

Randall Q Snurr

List of Publications by Year in descending order

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336
papers

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354
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354
docs citations

354
times ranked

24861
citing authors

#	ARTICLE	IF	CITATIONS
1	Ultrahigh Porosity in Metal-Organic Frameworks. <i>Science</i> , 2010, 329, 424-428.	6.0	3,306
2	De novo synthesis of a metal-organic framework material featuring ultrahigh surface area and gas storage capacities. <i>Nature Chemistry</i> , 2010, 2, 944-948.	6.6	1,535
3	Metal-Organic Framework Materials with Ultrahigh Surface Areas: Is the Sky the Limit?. <i>Journal of the American Chemical Society</i> , 2012, 134, 15016-15021.	6.6	1,497
4	A facile synthesis of UiO-66, UiO-67 and their derivatives. <i>Chemical Communications</i> , 2013, 49, 9449.	2.2	1,340
5	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. <i>Molecular Simulation</i> , 2016, 42, 81-101.	0.9	1,266
6	Large-scale screening of hypothetical metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 83-89.	6.6	1,098
7	Review and Analysis of Molecular Simulations of Methane, Hydrogen, and Acetylene Storage in Metal-Organic Frameworks. <i>Chemical Reviews</i> , 2012, 112, 703-723.	23.0	1,085
8	Development and Evaluation of Porous Materials for Carbon Dioxide Separation and Capture. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11586-11596.	7.2	1,025
9	Applicability of the BET Method for Determining Surface Areas of Microporous Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2007, 129, 8552-8556.	6.6	885
10	Vapor-Phase Metalation by Atomic Layer Deposition in a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2013, 135, 10294-10297.	6.6	821
11	Screening of Metal-Organic Frameworks for Carbon Dioxide Capture from Flue Gas Using a Combined Experimental and Modeling Approach. <i>Journal of the American Chemical Society</i> , 2009, 131, 18198-18199.	6.6	816
12	Destruction of chemical warfare agents using metal-organic frameworks. <i>Nature Materials</i> , 2015, 14, 512-516.	13.3	790
13	Metal-organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. <i>Chemical Society Reviews</i> , 2017, 46, 3357-3385.	18.7	707
14	Design of New Materials for Methane Storage. <i>Langmuir</i> , 2004, 20, 2683-2689.	1.6	663
15	Using molecular simulation to characterise metal-organic frameworks for adsorption applications. <i>Chemical Society Reviews</i> , 2009, 38, 1237.	18.7	613
16	Effects of Surface Area, Free Volume, and Heat of Adsorption on Hydrogen Uptake in Metal-Organic Frameworks. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9565-9570.	1.2	558
17	Separation of CO ₂ from CH ₄ Using Mixed-Ligand Metal-Organic Frameworks. <i>Langmuir</i> , 2008, 24, 8592-8598.	1.6	557
18	Computation-Ready, Experimental Metal-Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. <i>Chemistry of Materials</i> , 2014, 26, 6185-6192.	3.2	524

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19	Enhanced CO ₂ Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. <i>Chemistry of Materials</i> , 2009, 21, 1425-1430.	3.2	523
20	Light-Harvesting and Ultrafast Energy Migration in Porphyrin-Based Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2013, 135, 862-869.	6.6	510
21	Calculating Geometric Surface Areas as a Characterization Tool for Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15350-15356.	1.5	498
22	Understanding Inflections and Steps in Carbon Dioxide Adsorption Isotherms in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2008, 130, 406-407.	6.6	485
23	Perfluoroalkane Functionalization of NU-1000 via Solvent-Assisted Ligand Incorporation: Synthesis and CO ₂ Adsorption Studies. <i>Journal of the American Chemical Society</i> , 2013, 135, 16801-16804.	6.6	473
24	High Propene/Propane Selectivity in Isostructural Metal-Organic Frameworks with High Densities of Open Metal Sites. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1857-1860.	7.2	392
25	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal-Organic Framework Database: CoRE MOF 2019. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 5985-5998.	1.0	372
26	Enhancement of CO ₂ /N ₂ selectivity in a metal-organic framework by cavity modification. <i>Journal of Materials Chemistry</i> , 2009, 19, 2131.	6.7	370
27	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. <i>The Journal of Physical Chemistry</i> , 1993, 97, 13742-13752.	2.9	366
28	Object-oriented Programming Paradigms for Molecular Modeling. <i>Molecular Simulation</i> , 2003, 29, 29-46.	0.9	360
29	Carborane-based metal-organic frameworks as highly selective sorbents for CO ₂ over methane. <i>Chemical Communications</i> , 2008, , 4135.	2.2	349
30	High-throughput computational screening of metal-organic frameworks. <i>Chemical Society Reviews</i> , 2014, 43, 5735-5749.	18.7	336
31	Structure-property relationships of porous materials for carbon dioxide separation and capture. <i>Energy and Environmental Science</i> , 2012, 5, 9849.	15.6	334
32	Ultrahigh Surface Area Zirconium MOFs and Insights into the Applicability of the BET Theory. <i>Journal of the American Chemical Society</i> , 2015, 137, 3585-3591.	6.6	329
33	The materials genome in action: identifying the performance limits for methane storage. <i>Energy and Environmental Science</i> , 2015, 8, 1190-1199.	15.6	314
34	Highly Selective Carbon Dioxide Uptake by [Cu(bpy) ₂ (SiF ₆)] (bpy-1 =) Tj ETQq0 0 0 rgBT /Overlock 1 3663-3666.	6.6	303
35	Exceptional Negative Thermal Expansion in Isoreticular Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 4496-4499.	7.2	289
36	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. <i>CheM</i> , 2016, 1, 154-169.	5.8	286

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37	Synthesis, Properties, and Gas Separation Studies of a Robust Diimide-Based Microporous Organic Polymer. <i>Chemistry of Materials</i> , 2009, 21, 3033-3035.	3.2	272
38	Nanoporous Carbohydrate Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2012, 134, 406-417.	6.6	271
39	CD-MOF: A Versatile Separation Medium. <i>Journal of the American Chemical Society</i> , 2016, 138, 2292-2301.	6.6	269
40	Kinetic Separation of Propene and Propane in Metal-Organic Frameworks: Controlling Diffusion Rates in Plate-Shaped Crystals via Tuning of Pore Apertures and Crystallite Aspect Ratios. <i>Journal of the American Chemical Society</i> , 2011, 133, 5228-5231.	6.6	263
41	Evaluation of the BET Method for Determining Surface Areas of MOFs and Zeolites that Contain Ultra-Micropores. <i>Langmuir</i> , 2010, 26, 5475-5483.	1.6	257
42	Incorporation of an A1/A2-Difunctionalized Pillar[5]arene into a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2012, 134, 17436-17439.	6.6	254
43	An Extended Charge Equilibration Method. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2506-2511.	2.1	253
44	Prospects for nanoporous metal-organic materials in advanced separations processes. <i>AIChE Journal</i> , 2004, 50, 1090-1095.	1.8	249
45	Thermodynamic analysis of Xe/Kr selectivity in over 137,000 hypothetical metal-organic frameworks. <i>Chemical Science</i> , 2012, 3, 2217.	3.7	248
46	Evaluating topologically diverse metal-organic frameworks for cryo-adsorbed hydrogen storage. <i>Energy and Environmental Science</i> , 2016, 9, 3279-3289.	15.6	231
47	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. <i>Science Advances</i> , 2016, 2, e1600909.	4.7	231
48	Water adsorption in UiO-66: the importance of defects. <i>Chemical Communications</i> , 2014, 50, 11329-11331.	2.2	227
49	Molecular Modeling and Experimental Studies of the Thermodynamic and Transport Properties of Pyridinium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2821-2832.	1.2	226
50	Monomolecular cracking of n-hexane on Y, MOR, and ZSM-5 zeolites. <i>Applied Catalysis A: General</i> , 1999, 179, 71-86.	2.2	219
51	Gram-scale, high-yield synthesis of a robust metal-organic framework for storing methane and other gases. <i>Energy and Environmental Science</i> , 2013, 6, 1158.	15.6	219
52	Screening of bio-compatible metal-organic frameworks as potential drug carriers using Monte Carlo simulations. <i>Journal of Materials Chemistry B</i> , 2014, 2, 766-774.	2.9	215
53	Heats of Adsorption for Seven Gases in Three Metal-Organic Frameworks: Systematic Comparison of Experiment and Simulation. <i>Langmuir</i> , 2009, 25, 7383-7388.	1.6	212
54	Framework-Topology-Dependent Catalytic Activity of Zirconium-Based (Porphinato)zinc(II) MOFs. <i>Journal of the American Chemical Society</i> , 2016, 138, 14449-14457.	6.6	210

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55	Nanosizing a Metal-Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. ACS Nano, 2016, 10, 9174-9182.	7.3	202
56	Application of Consistency Criteria To Calculate BET Areas of Micro- And Mesoporous Metal-Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 215-224.	6.6	201
57	Designing Higher Surface Area Metal-Organic Frameworks: Are Triple Bonds Better Than Phenyls?. Journal of the American Chemical Society, 2012, 134, 9860-9863.	6.6	198
58	Computational Design of Metal-Organic Frameworks Based on Stable Zirconium Building Units for Storage and Delivery of Methane. Chemistry of Materials, 2014, 26, 5632-5639.	3.2	191
59	Design Requirements for Metal-Organic Frameworks as Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 18794-18803.	1.5	190
60	Energy-based descriptors to rapidly predict hydrogen storage in metal-organic frameworks. Molecular Systems Design and Engineering, 2019, 4, 162-174.	1.7	179
61	Topologically Guided, Automated Construction of Metal-Organic Frameworks and Their Evaluation for Energy-Related Applications. Crystal Growth and Design, 2017, 17, 5801-5810.	1.4	176
62	Large-Scale Quantitative Structure-Property Relationship (QSPR) Analysis of Methane Storage in Metal-Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	1.5	174
63	A combined experimental and quantum chemical study of CO ₂ adsorption in the metal-organic framework CPO-27 with different metals. Chemical Science, 2013, 4, 3544.	3.7	172
64	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	8.3	172
65	Machine learning the quantum-chemical properties of metal-organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
66	Recent developments in the molecular modeling of diffusion in nanoporous materials. Molecular Simulation, 2007, 33, 305-325.	0.9	166
67	Assessment of Isoreticular Metal-Organic Frameworks for Adsorption Separations: A Molecular Simulation Study of Methane/n-Butane Mixtures. Journal of Physical Chemistry B, 2004, 108, 15703-15708.	1.2	165
68	Molecular Simulations and NMR Measurements of Binary Diffusion in Zeolites. Journal of Physical Chemistry B, 1997, 101, 6469-6473.	1.2	154
69	Water-Stable Zirconium-Based Metal-Organic Framework Material with High Surface Area and Gas Storage Capacities. Chemistry - A European Journal, 2014, 20, 12389-12393.	1.7	150
70	Ultraporous, Water Stable, and Breathing Zirconium-Based Metal-Organic Frameworks with ftw Topology. Journal of the American Chemical Society, 2015, 137, 13183-13190.	6.6	149
71	Computational screening of metal-organic frameworks for xenon/krypton separation. AIChE Journal, 2011, 57, 1759-1766.	1.8	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.	2.2	144

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73	Chemical reduction of a diimide based porous polymer for selective uptake of carbon dioxide versus methane. <i>Chemical Communications</i> , 2010, 46, 1056.	2.2	144
74	Towards rapid computational screening of metal-organic frameworks for carbon dioxide capture: Calculation of framework charges via charge equilibration. <i>Chemical Engineering Journal</i> , 2011, 171, 775-781.	6.6	141
75	Simultaneously high gravimetric and volumetric methane uptake characteristics of the metal-organic framework NU-111. <i>Chemical Communications</i> , 2013, 49, 2992.	2.2	137
76	Adsorption of CH ₄ /CF ₄ Mixtures in Silicalite: Simulation, Experiment, and Theory. <i>Langmuir</i> , 1997, 13, 6795-6804.	1.6	136
77	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. <i>Nature Communications</i> , 2018, 9, 1378.	5.8	136
78	Separation of gas mixtures using Co(ii) carborane-based porous coordination polymers. <i>Chemical Communications</i> , 2010, 46, 3478.	2.2	135
79	Control over Catenation in Pillared Paddlewheel Metal-Organic Framework Materials via Solvent-Assisted Linker Exchange. <i>Chemistry of Materials</i> , 2013, 25, 739-744.	3.2	135
80	Optimal isosteric heat of adsorption for hydrogen storage and delivery using metal-organic frameworks. <i>Microporous and Mesoporous Materials</i> , 2010, 132, 300-303.	2.2	130
81	High-Throughput Screening of Metal-Organic Frameworks for Hydrogen Storage at Cryogenic Temperature. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27328-27341.	1.5	130
82	Molecular simulation of adsorption sites of light gases in the metal-organic framework IRMOF-1. <i>Fluid Phase Equilibria</i> , 2007, 261, 152-161.	1.4	129
83	Enhancement of CO ₂ /CH ₄ selectivity in metal-organic frameworks containing lithium cations. <i>Microporous and Mesoporous Materials</i> , 2011, 141, 231-235.	2.2	128
84	Molecular modelling of adsorption in novel nanoporous metal-organic materials. <i>Molecular Physics</i> , 2004, 102, 211-221.	0.8	126
85	High-Throughput Screening of Metal-Organic Frameworks for CO ₂ Capture in the Presence of Water. <i>Langmuir</i> , 2016, 32, 10368-10376.	1.6	124
86	Identification Schemes for Metal-Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. <i>Crystal Growth and Design</i> , 2019, 19, 6682-6697.	1.4	123
87	Separation and Molecular-Level Segregation of Complex Alkane Mixtures in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2008, 130, 10884-10885.	6.6	116
88	Carborane-Based Metal-Organic Framework with High Methane and Hydrogen Storage Capacities. <i>Chemistry of Materials</i> , 2013, 25, 3539-3543.	3.2	115
89	A Redox-Active Bistable Molecular Switch Mounted inside a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 14242-14245.	6.6	114
90	Carbohydrate-Mediated Purification of Petrochemicals. <i>Journal of the American Chemical Society</i> , 2015, 137, 5706-5719.	6.6	112

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91	Metal Alkoxide Functionalization in Metal-Organic Frameworks for Enhanced Ambient-Temperature Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2066-2075.	1.5	111
92	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Shortn-Alkanes in Faujasite. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13481-13491.	1.2	108
93	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6941-6951.	1.5	108
94	Ultrastable Mesoporous Hydrogen-Bonded Organic Framework-Based Fiber Composites toward Mustard Gas Detoxification. <i>Cell Reports Physical Science</i> , 2020, 1, 100024.	2.8	107
95	Zirconium-Based Metal-Organic Frameworks for the Removal of Protein-Bound Uremic Toxin from Human Serum Albumin. <i>Journal of the American Chemical Society</i> , 2019, 141, 2568-2576.	6.6	105
96	Structure-Activity Relationships That Identify Metal-Organic Framework Catalysts for Methane Activation. <i>ACS Catalysis</i> , 2019, 9, 3576-3587.	5.5	105
97	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 33419-33428.	4.0	104
98	Applications of molecular modeling in heterogeneous catalysis research. <i>Applied Catalysis A: General</i> , 2000, 200, 23-46.	2.2	103
99	Diffusion of binary mixtures of CF ₄ and n-alkanes in faujasite. <i>Separation and Purification Technology</i> , 2000, 20, 1-13.	3.9	103
100	Large-Scale Refinement of Metal-Organic Framework Structures Using Density Functional Theory. <i>Chemistry of Materials</i> , 2017, 29, 2521-2528.	3.2	103
101	Water stabilization of Zr ₆ -based metal-organic frameworks via solvent-assisted ligand incorporation. <i>Chemical Science</i> , 2015, 6, 5172-5176.	3.7	102
102	High volumetric uptake of ammonia using Cu-MOF-74/Cu-CPO-27. <i>Dalton Transactions</i> , 2016, 45, 4150-4153.	1.6	102
103	High xenon/krypton selectivity in a metal-organic framework with small pores and strong adsorption sites. <i>Microporous and Mesoporous Materials</i> , 2013, 169, 176-179.	2.2	101
104	G-quadruplex organic frameworks. <i>Nature Chemistry</i> , 2017, 9, 466-472.	6.6	99
105	Molecular mechanisms of liquid slip. <i>Journal of Fluid Mechanics</i> , 2008, 600, 257-269.	1.4	96
106	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. <i>The Journal of Physical Chemistry</i> , 1994, 98, 11948-11961.	2.9	93
107	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. <i>Journal of Materials Chemistry A</i> , 2016, 4, 529-536.	5.2	93
108	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20116-20126.	1.5	92

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109	Characterization of Acidic OH Groups in Zeolites of Different Types: An Interpretation of NH ₃ -TPD Results in the Light of Confinement Effects. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3882-3889.	1.2	89
110	A hierarchical atomistic/lattice simulation approach for the prediction of adsorption thermodynamics of benzene in silicalite. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5111-5119.	2.9	87
111	Identifying promising metal-organic frameworks for heterogeneous catalysis via high-throughput periodic density functional theory. <i>Journal of Computational Chemistry</i> , 2019, 40, 1305-1318.	1.5	87
112	Mesoporous Thin Films of α -Molecular Squares as Sensors for Volatile Organic Compounds. <i>Langmuir</i> , 2000, 16, 3964-3970.	1.6	86
113	One-dimensional zeolites as hydrocarbon traps. <i>Microporous and Mesoporous Materials</i> , 2002, 56, 55-64.	2.2	85
114	Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3143-3152.	1.5	85
115	Creating Optimal Pockets in a Clathrochelate-Based Metal-Organic Framework for Gas Adsorption and Separation: Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2022, 144, 3737-3745.	6.6	85
116	Water adsorption in hydrophobic nanopores: Monte Carlo simulations of water in silicalite. <i>Microporous and Mesoporous Materials</i> , 2006, 90, 293-298.	2.2	84
117	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5383-5389.	1.5	84
118	A thermodynamic tank model for studying the effect of higher hydrocarbons on natural gas storage in metal-organic frameworks. <i>Energy and Environmental Science</i> , 2015, 8, 1501-1510.	15.6	84
119	Electrochemically addressable trisradical rotaxanes organized within a metal-organic framework. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 11161-11168.	3.3	83
120	A new perspective on the order- n algorithm for computing correlation functions. <i>Molecular Simulation</i> , 2009, 35, 1084-1097.	0.9	82
121	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10527-10534.	1.5	82
122	High-Throughput Computational Screening of Multivariate Metal-Organic Frameworks (MTV-MOFs) for CO ₂ Capture. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 6135-6141.	2.1	82
123	How Reproducible are Surface Areas Calculated from the BET Equation?. <i>Advanced Materials</i> , 2022, 34, .	11.1	82
124	Is catenation beneficial for hydrogen storage in metal-organic frameworks?. <i>Chemical Communications</i> , 2008, , 4132.	2.2	80
125	Fine-Tuning a Robust Metal-Organic Framework toward Enhanced Clean Energy Gas Storage. <i>Journal of the American Chemical Society</i> , 2021, 143, 18838-18843.	6.6	79
126	Effects of Molecular Siting and Adsorbent Heterogeneity on the Ideality of Adsorption Equilibria. <i>Langmuir</i> , 2004, 20, 2489-2497.	1.6	78

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127	Isorecticular Series of (3,24)-Connected Metal-Organic Frameworks: Facile Synthesis and High Methane Uptake Properties. <i>Chemistry of Materials</i> , 2014, 26, 1912-1917.	3.2	76
128	Optimization of Two-Stage Pressure/Vacuum Swing Adsorption with Variable Dehydration Level for Postcombustion Carbon Capture. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 3338-3350.	1.8	75
129	Adsorption of Liquid-Phase Alkane Mixtures in Silicalite: Simulations and Experiment. <i>Langmuir</i> , 2004, 20, 150-156.	1.6	74
130	Enhanced Hydrogen Uptake and the Electronic Structure of Lithium-Doped Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9278-9284.	1.5	74
131	Development of a General Evaluation Metric for Rapid Screening of Adsorbent Materials for Postcombustion CO ₂ Capture. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 11529-11539.	3.2	74
132	Predicting membrane flux of CH ₄ and CF ₄ mixtures in Faujasite from molecular simulations. <i>AIChE Journal</i> , 2001, 47, 2032-2041.	1.8	73
133	Grand Canonical Monte Carlo Simulations of Nonrigid Molecules: Siting and Segregation in Silicalite Zeolite. <i>Langmuir</i> , 2000, 16, 3910-3919.	1.6	72
134	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. <i>Adsorption</i> , 2021, 27, 683-760.	1.4	72
135	Method for Analyzing Structural Changes of Flexible Metal-Organic Frameworks Induced by Adsorbates. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19317-19327.	1.5	71
136	Strategies for Characterization of Large-Pore Metal-Organic Frameworks by Combined Experimental and Computational Methods. <i>Chemistry of Materials</i> , 2009, 21, 4768-4777.	3.2	68
137	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. <i>Chemical Science</i> , 2015, 6, 384-389.	3.7	68
138	Monte Carlo simulation of n-alkane adsorption isotherms in carbon slit pores. <i>Journal of Chemical Physics</i> , 2007, 126, 134708.	1.2	67
139	Tuning the Redox Activity of Metal-Organic Frameworks for Enhanced, Selective O ₂ Binding: Design Rules and Ambient Temperature O ₂ Chemisorption in a Cobalt-Triazolate Framework. <i>Journal of the American Chemical Society</i> , 2020, 142, 4317-4328.	6.6	67
140	Nanoconfinement and mass transport in metal-organic frameworks. <i>Chemical Society Reviews</i> , 2021, 50, 11530-11558.	18.7	67
141	Molecular Traffic Control in a Nanoscale System. <i>Physical Review Letters</i> , 2000, 84, 2893-2896.	2.9	66
142	Siting and Segregation Effects of Simple Molecules in Zeolites MFI, MOR, and BOG. <i>Journal of Physical Chemistry B</i> , 1998, 102, 6720-6731.	1.2	65
143	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. <i>Chemistry of Materials</i> , 2017, 29, 6315-6328.	3.2	65
144	Computational Study of Water Adsorption in the Hydrophobic Metal-Organic Framework ZIF-8: Adsorption Mechanism and Acceleration of the Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24000-24010.	1.5	62

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145	Molecular modelling and machine learning for high-throughput screening of metal-organic frameworks for hydrogen storage. <i>Molecular Simulation</i> , 2019, 45, 1069-1081.	0.9	62
146	Molecular Simulations of Methane Adsorption in Silicalite. <i>Molecular Simulation</i> , 1991, 8, 73-92.	0.9	61
147	<i><i>110th Anniversary</i></i> : Surrogate Models Based on Artificial Neural Networks To Simulate and Optimize Pressure Swing Adsorption Cycles for CO ₂ Capture. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 18241-18252.	1.8	61
148	Stepwise adsorption in a mesoporous metal-organic framework: experimental and computational analysis. <i>Chemical Communications</i> , 2012, 48, 3297.	2.2	60
149	Adsorption and molecular siting of CO ₂ , water, and other gases in the superhydrophobic, flexible pores of FMOF-1 from experiment and simulation. <i>Chemical Science</i> , 2017, 8, 3989-4000.	3.7	60
150	Adsorption isotherm sensitivity to small changes in zeolite structure. <i>Chemical Physics Letters</i> , 1999, 308, 155-159.	1.2	59
151	Molecular modeling of binary liquid-phase adsorption of aromatics in silicalite. <i>AIChE Journal</i> , 2004, 50, 463-469.	1.8	59
152	Self-Diffusion of Chain Molecules in the Metal-Organic Framework IRMOF-1: Simulation and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 930-933.	2.1	59
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