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	Realizing the data-driven, computational discovery of metal-organic framework catalysts. Current Opinion in Chemical Engineering, 2022, 35, 100760.	7.8	28
2	Applying design principles to improve hydrogen storage capacity in nanoporous materials. Brazilian Journal of Chemical Engineering, 2022, 39, 919-931.	1.3	3
3	Gating effect for gas adsorption in microporous materialsâ€"mechanisms and applications. Chemical Society Reviews, 2022, 51, 1139-1166.	38.1	34
4	In silico design of microporous polymers for chemical separations and storage. Current Opinion in Chemical Engineering, 2022, 36, 100795.	7.8	6
5	Exploring mechanistic routes for light alkane oxidation with an ironâ€"triazolate metalâ€"organic framework. Physical Chemistry Chemical Physics, 2022, 24, 8129-8141.	2.8	6
6	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
7	Electrical Regulation of CO₂ Adsorption in the Metalâ€"Organic Framework MIL-53. ACS Applied Materials & Interfaces, 2022, 14, 13904-13913.	8.0	6
8	Insights into Mass Transfer Barriers in Metalâ€"Organic Frameworks. Chemistry of Materials, 2022, 34, 4134-4141.	6.7	16
9	High-throughput predictions of metalâ€"organic framework electronic properties: theoretical challenges, graph neural networks, and data exploration. Npj Computational Materials, 2022, 8, .	8.7	43
10	How Reproducible are Surface Areas Calculated from the BET Equation?. Advanced Materials, 2022, 34, .	21.0	82
11	Interfacial Unit-Dependent Catalytic Activity for CO Oxidation over Cerium Oxysulfate Cluster Assemblies. ACS Applied Materials & Interfaces, 2022, 14, 33515-33524.	8.0	2
12	Separation of Aromatic Hydrocarbons in Porous Materials. Journal of the American Chemical Society, 2022, 144, 12212-12218.	13.7	47
13	Molecular Simulations of Adsorption and Diffusion in Crystalline Nanoporous Materials. , 2021, , 199-319.		2
14	Nanoconfinement and mass transport in metalâ€"organic frameworks. Chemical Society Reviews, 2021, 50, 11530-11558.	38.1	67
15	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
16	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
17	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. Adsorption, 2021, 27, 683-760.	3.0	72
18	Ammonia Capture within Zirconium Metalâ€"Organic Frameworks: Reversible and Irreversible Uptake. ACS Applied Materials & Interfaces, 2021, 13, 20081-20093.	8.0	36

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19	Zirconium Metalâ€“Organic Frameworks Integrating Chloride Ions for Ammonia Capture and/or Chemical Separation. ACS Applied Materials & Interfaces, 2021, 13, 22485-22494.	8.0	27
20	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	10.0	170
21	Insights into Catalytic Hydrolysis of Organophosphonates at Mâ€“OH Sites of Azolate-Based Metal Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 9893-9900.	13.7	45
22	Selective Photodimerization in a Cyclodextrin Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 9129-9139.	13.7	34
23	Molecular fingerprint and machine learning to accelerate design of <scp>highâ€performance</scp> homochiral metalâ€“organic frameworks. AICHE Journal, 2021, 67, e17352.	3.6	15
24	Machine learning using host/guest energy histograms to predict adsorption in metalâ€“organic frameworks: Application to short alkanes and Xe/Kr mixtures. Journal of Chemical Physics, 2021, 155, 014701.	3.0	24
25	Molecular Siting of C1â€“C6 n-Alkanes in ZIF-4: A Hybrid Monte Carlo Study. Journal of Physical Chemistry C, 2021, 125, 16256-16267.	3.1	3
26	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. Science Advances, 2021, 7, .	10.3	47
27	Art of Architecture: Efficient Transport through Solvent-Filled Metalâ€“Organic Frameworks Regulated by Topology. Chemistry of Materials, 2021, 33, 6832-6840.	6.7	12
28	Transport Diffusion of Linear Alkanes (C₅â€“C₁₆) through Thin Films of ZIF-8 as Assessed by Quartz Crystal Microgravimetry. Langmuir, 2021, 37, 9405-9414.	3.5	9
29	Computational Screening of Metal-Catecholate-Functionalized Metalâ€“Organic Frameworks for Room-Temperature Hydrogen Storage. Journal of Physical Chemistry C, 2021, 125, 21701-21708.	3.1	9
30	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
31	Computational Predictions and Experimental Validation of Alkane Oxidative Dehydrogenation by Fe₂M MOF Nodes. ACS Catalysis, 2020, 10, 1460-1469.	11.2	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.	8.0	18
33	Computational Screening of Metalâ€“Organic Framework-Supported Single-Atom Transition-Metal Catalysts for the Gas-Phase Hydrolysis of Nerve Agents. ACS Catalysis, 2020, 10, 1310-1323.	11.2	39
34	Exploring the Effects of Node Topology, Connectivity, and Metal Identity on the Binding of Nerve Agents and Their Hydrolysis Products in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 35657-35675.	8.0	17
35	Topology-Dependent Alkane Diffusion in Zirconium Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 56049-56059.	8.0	18
36	Zr₆O₈ Node-Catalyzed Butene Hydrogenation and Isomerization in the Metalâ€“Organic Framework NU-1000. ACS Catalysis, 2020, 10, 14959-14970.	11.2	24

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37	Do Internal and External Surfaces of Metalâ€“Organic Frameworks Have the Same Hydrophobicity? Insights from Molecular Simulations. Langmuir, 2020, 36, 13070-13078.	3.5	9
38	Investigating the Process and Mechanism of Molecular Transport within a Representative Solvent-Filled Metalâ€“Organic Framework. Langmuir, 2020, 36, 10853-10859.	3.5	18
39	Supramolecular Porous Assemblies of Atomically Precise Catalytically Active Cerium-Based Clusters. Chemistry of Materials, 2020, 32, 8522-8529.	6.7	23
40	Tuning the Atrazine Binding Sites in an Indium-Based Flexible Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2020, 12, 44762-44768.	8.0	11
41	Exploring the Tunability of Trimetallic MOF Nodes for Partial Oxidation of Methane to Methanol. ACS Applied Materials & Interfaces, 2020, 12, 28217-28231.	8.0	46
42	Topological effects on separation of alkane isomers in metalâ^'organic frameworks. Fluid Phase Equilibria, 2020, 519, 112642.	2.5	8
43	Comparing GGA, GGA+U, and meta-GGA functionals for redox-dependent binding at open metal sites in metalâ€“organic frameworks. Journal of Chemical Physics, 2020, 152, 224101.	3.0	16
44	Structure and activity of mixed VOx-CeO2 domains supported on alumina in cyclohexane oxidative dehydrogenation. Journal of Catalysis, 2020, 384, 147-158.	6.2	17
45	Highâ€Valent Metalâ€“Oxo Species at the Nodes of Metalâ€“Triazolate Frameworks: The Effects of Ligand Exchange and Twoâ€State Reactivity for Câ^'H Bond Activation. Angewandte Chemie - International Edition, 2020, 59, 19494-19502.	13.8	14
46	Highâ€Valent Metalâ€“Oxo Species at the Nodes of Metalâ€“Triazolate Frameworks: The Effects of Ligand Exchange and Twoâ€State Reactivity for Câ^'H Bond Activation. Angewandte Chemie, 2020, 132, 19662-19670.	2.0	9
47	Process-level modelling and optimization to evaluate metalâ€“organic frameworks for post-combustion capture of CO₂. Molecular Systems Design and Engineering, 2020, 5, 1205-1218.	3.4	37
48	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
49	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
50	Ultrastable Mesoporous Hydrogen-Bonded Organic Framework-Based Fiber Composites toward Mustard Gas Detoxification. Cell Reports Physical Science, 2020, 1, 100024.	5.6	107
51	Understanding the Loading Dependence of Adsorbate Diffusivities in Hierarchical Metalâ€“Organic Frameworks. Langmuir, 2020, 36, 1372-1378.	3.5	18
52	Single-Crystal Polycationic Polymers Obtained by Single-Crystal-to-Single-Crystal Photopolymerization. Journal of the American Chemical Society, 2020, 142, 6180-6187.	13.7	50
53	DFT Study on the Catalytic Activity of ALD-Grown Diiron Oxide Nanoclusters for Partial Oxidation of Methane to Methanol. Journal of Physical Chemistry A, 2020, 124, 1580-1592.	2.5	7
54	Interplay of Lewis and BrÃ¸nsted Acid Sites in Zr-Based Metalâ€“Organic Frameworks for Efficient Esterification of Biomass-Derived Levulinic Acid. ACS Applied Materials & Interfaces, 2019, 11, 32090-32096.	8.0	44

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55	A Hierarchical Nanoporous Diamondoid Superstructure. CheM, 2019, 5, 2353-2364.	11.7	23
56	Itâ€™s an Interesting MOF, but Is It Stable?. Matter, 2019, 1, 26-27.	10.0	4
57	Computational screening, synthesis and testing of metalâ€“organic frameworks with a bithiazole linker for carbon dioxide capture and its green conversion into cyclic carbonates. Molecular Systems Design and Engineering, 2019, 4, 1000-1013.	3.4	24
58	High Propane and Isobutane Adsorption Cooling Capacities in Zirconium-Based Metalâ€“Organic Frameworks Predicted by Molecular Simulations. ACS Sustainable Chemistry and Engineering, 2019, 7, 18242-18246.	6.7	14
59	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
60	Prediction of hydrogen adsorption in nanoporous materials from the energy distribution of adsorption sites. Molecular Physics, 2019, 117, 3683-3694.	1.7	23
61	Impact of H2O and CO2 on methane storage in metalâ€“organic frameworks. Adsorption, 2019, 25, 1633-1642.	3.0	8
62	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	3.0	123
63	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
64	Energy-based descriptors to rapidly predict hydrogen storage in metalâ€“organic frameworks. Molecular Systems Design and Engineering, 2019, 4, 162-174.	3.4	179
65	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
66	Elucidating the mechanism of the UiO-66-catalyzed sulfide oxidation: activity and selectivity enhancements through changes in the node coordination environment and solvent. Catalysis Science and Technology, 2019, 9, 327-335.	4.1	40
67	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
68	Investigation of the Hydrophobic Nature of Metal Oxide Surfaces Created by Atomic Layer Deposition. Langmuir, 2019, 35, 5762-5769.	3.5	31
69	Structureâ€“Activity Relationships That Identify Metalâ€“Organic Framework Catalysts for Methane Activation. ACS Catalysis, 2019, 9, 3576-3587.	11.2	105
70	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
71	The effect of co-adsorbed solvent molecules on H₂ binding to metal alkoxides. Physical Chemistry Chemical Physics, 2019, 21, 9218-9224.	2.8	2
72	Screening for Improved Nerve Agent Simulants and Insights into Organophosphate Hydrolysis Reactions from DFT and QSAR Modeling. Chemistry - A European Journal, 2019, 25, 9217-9229.	3.3	26

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73	Toward Design Rules of Metalâ€“Organic Frameworks for Adsorption Cooling: Effect of Topology on the Ethanol Working Capacity. Chemistry of Materials, 2019, 31, 2702-2706.	6.7	27
74	Interactions of VOx Species with Amorphous TiO2 Domains on ALD-Derived Alumina-Supported Materials. Journal of Physical Chemistry C, 2019, 123, 7988-7999.	3.1	11
75	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
76	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157.	4.4	16
77	Tunable Crystallinity and Charge Transfer in Twoâ€Dimensional Gâ€Quadruplex Organic Frameworks. Angewandte Chemie, 2018, 130, 4049-4053.	2.0	10
78	Theoretical insights into direct methane to methanol conversion over supported dicopper oxo nanoclusters. Catalysis Today, 2018, 312, 2-9.	4.4	23
79	Computer-aided discovery of a metalâ€“organic framework with superior oxygen uptake. Nature Communications, 2018, 9, 1378.	12.8	136
80	Tunable Crystallinity and Charge Transfer in Twoâ€Dimensional Gâ€Quadruplex Organic Frameworks. Angewandte Chemie - International Edition, 2018, 57, 3985-3989.	13.8	26
81	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metalâ€“Organic Frameworks for Adsorption Applications. Journal of Chemical Theory and Computation, 2018, 14, 365-376.	5.3	18
82	Competitive Adsorption of Methyl Bromide and Water on Metal Catecholates: Insights from Density Functional Theory. Industrial & Engineering Chemistry Research, 2018, 57, 17488-17495.	3.7	5
83	Evidence for Copper Dimers in Low-Loaded CuO_x/SiO₂ Catalysts for Cyclohexane Oxidative Dehydrogenation. ACS Catalysis, 2018, 8, 9775-9789.	11.2	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 Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry C, 2018, 122, 12362-12368.	3.1	55
86	Anomaly in the Chain Length Dependence of n-Alkane Diffusion in ZIF-4 Metal-Organic Frameworks. Molecules, 2018, 23, 668.	3.8	15
87	Proton Conduction in TrÃ¶gerâ€™s Base-Linked Poly(crown ether)s. ACS Applied Materials & Interfaces, 2018, 10, 25303-25310.	8.0	27
88	Comprehensive Phase Diagrams of MoS₂ Edge Sites Using Dispersion-Corrected DFT Free Energy Calculations. Journal of Physical Chemistry C, 2018, 122, 15318-15329.	3.1	18
89	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. Chemical Engineering Science, 2017, 159, 18-30.	3.8	26
90	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

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91	Optimizing Open Iron Sites in Metalâ€“Organic Frameworks for Ethane Oxidation: A First-Principles Study. ACS Applied Materials & Interfaces, 2017, 9, 33484-33492.	8.0	44
92	Metalâ€“organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. Chemical Society Reviews, 2017, 46, 3357-3385.	38.1	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.	3.1	20
94	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2017, 9, 33419-33428.	8.0	104
95	G-quadruplex organic frameworks. Nature Chemistry, 2017, 9, 466-472.	13.6	99
96	Correction to â€œCatechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separationâ€• Journal of Physical Chemistry C, 2017, 121, 20553-20553.	3.1	1
97	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
98	Elucidating the Nanoparticleâ€“Metal Organic Framework Interface of Pt@ZIF-8 Catalysts. Journal of Physical Chemistry C, 2017, 121, 25079-25091.	3.1	28
99	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
100	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
101	Ab Initio Screening of Metal Catecholates for Adsorption of Toxic Pnictogen Hydride Gases. Industrial & Engineering Chemistry Research, 2017, 56, 14324-14336.	3.7	8
102	Computational screening of functional groups for capture of toxic industrial chemicals in porous materials. Physical Chemistry Chemical Physics, 2017, 19, 31766-31772.	2.8	1
103	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. Chemistry of Materials, 2017, 29, 6315-6328.	6.7	65
104	Large-Scale Refinement of Metalâ€'Organic Framework Structures Using Density Functional Theory. Chemistry of Materials, 2017, 29, 2521-2528.	6.7	103
105	Evaluating topologically diverse metalâ€“organic frameworks for cryo-adsorbed hydrogen storage. Energy and Environmental Science, 2016, 9, 3279-3289.	30.8	231
106	Alkaline-earth metal-oxide overlayers on TiO₂: application toward CO₂ photoreduction. Catalysis Science and Technology, 2016, 6, 7885-7895.	4.1	29
107	Nanosizing a Metalâ€“Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. ACS Nano, 2016, 10, 9174-9182.	14.6	202
108	High-Throughput Screening of Metalâ€“Organic Frameworks for CO₂ Capture in the Presence of Water. Langmuir, 2016, 32, 10368-10376.	3.5	124

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109	CO₂ adsorption-induced structural changes in coordination polymer ligands elucidated via molecular simulations and experiments. Dalton Transactions, 2016, 45, 17168-17178.	3.3	11
110	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. CheM, 2016, 1, 154-169.	11.7	286
111	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
112	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. Science Advances, 2016, 2, e1600909.	10.3	231
113	Using Gas-Phase Clusters to Screen Porphyrin-Supported Nanocluster Catalysts for Ethane Oxidation to Ethanol. Catalysis Letters, 2016, 146, 2566-2573.	2.6	10
114	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
115	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
116	CD-MOF: A Versatile Separation Medium. Journal of the American Chemical Society, 2016, 138, 2292-2301.	13.7	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.	3.7	75
118	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
119	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
120	High volumetric uptake of ammonia using Cu-MOF-74/Cu-CPO-27. Dalton Transactions, 2016, 45, 4150-4153.	3.3	102
121	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. Molecular Simulation, 2016, 42, 81-101.	2.0	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.	3.1	20
124	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	30.8	314
125	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
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.	13.7	329

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127	Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516.	27.5	790
128	A MOF platform for incorporation of complementary organic motifs for CO₂ binding. Chemical Communications, 2015, 51, 12478-12481.	4.1	45
129	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. Chemical Science, 2015, 6, 384-389.	7.4	68
130	Continuous fractional component Monte Carlo simulations of high-density adsorption in metalâ€“organic frameworks. Molecular Simulation, 2015, 41, 1339-1347.	2.0	6
131	Pore Size Dependence of Adsorption and Separation of Thiophene/Benzene Mixtures in Zeolites. Journal of Physical Chemistry C, 2015, 119, 15263-15273.	3.1	39
132	Water stabilization of Zr₆-based metalâ€“organic frameworks via solvent-assisted ligand incorporation. Chemical Science, 2015, 6, 5172-5176.	7.4	102
133	A kinetic study of vapor-phase cyclohexene epoxidation by H2O2 over mesoporous TS-1. Journal of Catalysis, 2015, 326, 107-115.	6.2	51
134	Carbohydrate-Mediated Purification of Petrochemicals. Journal of the American Chemical Society, 2015, 137, 5706-5719.	13.7	112
135	Computational Screening of Metal Catecholates for Ammonia Capture in Metalâ€“Organic Frameworks. Industrial & Engineering Chemistry Research, 2015, 54, 3257-3267.	3.7	27
136	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
137	A modelling approach for MOF-encapsulated metal catalysts and application to n-butane oxidation. Physical Chemistry Chemical Physics, 2015, 17, 27596-27608.	2.8	19
138	Optimization of Pressure/Vacuum Swing Adsorption with Variable Dehydration Levels for Post Combustion Carbon Capture. Computer Aided Chemical Engineering, 2015, 37, 2447-2452.	0.5	0
139	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
140	Heterogeneous Diffusion of Alkanes in the Hierarchical Metalâ€“Organic Framework NU-1000. Langmuir, 2015, 31, 10056-10065.	3.5	32
141	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
142	Diffusion of methane and other alkanes in metal-organic frameworks for natural gas storage. Chemical Engineering Science, 2015, 124, 135-143.	3.8	34
143	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metalâ€organic framework. AICHE Journal, 2014, 60, 2324-2334.	3.6	14
144	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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145	High-throughput computational screening of metalâ€“organic frameworks. Chemical Society Reviews, 2014, 43, 5735-5749.	38.1	336
146	Metallacarborane-Based Metalâ€“Organic Framework with a Complex Topology. Crystal Growth and Design, 2014, 14, 1324-1330.	3.0	28
147	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
148	Textural properties of a large collection of computationally constructed MOFs and zeolites. Microporous and Mesoporous Materials, 2014, 186, 207-213.	4.4	38
149	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
150	High propylene/propane adsorption selectivity in a copper(catecholate)-decorated porous organic polymer. Journal of Materials Chemistry A, 2014, 2, 299-302.	10.3	46
151	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
152	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
153	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
154	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
155	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
156	Water adsorption in UiO-66: the importance of defects. Chemical Communications, 2014, 50, 11329-11331.	4.1	227
157	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. Journal of Physical Chemistry C, 2014, 118, 6941-6951.	3.1	108
158	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. Fluid Phase Equilibria, 2014, 366, 146-151.	2.5	14
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