications, 2012, 48, 3297.	4.1	60
149	Adsorption and molecular siting of CO₂, water, and other gases in the superhydrophobic, flexible pores of FMOF-1 from experiment and simulation. Chemical Science, 2017, 8, 3989-4000.	7.4	60
150	Adsorption isotherm sensitivity to small changes in zeolite structure. Chemical Physics Letters, 1999, 308, 155-159.	2.6	59
151	Molecular modeling of binary liquid-phase adsorption of aromatics in silicalite. AICHE Journal, 2004, 50, 463-469.	3.6	59
152	Self-Diffusion of Chain Molecules in the Metalâ€“Organic Framework IRMOF-1: Simulation and Experiment. Journal of Physical Chemistry Letters, 2012, 3, 930-933.	4.6	59
153	Liquid Slip in Nanoscale Channels as a Rate Process. Physical Review Letters, 2007, 98, 226001.	7.8	58
154	Modeling Water and Ammonia Adsorption in Hydrophobic Metalâ€“Organic Frameworks: Single Components and Mixtures. Journal of Physical Chemistry C, 2014, 118, 1102-1110.	3.1	57
155	Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry C, 2018, 122, 12362-12368.	3.1	55
156	Molecular Squares as Molecular Sieves: Size-Selective Transport Through Porous-Membrane-Supported Thin-Film Materials. Advanced Materials, 2001, 13, 1895.	21.0	53
157	Chiral Co(II) Metalâ€“Organic Framework in the Heterogeneous Catalytic Oxidation of Alkenes under Aerobic and Anaerobic Conditions. ACS Catalysis, 2014, 4, 1032-1039.	11.2	53
158	Computational Predictions and Experimental Validation of Alkane Oxidative Dehydrogenation by Fe₂M MOF Nodes. ACS Catalysis, 2020, 10, 1460-1469.	11.2	53
159	Isothermal Titration Calorimetry to Explore the Parameter Space of Organophosphorus Agrochemical Adsorption in MOFs. Journal of the American Chemical Society, 2020, 142, 12357-12366.	13.7	53
160	Fast and Accurate Machine Learning Strategy for Calculating Partial Atomic Charges in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2021, 17, 3052-3064.	5.3	53
161	Prediction of Structure and Properties of Boron-Based Covalent Organic Frameworks by a First-Principles Derived Force Field. Journal of Physical Chemistry C, 2012, 116, 4921-4929.	3.1	52
162	The effect of pyridine modification of Niâ€“DOBDC on CO₂ capture under humid conditions. Chemical Communications, 2014, 50, 3296-3298.	4.1	52

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163	Packing Effects in the Liquid-Phase Adsorption of C5-C22n-Alkanes on ZSM-5. Journal of Physical Chemistry B, 2003, 107, 10760-10766.	2.6	51
164	A kinetic study of vapor-phase cyclohexene epoxidation by H2O2 over mesoporous TS-1. Journal of Catalysis, 2015, 326, 107-115.	6.2	51
165	Investigation of particle damping mechanism via particle dynamics simulations. Granular Matter, 2009, 11, 417-429.	2.2	50
166	Particle dynamics simulations of a piston-based particle damper. Powder Technology, 2009, 189, 115-125.	4.2	50
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