Randall Q Snurr

List of Publications by Year in Descending Order

334 papers	36,690 citations	90 h-index	187 g-index
353 ext. papers	41,027 ext. citations	8.5 avg, IF	7.61 L-index

#	Paper	IF	Citations
334	Gating effect for gas adsorption in microporous materials-mechanisms and applications.. *Chemical Society Reviews*, **2022**,	58.5	5
333	In silico design of microporous polymers for chemical separations and storage. *Current Opinion in Chemical Engineering*, **2022**, 36, 100795	5.4	1
332	Realizing the data-driven, computational discovery of metal-organic framework catalysts. *Current Opinion in Chemical Engineering*, **2022**, 35, 100760	5.4	2
331	Exploring mechanistic routes for light alkane oxidation with an iron-triazolate metal-organic framework.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
330	Creating Optimal Pockets in a Clathrochelate-Based Metal-Organic Framework for Gas Adsorption and Separation: Experimental and Computational Studies.. *Journal of the American Chemical Society* , **2022**,	16.4	9
329	Insights into Mass Transfer Barriers in Metal□Organic Frameworks. *Chemistry of Materials*, **2022**, 34, 4134-4141	9.6	2
328	Fine-Tuning a Robust Metal-Organic Framework toward Enhanced Clean Energy Gas Storage. *Journal of the American Chemical Society*, **2021**, 143, 18838-18843	16.4	14
327	Fast and Accurate Machine Learning Strategy for Calculating Partial Atomic Charges in Metal-Organic Frameworks. *Journal of Chemical Theory and Computation*, **2021**, 17, 3052-3064	6.4	15
326	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. *Adsorption*, **2021**, 27, 683-760	2.6	25
325	Ammonia Capture within Zirconium Metal-Organic Frameworks: Reversible and Irreversible Uptake. *ACS Applied Materials & Interfaces*, **2021**, 13, 20081-20093	9.5	15
324	Zirconium Metal-Organic Frameworks Integrating Chloride Ions for Ammonia Capture and/or Chemical Separation. *ACS Applied Materials & Interfaces*, **2021**, 13, 22485-22494	9.5	10
323	Machine learning the quantum-chemical properties of metal□organic frameworks for accelerated materials discovery. *Matter*, **2021**, 4, 1578-1597	12.7	43
322	Insights into Catalytic Hydrolysis of Organophosphonates at M-OH Sites of Azolate-Based Metal Organic Frameworks. *Journal of the American Chemical Society*, **2021**, 143, 9893-9900	16.4	10
321	Selective Photodimerization in a Cyclodextrin Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 9129-9139	16.4	9
320	Molecular fingerprint and machine learning to accelerate design of high-performance homochiral metal□organic frameworks. *AICHE Journal*, **2021**, 67, e17352	3.6	2
319	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	3.9	6
318	Molecular Simulations of Adsorption and Diffusion in Crystalline Nanoporous Materials **2021**, 199-319		0

317	Nanoconfinement and mass transport in metal-organic frameworks. *Chemical Society Reviews*, **2021**, 50, 11530-11558	58.5	11
316	Inverse design of nanoporous crystalline reticular materials with deep generative models. *Nature Machine Intelligence*, **2021**, 3, 76-86	22.5	58
315	Molecular Siting of C1–C6 n-Alkanes in ZIF-4: A Hybrid Monte Carlo Study. *Journal of Physical Chemistry C*, **2021**, 125, 16256-16267	3.8	
314	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. *Science Advances*, **2021**, 7,	14.3	8
313	Art of Architecture: Efficient Transport through Solvent-Filled Metal–Organic Frameworks Regulated by Topology. *Chemistry of Materials*, **2021**, 33, 6832-6840	9.6	3
312	Transport Diffusion of Linear Alkanes (C-C) through Thin Films of ZIF-8 as Assessed by Quartz Crystal Microgravimetry. *Langmuir*, **2021**, 37, 9405-9414	4	2
311	Exploring the Tunability of Trimetallic MOF Nodes for Partial Oxidation of Methane to Methanol. *ACS Applied Materials & Interfaces*, **2020**, 12, 28217-28231	9.5	27
310	Topological effects on separation of alkane isomers in metal–organic frameworks. *Fluid Phase Equilibria*, **2020**, 519, 112642	2.5	5
309	Comparing GGA, GGA+U, and meta-GGA functionals for redox-dependent binding at open metal sites in metal-organic frameworks. *Journal of Chemical Physics*, **2020**, 152, 224101	3.9	8
308	Structure and activity of mixed VOx-CeO2 domains supported on alumina in cyclohexane oxidative dehydrogenation. *Journal of Catalysis*, **2020**, 384, 147-158	7.3	8
307	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. *Angewandte Chemie - International Edition*, **2020**, 59, 19494-19502	16.4	8
306	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. *Angewandte Chemie*, **2020**, 132, 19662-19670	3.6	6
305	Process-level modelling and optimization to evaluate metal–organic frameworks for post-combustion capture of CO2. *Molecular Systems Design and Engineering*, **2020**, 5, 1205-1218	4.6	17
304	Isothermal Titration Calorimetry to Explore the Parameter Space of Organophosphorus Agrochemical Adsorption in MOFs. *Journal of the American Chemical Society*, **2020**, 142, 12357-12366	16.4	26
303	Tuning the Redox Activity of Metal-Organic Frameworks for Enhanced, Selective O Binding: Design Rules and Ambient Temperature O Chemisorption in a Cobalt-Triazolate Framework. *Journal of the American Chemical Society*, **2020**, 142, 4317-4328	16.4	36
302	Ultrastable Mesoporous Hydrogen-Bonded Organic Framework-Based Fiber Composites toward Mustard Gas Detoxification. *Cell Reports Physical Science*, **2020**, 1, 100024	6.1	36
301	Understanding the Loading Dependence of Adsorbate Diffusivities in Hierarchical Metal-Organic Frameworks. *Langmuir*, **2020**, 36, 1372-1378	4	15
300	Single-Crystal Polycationic Polymers Obtained by Single-Crystal-to-Single-Crystal Photopolymerization. *Journal of the American Chemical Society*, **2020**, 142, 6180-6187	16.4	18

299	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	2.8	0
298	Computational Predictions and Experimental Validation of Alkane Oxidative Dehydrogenation by Fe2M MOF Nodes. *ACS Catalysis*, **2020**, 10, 1460-1469	13.1	27
297	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	9.5	12
296	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	13.1	25
295	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	9.5	10
294	Topology-Dependent Alkane Diffusion in Zirconium Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2020**, 12, 56049-56059	9.5	9
293	Zr6O8 Node-Catalyzed Butene Hydrogenation and Isomerization in the Metal□Organic Framework NU-1000. *ACS Catalysis*, **2020**, 10, 14959-14970	13.1	9
292	Do Internal and External Surfaces of Metal-Organic Frameworks Have the Same Hydrophobicity? Insights from Molecular Simulations. *Langmuir*, **2020**, 36, 13070-13078	4	4
291	Investigating the Process and Mechanism of Molecular Transport within a Representative Solvent-Filled Metal-Organic Framework. *Langmuir*, **2020**, 36, 10853-10859	4	10
290	Supramolecular Porous Assemblies of Atomically Precise Catalytically Active Cerium-Based Clusters. *Chemistry of Materials*, **2020**, 32, 8522-8529	9.6	10
289	Tuning the Atrazine Binding Sites in an Indium-Based Flexible Metal-Organic Framework. *ACS Applied Materials & Interfaces*, **2020**, 12, 44762-44768	9.5	9
288	Prediction of hydrogen adsorption in nanoporous materials from the energy distribution of adsorption sites** The isotherm prediction algorithm presented in this research along with some additional functionality is packaged as a python software Python Isotherm Prediction (PyIsoP) for easy use and is available on the Snurr Group GitHub https://github.com/snurr-group.View all notes. *Molecular Physics*, **2019**, 117, 3683-3694	1.7	12
287	Impact of H2O and CO2 on methane storage in metal□organic frameworks. *Adsorption*, **2019**, 25, 1633-1642	2.6	6
286	Identification Schemes for Metal□Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
285	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	3.9	32
284	Energy-based descriptors to rapidly predict hydrogen storage in metal□organic frameworks. *Molecular Systems Design and Engineering*, **2019**, 4, 162-174	4.6	100
283	Zirconium-Based Metal-Organic Frameworks for the Removal of Protein-Bound Uremic Toxin from Human Serum Albumin. *Journal of the American Chemical Society*, **2019**, 141, 2568-2576	16.4	63
282	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	5.5	27

281	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	8.3	48
280	Investigation of the Hydrophobic Nature of Metal Oxide Surfaces Created by Atomic Layer Deposition. *Langmuir*, **2019**, 35, 5762-5769	4	16
279	Structure–Activity Relationships That Identify Metal–Organic Framework Catalysts for Methane Activation. *ACS Catalysis*, **2019**, 9, 3576-3587	13.1	63
278	Molecular modelling and machine learning for high-throughput screening of metal-organic frameworks for hydrogen storage. *Molecular Simulation*, **2019**, 45, 1069-1081	2	35
277	The effect of co-adsorbed solvent molecules on H binding to metal alkoxides. *Physical Chemistry Chemical Physics*, **2019**, 21, 9218-9224	3.6	0
276	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	4.8	20
275	Toward Design Rules of Metal–Organic Frameworks for Adsorption Cooling: Effect of Topology on the Ethanol Working Capacity. *Chemistry of Materials*, **2019**, 31, 2702-2706	9.6	19
274	Interplay of Lewis and Brønsted Acid Sites in Zr-Based Metal-Organic Frameworks for Efficient Esterification of Biomass-Derived Levulinic Acid. *ACS Applied Materials & Interfaces*, **2019**, 11, 32090-32096	9.5	25
273	A Hierarchical Nanoporous Diamondoid Superstructure. *CheM*, **2019**, 5, 2353-2364	16.2	12
272	It's an Interesting MOF, but Is It Stable?. *Matter*, **2019**, 1, 26-27	12.7	3
271	Computational screening, synthesis and testing of metal–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	4.6	14
270	High Propane and Isobutane Adsorption Cooling Capacities in Zirconium-Based Metal–Organic Frameworks Predicted by Molecular Simulations. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 18242-18246	8.3	9
269	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal–Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*, **2019**, 64, 5985-5998	2.8	183
268	Interactions of VOx Species with Amorphous TiO2 Domains on ALD-Derived Alumina-Supported Materials. *Journal of Physical Chemistry C*, **2019**, 123, 7988-7999	3.8	7
267	Identifying promising metal-organic frameworks for heterogeneous catalysis via high-throughput periodic density functional theory. *Journal of Computational Chemistry*, **2019**, 40, 1305-1318	3.5	51
266	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. *Catalysis Today*, **2018**, 312, 149-157	5.3	11
265	Tunable Crystallinity and Charge Transfer in Two-Dimensional G-Quadruplex Organic Frameworks. *Angewandte Chemie*, **2018**, 130, 4049-4053	3.6	7
264	Theoretical insights into direct methane to methanol conversion over supported dicopper oxo nanoclusters. *Catalysis Today*, **2018**, 312, 2-9	5.3	16

263	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. *Nature Communications*, **2018**, 9, 1378	17.4	100
262	Tunable Crystallinity and Charge Transfer in Two-Dimensional G-Quadruplex Organic Frameworks. *Angewandte Chemie - International Edition*, **2018**, 57, 3985-3989	16.4	18
261	Anomaly in the Chain Length Dependence of n-Alkane Diffusion in ZIF-4 Metal-Organic Frameworks. *Molecules*, **2018**, 23,	4.8	12
260	Proton Conduction in Tr□ger's Base-Linked Poly(crown ether)s. *ACS Applied Materials & Interfaces*, **2018**, 10, 25303-25310	9.5	16
259	Comprehensive Phase Diagrams of MoS2 Edge Sites Using Dispersion-Corrected DFT Free Energy Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 15318-15329	3.8	15
258	Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metal-Organic Frameworks for Adsorption Applications. *Journal of Chemical Theory and Computation*, **2018**, 14, 365-376	6.4	16
257	Competitive Adsorption of Methyl Bromide and Water on Metal Catecholates: Insights from Density Functional Theory. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17488-17495	3.9	2
256	Evidence for Copper Dimers in Low-Loaded CuOx/SiO2 Catalysts for Cyclohexane Oxidative Dehydrogenation. *ACS Catalysis*, **2018**, 8, 9775-9789	13.1	8
255	Molecular Modeling of Carbon Dioxide Adsorption in Metal-Organic Frameworks **2018**, 99-149		3
254	Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metal□Organic Framework NU-1000. *Journal of Physical Chemistry C*, **2018**, 122, 12362-12368	3.8	36
253	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. *Chemical Engineering Science*, **2017**, 159, 18-30	4.4	23
252	Adsorption and molecular siting of CO, water, and other gases in the superhydrophobic, flexible pores of FMOF-1 from experiment and simulation. *Chemical Science*, **2017**, 8, 3989-4000	9.4	51
251	Optimizing Open Iron Sites in Metal-Organic Frameworks for Ethane Oxidation: A First-Principles Study. *ACS Applied Materials & Interfaces*, **2017**, 9, 33484-33492	9.5	31
250	Metal-organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. *Chemical Society Reviews*, **2017**, 46, 3357-3385	58.5	557
249	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. *Journal of Physical Chemistry C*, **2017**, 121, 10463-10469	3.8	14
248	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2017**, 9, 33419-33428	9.5	73
247	G-quadruplex organic frameworks. *Nature Chemistry*, **2017**, 9, 466-472	17.6	72
246	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	3.8	33

245	Elucidating the Nanoparticle Metal Organic Framework Interface of Catalysts. *Journal of Physical Chemistry C*, **2017**, 121, 25079-25091	3.8	22
244	Topologically Guided, Automated Construction of Metal Organic Frameworks and Their Evaluation for Energy-Related Applications. *Crystal Growth and Design*, **2017**, 17, 5801-5810	3.5	99
243	High-Throughput Computational Screening of Multivariate Metal-Organic Frameworks (MTV-MOFs) for CO Capture. *Journal of Physical Chemistry Letters*, **2017**, 8, 6135-6141	6.4	53
242	Ab Initio Screening of Metal Catecholates for Adsorption of Toxic Pnictogen Hydride Gases. *Industrial & Engineering Chemistry Research*, **2017**, 56, 14324-14336	3.9	5
241	Computational screening of functional groups for capture of toxic industrial chemicals in porous materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 31766-31772	3.6	1
240	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. *Chemistry of Materials*, **2017**, 29, 6315-6328	9.6	46
239	Large-Scale Refinement of Metal Organic Framework Structures Using Density Functional Theory. *Chemistry of Materials*, **2017**, 29, 2521-2528	9.6	74
238	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. *Molecular Simulation*, **2016**, 42, 81-101	2	807
237	High-Throughput Screening of Metal-Organic Frameworks for CO Capture in the Presence of Water. *Langmuir*, **2016**, 32, 10368-10376	4	93
236	CO adsorption-induced structural changes in coordination polymer ligands elucidated via molecular simulations and experiments. *Dalton Transactions*, **2016**, 45, 17168-17178	4.3	10
235	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. *CheM*, **2016**, 1, 154-169	16.2	217
234	High-Throughput Screening of Metal Organic Frameworks for Hydrogen Storage at Cryogenic Temperature. *Journal of Physical Chemistry C*, **2016**, 120, 27328-27341	3.8	81
233	In silico discovery of metal-organic frameworks for precombustion CO capture using a genetic algorithm. *Science Advances*, **2016**, 2, e1600909	14.3	164
232	Using Gas-Phase Clusters to Screen Porphyrin-Supported Nanocluster Catalysts for Ethane Oxidation to Ethanol. *Catalysis Letters*, **2016**, 146, 2566-2573	2.8	7
231	A Redox-Active Bistable Molecular Switch Mounted inside a Metal-Organic Framework. *Journal of the American Chemical Society*, **2016**, 138, 14242-14245	16.4	95
230	Framework-Topology-Dependent Catalytic Activity of Zirconium-Based (Porphinato)zinc(II) MOFs. *Journal of the American Chemical Society*, **2016**, 138, 14449-14457	16.4	151
229	CD-MOF: A Versatile Separation Medium. *Journal of the American Chemical Society*, **2016**, 138, 2292-301	16.4	203
228	Optimization of Two-Stage Pressure/Vacuum Swing Adsorption with Variable Dehydration Level for Postcombustion Carbon Capture. *Industrial & Engineering Chemistry Research*, **2016**, 55, 3338-3350	3.9	55

227	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. *Journal of Materials Chemistry A*, **2016**, 4, 529-536	13	71
226	Application of Consistency Criteria To Calculate BET Areas of Micro- And Mesoporous Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2016**, 138, 215-24	16.4	145
225	High volumetric uptake of ammonia using Cu-MOF-74/Cu-CPO-27. *Dalton Transactions*, **2016**, 45, 4150-3	4.3	71
224	Evaluating topologically diverse metal□rganic frameworks for cryo-adsorbed hydrogen storage. *Energy and Environmental Science*, **2016**, 9, 3279-3289	35.4	151
223	Alkaline-earth metal-oxide overlayers on TiO2: application toward CO2 photoreduction. *Catalysis Science and Technology*, **2016**, 6, 7885-7895	5.5	22
222	Nanosizing a Metal-Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. *ACS Nano*, **2016**, 10, 9174-9182	16.7	157
221	Ultrahigh surface area zirconium MOFs and insights into the applicability of the BET theory. *Journal of the American Chemical Society*, **2015**, 137, 3585-91	16.4	249
220	Destruction of chemical warfare agents using metal-organic frameworks. *Nature Materials*, **2015**, 14, 512-6	27	647
219	A MOF platform for incorporation of complementary organic motifs for CO2 binding. *Chemical Communications*, **2015**, 51, 12478-81	5.8	39
218	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. *Chemical Science*, **2015**, 6, 384-389	9.4	61
217	Continuous fractional component Monte Carlo simulations of high-density adsorption in metal□rganic frameworks. *Molecular Simulation*, **2015**, 41, 1339-1347	2	6
216	Pore Size Dependence of Adsorption and Separation of Thiophene/Benzene Mixtures in Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 15263-15273	3.8	34
215	Water stabilization of Zr-based metal-organic frameworks solvent-assisted ligand incorporation. *Chemical Science*, **2015**, 6, 5172-5176	9.4	75
214	A kinetic study of vapor-phase cyclohexene epoxidation by H2O2 over mesoporous TS-1. *Journal of Catalysis*, **2015**, 326, 107-115	7.3	41
213	Carbohydrate-mediated purification of petrochemicals. *Journal of the American Chemical Society*, **2015**, 137, 5706-19	16.4	95
212	Computational Screening of Metal Catecholates for Ammonia Capture in Metal□rganic Frameworks. *Industrial & Engineering Chemistry Research*, **2015**, 54, 3257-3267	3.9	26
211	A thermodynamic tank model for studying the effect of higher hydrocarbons on natural gas storage in metal□rganic frameworks. *Energy and Environmental Science*, **2015**, 8, 1501-1510	35.4	70
210	A modelling approach for MOF-encapsulated metal catalysts and application to n-butane oxidation. *Physical Chemistry Chemical Physics*, **2015**, 17, 27596-608	3.6	18

209	Optimization of Pressure/Vacuum Swing Adsorption with Variable Dehydration Levels for Post Combustion Carbon Capture. *Computer Aided Chemical Engineering*, **2015**, 37, 2447-2452	0.6	
208	Electrochemically addressable trisradical rotaxanes organized within a metal-organic framework. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 11161-8	11.5	71
207	Heterogeneous Diffusion of Alkanes in the Hierarchical Metal-Organic Framework NU-1000. *Langmuir*, **2015**, 31, 10056-65	4	25
206	Ultraporous, Water Stable, and Breathing Zirconium-Based Metal-Organic Frameworks with ftw Topology. *Journal of the American Chemical Society*, **2015**, 137, 13183-90	16.4	125
205	Diffusion of methane and other alkanes in metal-organic frameworks for natural gas storage. *Chemical Engineering Science*, **2015**, 124, 135-143	4.4	28
204	Computer-Aided Search for Materials to Store Natural Gas for Vehicles. *Frontiers for Young Minds*, **2015**, 3,	1.5	2
203	Understanding the Effects of Preadsorbed Perfluoroalkanes on the Adsorption of Water and Ammonia in MOFs. *Journal of Physical Chemistry C*, **2015**, 119, 3163-3170	3.8	17
202	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
201	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	3.8	64
200	The effect of pyridine modification of Ni-DOBDC on CO2 capture under humid conditions. *Chemical Communications*, **2014**, 50, 3296-8	5.8	41
199	High-throughput computational screening of metal-organic frameworks. *Chemical Society Reviews*, **2014**, 43, 5735-49	58.5	251
198	Metallacarborane-Based Metal□Organic Framework with a Complex Topology. *Crystal Growth and Design*, **2014**, 14, 1324-1330	3.5	23
197	Chiral Co(II) Metal□Organic Framework in the Heterogeneous Catalytic Oxidation of Alkenes under Aerobic and Anaerobic Conditions. *ACS Catalysis*, **2014**, 4, 1032-1039	13.1	47
196	Textural properties of a large collection of computationally constructed MOFs and zeolites. *Microporous and Mesoporous Materials*, **2014**, 186, 207-213	5.3	31
195	Screening of bio-compatible metal-organic frameworks as potential drug carriers using Monte Carlo simulations. *Journal of Materials Chemistry B*, **2014**, 2, 766-774	7.3	171
194	High propylene/propane adsorption selectivity in a copper(catecholate)-decorated porous organic polymer. *Journal of Materials Chemistry A*, **2014**, 2, 299-302	13	40
193	Modeling Water and Ammonia Adsorption in Hydrophobic Metal□Organic Frameworks: Single Components and Mixtures. *Journal of Physical Chemistry C*, **2014**, 118, 1102-1110	3.8	50
192	Computation-Ready, Experimental Metal□Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. *Chemistry of Materials*, **2014**, 26, 6185-6192	9.6	387

191	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	9.6	158
190	Water-stable zirconium-based metal-organic framework material with high-surface area and gas-storage capacities. *Chemistry - A European Journal*, **2014**, 20, 12389-93	4.8	124
189	Isoreticular Series of (3,24)-Connected Metal–Organic Frameworks: Facile Synthesis and High Methane Uptake Properties. *Chemistry of Materials*, **2014**, 26, 1912-1917	9.6	69
188	Water adsorption in UiO-66: the importance of defects. *Chemical Communications*, **2014**, 50, 11329-31	5.8	175
187	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. *Journal of Physical Chemistry C*, **2014**, 118, 6941-6951	3.8	94
186	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. *Fluid Phase Equilibria*, **2014**, 366, 146-151	2.5	13
185	Strong influence of the H2 binding energy on the Maxwell–Stefan diffusivity in NU-100, UiO-68, and IRMOF-16. *Microporous and Mesoporous Materials*, **2014**, 185, 190-196	5.3	7
184	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. *Journal of Physical Chemistry C*, **2014**, 118, 5383-5389	3.8	74
183	Computational Study of Propylene and Propane Binding in Metal–Organic Frameworks Containing Highly Exposed Cu+ or Ag+ Cations. *Journal of Physical Chemistry C*, **2014**, 118, 9086-9092	3.8	14
182	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework. *AICHE Journal*, **2014**, 60, 2324-2334	3.6	13
181	Large-scale generation and screening of hypothetical metal-organic frameworks for applications in gas storage and separations. *Topics in Current Chemistry*, **2014**, 345, 257-89		6
180	Insights into the complexity of chiral recognition by a three-point model. *Microporous and Mesoporous Materials*, **2013**, 172, 44-50	5.3	16
179	A combined experimental and quantum chemical study of CO2 adsorption in the metal–organic framework CPO-27 with different metals. *Chemical Science*, **2013**, 4, 3544	9.4	142
178	Carborane-Based Metal–Organic Framework with High Methane and Hydrogen Storage Capacities. *Chemistry of Materials*, **2013**, 25, 3539-3543	9.6	98
177	Perfluoroalkane functionalization of NU-1000 via solvent-assisted ligand incorporation: synthesis and CO2 adsorption studies. *Journal of the American Chemical Society*, **2013**, 135, 16801-4	16.4	370
176	High xenon/krypton selectivity in a metal-organic framework with small pores and strong adsorption sites. *Microporous and Mesoporous Materials*, **2013**, 169, 176-179	5.3	80
175	Experiences with the publicly available multipurpose simulation code, Music. *Molecular Simulation*, **2013**, 39, 1223-1232	2	28
174	A facile synthesis of UiO-66, UiO-67 and their derivatives. *Chemical Communications*, **2013**, 49, 9449-51	5.8	1013

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