

Randall Q Snurr

List of Publications by Year in descending order

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336
papers

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docs citations

354
times ranked

24861
citing authors

#	ARTICLE	IF	CITATIONS
1	Realizing the data-driven, computational discovery of metal-organic framework catalysts. <i>Current Opinion in Chemical Engineering</i> , 2022, 35, 100760.	3.8	28
2	Applying design principles to improve hydrogen storage capacity in nanoporous materials. <i>Brazilian Journal of Chemical Engineering</i> , 2022, 39, 919-931.	0.7	3
3	Gating effect for gas adsorption in microporous materials—mechanisms and applications. <i>Chemical Society Reviews</i> , 2022, 51, 1139-1166.	18.7	34
4	In silico design of microporous polymers for chemical separations and storage. <i>Current Opinion in Chemical Engineering</i> , 2022, 36, 100795.	3.8	6
5	Exploring mechanistic routes for light alkane oxidation with an iron—triazolate metal—organic framework. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8129-8141.	1.3	6
6	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
7	Electrical Regulation of CO ₂ Adsorption in the Metal—Organic Framework MIL-53. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 13904-13913.	4.0	6
8	Insights into Mass Transfer Barriers in Metal—Organic Frameworks. <i>Chemistry of Materials</i> , 2022, 34, 4134-4141.	3.2	16
9	High-throughput predictions of metal—organic framework electronic properties: theoretical challenges, graph neural networks, and data exploration. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	43
10	How Reproducible are Surface Areas Calculated from the BET Equation?. <i>Advanced Materials</i> , 2022, 34, .	11.1	82
11	Interfacial Unit-Dependent Catalytic Activity for CO Oxidation over Cerium Oxysulfate Cluster Assemblies. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 33515-33524.	4.0	2
12	Separation of Aromatic Hydrocarbons in Porous Materials. <i>Journal of the American Chemical Society</i> , 2022, 144, 12212-12218.	6.6	47
13	Molecular Simulations of Adsorption and Diffusion in Crystalline Nanoporous Materials. , 2021, , 199-319.		2
14	Nanoconfinement and mass transport in metal—organic frameworks. <i>Chemical Society Reviews</i> , 2021, 50, 11530-11558.	18.7	67
15	Inverse design of nanoporous crystalline reticular materials with deep generative models. <i>Nature Machine Intelligence</i> , 2021, 3, 76-86.	8.3	172
16	Fast and Accurate Machine Learning Strategy for Calculating Partial Atomic Charges in Metal—Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3052-3064.	2.3	53
17	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. <i>Adsorption</i> , 2021, 27, 683-760.	1.4	72
18	Ammonia Capture within Zirconium Metal—Organic Frameworks: Reversible and Irreversible Uptake. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 20081-20093.	4.0	36

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19	Zirconium Metal-Organic Frameworks Integrating Chloride Ions for Ammonia Capture and/or Chemical Separation. ACS Applied Materials & Interfaces, 2021, 13, 22485-22494.	4.0	27
20	Machine learning the quantum-chemical properties of metal-organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
21	Insights into Catalytic Hydrolysis of Organophosphonates at -OH Sites of Azolate-Based Metal Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 9893-9900.	6.6	45
22	Selective Photodimerization in a Cyclodextrin Metal-Organic Framework. Journal of the American Chemical Society, 2021, 143, 9129-9139.	6.6	34
23	Molecular fingerprint and machine learning to accelerate design of high-performance homochiral metal-organic frameworks. AIChE Journal, 2021, 67, e17352.	1.8	15
24	Machine learning using host/guest energy histograms to predict adsorption in metal-organic frameworks: Application to short alkanes and Xe/Kr mixtures. Journal of Chemical Physics, 2021, 155, 014701.	1.2	24
25	Molecular Siting of C1-C6 Alkanes in ZIF-4: A Hybrid Monte Carlo Study. Journal of Physical Chemistry C, 2021, 125, 16256-16267.	1.5	3
26	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. Science Advances, 2021, 7, .	4.7	47
27	Art of Architecture: Efficient Transport through Solvent-Filled Metal-Organic Frameworks Regulated by Topology. Chemistry of Materials, 2021, 33, 6832-6840.	3.2	12
28	Transport Diffusion of Linear Alkanes (C ₅ -C ₁₆) through Thin Films of ZIF-8 as Assessed by Quartz Crystal Microgravimetry. Langmuir, 2021, 37, 9405-9414.	1.6	9
29	Computational Screening of Metal-Catecholate-Functionalized Metal-Organic Frameworks for Room-Temperature Hydrogen Storage. Journal of Physical Chemistry C, 2021, 125, 21701-21708.	1.5	9
30	Fine-Tuning a Robust Metal-Organic Framework toward Enhanced Clean Energy Gas Storage. Journal of the American Chemical Society, 2021, 143, 18838-18843.	6.6	79
31	Computational Predictions and Experimental Validation of Alkane Oxidative Dehydrogenation by Fe ₂ M MOF Nodes. ACS Catalysis, 2020, 10, 1460-1469.	5.5	53
32	Insights into Catalytic Gas-Phase Hydrolysis of Organophosphate Chemical Warfare Agents by MOF-Supported Bimetallic Metal-Oxo Clusters. ACS Applied Materials & Interfaces, 2020, 12, 14631-14640.	4.0	18
33	Computational Screening of Metal-Organic Framework-Supported Single-Atom Transition-Metal Catalysts for the Gas-Phase Hydrolysis of Nerve Agents. ACS Catalysis, 2020, 10, 1310-1323.	5.5	39
34	Exploring the Effects of Node Topology, Connectivity, and Metal Identity on the Binding of Nerve Agents and Their Hydrolysis Products in Metal-Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 35657-35675.	4.0	17
35	Topology-Dependent Alkane Diffusion in Zirconium Metal-Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 56049-56059.	4.0	18
36	Zr ₆ O ₈ Node-Catalyzed Butene Hydrogenation and Isomerization in the Metal-Organic Framework NU-1000. ACS Catalysis, 2020, 10, 14959-14970.	5.5	24

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37	Do Internal and External Surfaces of Metal-Organic Frameworks Have the Same Hydrophobicity? Insights from Molecular Simulations. <i>Langmuir</i> , 2020, 36, 13070-13078.	1.6	9
38	Investigating the Process and Mechanism of Molecular Transport within a Representative Solvent-Filled Metal-Organic Framework. <i>Langmuir</i> , 2020, 36, 10853-10859.	1.6	18
39	Supramolecular Porous Assemblies of Atomically Precise Catalytically Active Cerium-Based Clusters. <i>Chemistry of Materials</i> , 2020, 32, 8522-8529.	3.2	23
40	Tuning the Atrazine Binding Sites in an Indium-Based Flexible Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 44762-44768.	4.0	11
41	Exploring the Tunability of Trimetallic MOF Nodes for Partial Oxidation of Methane to Methanol. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 28217-28231.	4.0	46
42	Topological effects on separation of alkane isomers in metal-organic frameworks. <i>Fluid Phase Equilibria</i> , 2020, 519, 112642.	1.4	8
43	Comparing GGA, GGA+ <i>U</i> , and meta-GGA functionals for redox-dependent binding at open metal sites in metal-organic frameworks. <i>Journal of Chemical Physics</i> , 2020, 152, 224101.	1.2	16
44	Structure and activity of mixed VO _x -CeO ₂ domains supported on alumina in cyclohexane oxidative dehydrogenation. <i>Journal of Catalysis</i> , 2020, 384, 147-158.	3.1	17
45	High-Valent Metal-Oxo Species at the Nodes of Metal-Triazolate Frameworks: The Effects of Ligand Exchange and Two-State Reactivity for C-H Bond Activation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19494-19502.	7.2	14
46	High-Valent Metal-Oxo Species at the Nodes of Metal-Triazolate Frameworks: The Effects of Ligand Exchange and Two-State Reactivity for C-H Bond Activation. <i>Angewandte Chemie</i> , 2020, 132, 19662-19670.	1.6	9
47	Process-level modelling and optimization to evaluate metal-organic frameworks for post-combustion capture of CO ₂ . <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1205-1218.	1.7	37
48	Isothermal Titration Calorimetry to Explore the Parameter Space of Organophosphorus Agrochemical Adsorption in MOFs. <i>Journal of the American Chemical Society</i> , 2020, 142, 12357-12366.	6.6	53
49	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
50	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
51	Understanding the Loading Dependence of Adsorbate Diffusivities in Hierarchical Metal-Organic Frameworks. <i>Langmuir</i> , 2020, 36, 1372-1378.	1.6	18
52	Single-Crystal Polycationic Polymers Obtained by Single-Crystal-to-Single-Crystal Photopolymerization. <i>Journal of the American Chemical Society</i> , 2020, 142, 6180-6187.	6.6	50
53	DFT Study on the Catalytic Activity of ALD-Grown Iron Oxide Nanoclusters for Partial Oxidation of Methane to Methanol. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1580-1592.	1.1	7
54	Interplay of Lewis and Brønsted Acid Sites in Zr-Based Metal-Organic Frameworks for Efficient Esterification of Biomass-Derived Levulinic Acid. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 32090-32096.	4.0	44

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55	A Hierarchical Nanoporous Diamondoid Superstructure. <i>CheM</i> , 2019, 5, 2353-2364.	5.8	23
56	It's an Interesting MOF, but Is It Stable?. <i>Matter</i> , 2019, 1, 26-27.	5.0	4
57	Computational screening, synthesis and testing of metal-organic frameworks with a bithiazole linker for carbon dioxide capture and its green conversion into cyclic carbonates. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 1000-1013.	1.7	24
58	High Propane and Isobutane Adsorption Cooling Capacities in Zirconium-Based Metal-Organic Frameworks Predicted by Molecular Simulations. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 18242-18246.	3.2	14
59	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
60	Prediction of hydrogen adsorption in nanoporous materials from the energy distribution of adsorption sites. <i>Molecular Physics</i> , 2019, 117, 3683-3694.	0.8	23
61	Impact of H ₂ O and CO ₂ on methane storage in metal-organic frameworks. <i>Adsorption</i> , 2019, 25, 1633-1642.	1.4	8
62	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
63	110th Anniversary: 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
64	Energy-based descriptors to rapidly predict hydrogen storage in metal-organic frameworks. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 162-174.	1.7	179
65	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
66	Elucidating the mechanism of the UiO-66-catalyzed sulfide oxidation: activity and selectivity enhancements through changes in the node coordination environment and solvent. <i>Catalysis Science and Technology</i> , 2019, 9, 327-335.	2.1	40
67	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
68	Investigation of the Hydrophobic Nature of Metal Oxide Surfaces Created by Atomic Layer Deposition. <i>Langmuir</i> , 2019, 35, 5762-5769.	1.6	31
69	Structure-Activity Relationships That Identify Metal-Organic Framework Catalysts for Methane Activation. <i>ACS Catalysis</i> , 2019, 9, 3576-3587.	5.5	105
70	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
71	The effect of co-adsorbed solvent molecules on H ₂ binding to metal alkoxides. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9218-9224.	1.3	2
72	Screening for Improved Nerve Agent Simulants and Insights into Organophosphate Hydrolysis Reactions from DFT and QSAR Modeling. <i>Chemistry - A European Journal</i> , 2019, 25, 9217-9229.	1.7	26

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73	Toward Design Rules of Metal-Organic Frameworks for Adsorption Cooling: Effect of Topology on the Ethanol Working Capacity. <i>Chemistry of Materials</i> , 2019, 31, 2702-2706.	3.2	27
74	Interactions of VO _x Species with Amorphous TiO ₂ Domains on ALD-Derived Alumina-Supported Materials. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7988-7999.	1.5	11
75	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
76	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. <i>Catalysis Today</i> , 2018, 312, 149-157.	2.2	16
77	Tunable Crystallinity and Charge Transfer in Two-Dimensional G-Quadruplex Organic Frameworks. <i>Angewandte Chemie</i> , 2018, 130, 4049-4053.	1.6	10
78	Theoretical insights into direct methane to methanol conversion over supported dicopper oxo nanoclusters. <i>Catalysis Today</i> , 2018, 312, 2-9.	2.2	23
79	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. <i>Nature Communications</i> , 2018, 9, 1378.	5.8	136
80	Tunable Crystallinity and Charge Transfer in Two-Dimensional G-Quadruplex Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3985-3989.	7.2	26
81	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metal-Organic Frameworks for Adsorption Applications. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 365-376.	2.3	18
82	Competitive Adsorption of Methyl Bromide and Water on Metal Catecholates: Insights from Density Functional Theory. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 17488-17495.	1.8	5
83	Evidence for Copper Dimers in Low-Loaded CuO/SiO ₂ Catalysts for Cyclohexane Oxidative Dehydrogenation. <i>ACS Catalysis</i> , 2018, 8, 9775-9789.	5.5	11
84	Molecular Modeling of Carbon Dioxide Adsorption in Metal-Organic Frameworks. , 2018, , 99-149.		6
85	Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metal-Organic Framework NU-1000. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12362-12368.	1.5	55
86	Anomaly in the Chain Length Dependence of n-Alkane Diffusion in ZIF-4 Metal-Organic Frameworks. <i>Molecules</i> , 2018, 23, 668.	1.7	15
87	Proton Conduction in Tröger's Base-Linked Poly(crown ether)s. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 25303-25310.	4.0	27
88	Comprehensive Phase Diagrams of MoS ₂ Edge Sites Using Dispersion-Corrected DFT Free Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15318-15329.	1.5	18
89	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. <i>Chemical Engineering Science</i> , 2017, 159, 18-30.	1.9	26
90	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

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91	Optimizing Open Iron Sites in Metal-Organic Frameworks for Ethane Oxidation: A First-Principles Study. ACS Applied Materials & Interfaces, 2017, 9, 33484-33492.	4.0	44
92	Metal-organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. Chemical Society Reviews, 2017, 46, 3357-3385.	18.7	707
93	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. Journal of Physical Chemistry C, 2017, 121, 10463-10469.	1.5	20
94	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metal-Organic Frameworks. ACS Applied Materials & Interfaces, 2017, 9, 33419-33428.	4.0	104
95	G-quadruplex organic frameworks. Nature Chemistry, 2017, 9, 466-472.	6.6	99
96	Correction to "Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation". Journal of Physical Chemistry C, 2017, 121, 20553-20553.	1.5	1
97	Computational Study of Water Adsorption in the Hydrophobic Metal-Organic Framework ZIF-8: Adsorption Mechanism and Acceleration of the Simulations. Journal of Physical Chemistry C, 2017, 121, 24000-24010.	1.5	62
98	Elucidating the Nanoparticle-Metal Organic Framework Interface of Pt@ZIF-8 Catalysts. Journal of Physical Chemistry C, 2017, 121, 25079-25091.	1.5	28
99	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
100	High-Throughput Computational Screening of Multivariate Metal-Organic Frameworks (MTV-MOFs) for CO ₂ Capture. Journal of Physical Chemistry Letters, 2017, 8, 6135-6141.	2.1	82
101	Ab Initio Screening of Metal Catecholates for Adsorption of Toxic Pnictogen Hydride Gases. Industrial & Engineering Chemistry Research, 2017, 56, 14324-14336.	1.8	8
102	Computational screening of functional groups for capture of toxic industrial chemicals in porous materials. Physical Chemistry Chemical Physics, 2017, 19, 31766-31772.	1.3	1
103	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. Chemistry of Materials, 2017, 29, 6315-6328.	3.2	65
104	Large-Scale Refinement of Metal-Organic Framework Structures Using Density Functional Theory. Chemistry of Materials, 2017, 29, 2521-2528.	3.2	103
105	Evaluating topologically diverse metal-organic frameworks for cryo-adsorbed hydrogen storage. Energy and Environmental Science, 2016, 9, 3279-3289.	15.6	231
106	Alkaline-earth metal-oxide overlayers on TiO ₂ : application toward CO ₂ photoreduction. Catalysis Science and Technology, 2016, 6, 7885-7895.	2.1	29
107	Nanosizing a Metal-Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. ACS Nano, 2016, 10, 9174-9182.	7.3	202
108	High-Throughput Screening of Metal-Organic Frameworks for CO ₂ Capture in the Presence of Water. Langmuir, 2016, 32, 10368-10376.	1.6	124

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109	CO ₂ adsorption-induced structural changes in coordination polymer ligands elucidated via molecular simulations and experiments. Dalton Transactions, 2016, 45, 17168-17178.	1.6	11
110	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. Chem, 2016, 1, 154-169.	5.8	286
111	High-Throughput Screening of Metal-Organic Frameworks for Hydrogen Storage at Cryogenic Temperature. Journal of Physical Chemistry C, 2016, 120, 27328-27341.	1.5	130
112	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. Science Advances, 2016, 2, e1600909.	4.7	231
113	Using Gas-Phase Clusters to Screen Porphyrin-Supported Nanocluster Catalysts for Ethane Oxidation to Ethanol. Catalysis Letters, 2016, 146, 2566-2573.	1.4	10
114	A Redox-Active Bistable Molecular Switch Mounted inside a Metal-Organic Framework. Journal of the American Chemical Society, 2016, 138, 14242-14245.	6.6	114
115	Framework-Topology-Dependent Catalytic Activity of Zirconium-Based (Porphinato)zinc(II) MOFs. Journal of the American Chemical Society, 2016, 138, 14449-14457.	6.6	210
116	CD-MOF: A Versatile Separation Medium. Journal of the American Chemical Society, 2016, 138, 2292-2301.	6.6	269
117	Optimization of Two-Stage Pressure/Vacuum Swing Adsorption with Variable Dehydration Level for Postcombustion Carbon Capture. Industrial & Engineering Chemistry Research, 2016, 55, 3338-3350.	1.8	75
118	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. Journal of Materials Chemistry A, 2016, 4, 529-536.	5.2	93
119	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
120	High volumetric uptake of ammonia using Cu-MOF-74/Cu-CPO-27. Dalton Transactions, 2016, 45, 4150-4153.	1.6	102
121	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. Molecular Simulation, 2016, 42, 81-101.	0.9	1,266
122	Computer-Aided Search for Materials to Store Natural Gas for Vehicles. Frontiers for Young Minds, 2015, 3, .	0.8	2
123	Understanding the Effects of Preadsorbed Perfluoroalkanes on the Adsorption of Water and Ammonia in MOFs. Journal of Physical Chemistry C, 2015, 119, 3163-3170.	1.5	20
124	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	15.6	314
125	Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metal-Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 3143-3152.	1.5	85
126	Ultrahigh Surface Area Zirconium MOFs and Insights into the Applicability of the BET Theory. Journal of the American Chemical Society, 2015, 137, 3585-3591.	6.6	329

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127	Destruction of chemical warfare agents using metal-organic frameworks. <i>Nature Materials</i> , 2015, 14, 512-516.	13.3	790
128	A MOF platform for incorporation of complementary organic motifs for CO ₂ binding. <i>Chemical Communications</i> , 2015, 51, 12478-12481.	2.2	45
129	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. <i>Chemical Science</i> , 2015, 6, 384-389.	3.7	68
130	Continuous fractional component Monte Carlo simulations of high-density adsorption in metal-organic frameworks. <i>Molecular Simulation</i> , 2015, 41, 1339-1347.	0.9	6
131	Pore Size Dependence of Adsorption and Separation of Thiophene/Benzene Mixtures in Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15263-15273.	1.5	39
132	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
133	A kinetic study of vapor-phase cyclohexene epoxidation by H ₂ O ₂ over mesoporous TS-1. <i>Journal of Catalysis</i> , 2015, 326, 107-115.	3.1	51
134	Carbohydrate-Mediated Purification of Petrochemicals. <i>Journal of the American Chemical Society</i> , 2015, 137, 5706-5719.	6.6	112
135	Computational Screening of Metal Catecholates for Ammonia Capture in Metal-Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 3257-3267.	1.8	27
136	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
137	A modelling approach for MOF-encapsulated metal catalysts and application to n-butane oxidation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27596-27608.	1.3	19
138	Optimization of Pressure/Vacuum Swing Adsorption with Variable Dehydration Levels for Post Combustion Carbon Capture. <i>Computer Aided Chemical Engineering</i> , 2015, 37, 2447-2452.	0.3	0
139	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
140	Heterogeneous Diffusion of Alkanes in the Hierarchical Metal-Organic Framework NU-1000. <i>Langmuir</i> , 2015, 31, 10056-10065.	1.6	32
141	Ultraporous, Water Stable, and Breathing Zirconium-Based Metal-Organic Frameworks with ftw Topology. <i>Journal of the American Chemical Society</i> , 2015, 137, 13183-13190.	6.6	149
142	Diffusion of methane and other alkanes in metal-organic frameworks for natural gas storage. <i>Chemical Engineering Science</i> , 2015, 124, 135-143.	1.9	34
143	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework. <i>AIChE Journal</i> , 2014, 60, 2324-2334.	1.8	14
144	The effect of pyridine modification of Ni-DOBDC on CO ₂ capture under humid conditions. <i>Chemical Communications</i> , 2014, 50, 3296-3298.	2.2	52

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145	High-throughput computational screening of metal-organic frameworks. <i>Chemical Society Reviews</i> , 2014, 43, 5735-5749.	18.7	336
146	Metallacarborane-Based Metal-Organic Framework with a Complex Topology. <i>Crystal Growth and Design</i> , 2014, 14, 1324-1330.	1.4	28
147	Chiral Co(II) Metal-Organic Framework in the Heterogeneous Catalytic Oxidation of Alkenes under Aerobic and Anaerobic Conditions. <i>ACS Catalysis</i> , 2014, 4, 1032-1039.	5.5	53
148	Textural properties of a large collection of computationally constructed MOFs and zeolites. <i>Microporous and Mesoporous Materials</i> , 2014, 186, 207-213.	2.2	38
149	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
150	High propylene/propane adsorption selectivity in a copper(catecholate)-decorated porous organic polymer. <i>Journal of Materials Chemistry A</i> , 2014, 2, 299-302.	5.2	46
151	Modeling Water and Ammonia Adsorption in Hydrophobic Metal-Organic Frameworks: Single Components and Mixtures. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1102-1110.	1.5	57
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