Randall Q Snurr

List of Publications by Citations

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	Ultrahigh porosity in metal-organic frameworks. *Science*, **2010**, 329, 424-8	33.3	2869
333	De novo synthesis of a metal-organic framework material featuring ultrahigh surface area and gas storage capacities. *Nature Chemistry*, **2010**, 2, 944-8	17.6	1350
332	Metal-organic framework materials with ultrahigh surface areas: is the sky the limit?. *Journal of the American Chemical Society*, **2012**, 134, 15016-21	16.4	1210
331	A facile synthesis of UiO-66, UiO-67 and their derivatives. *Chemical Communications*, **2013**, 49, 9449-51	5.8	1013
330	Review and analysis of molecular simulations of methane, hydrogen, and acetylene storage in metal-organic frameworks. *Chemical Reviews*, **2012**, 112, 703-23	68.1	983
329	Development and evaluation of porous materials for carbon dioxide separation and capture. *Angewandte Chemie - International Edition*, **2011**, 50, 11586-96	16.4	907
328	Large-scale screening of hypothetical metal-organic frameworks. *Nature Chemistry*, **2011**, 4, 83-9	17.6	882
327	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. *Molecular Simulation*, **2016**, 42, 81-101	2	807
326	Applicability of the BET method for determining surface areas of microporous metal-organic frameworks. *Journal of the American Chemical Society*, **2007**, 129, 8552-6	16.4	738
325	Screening of metal-organic frameworks for carbon dioxide capture from flue gas using a combined experimental and modeling approach. *Journal of the American Chemical Society*, **2009**, 131, 18198-9	16.4	737
324	Vapor-phase metalation by atomic layer deposition in a metal-organic framework. *Journal of the American Chemical Society*, **2013**, 135, 10294-7	16.4	659
323	Destruction of chemical warfare agents using metal-organic frameworks. *Nature Materials*, **2015**, 14, 512-6	27	647
322	Design of new materials for methane storage. *Langmuir*, **2004**, 20, 2683-9	4	621
321	Using molecular simulation to characterise metal-organic frameworks for adsorption applications. *Chemical Society Reviews*, **2009**, 38, 1237-47	58.5	565
320	Metal-organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. *Chemical Society Reviews*, **2017**, 46, 3357-3385	58.5	557
319	Separation of CO2 from CH4 using mixed-ligand metal-organic frameworks. *Langmuir*, **2008**, 24, 8592-8	4	522
318	Effects of surface area, free volume, and heat of adsorption on hydrogen uptake in metal-organic frameworks. *Journal of Physical Chemistry B*, **2006**, 110, 9565-70	3.4	521

317	Enhanced CO2 Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. *Chemistry of Materials*, **2009**, 21, 1425-1430	9.6	472
316	Light-harvesting and ultrafast energy migration in porphyrin-based metal-organic frameworks. *Journal of the American Chemical Society*, **2013**, 135, 862-9	16.4	461
315	Understanding inflections and steps in carbon dioxide adsorption isotherms in metal-organic frameworks. *Journal of the American Chemical Society*, **2008**, 130, 406-7	16.4	458
314	Calculating Geometric Surface Areas as a Characterization Tool for Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2007**, 111, 15350-15356	3.8	446
313	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
312	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
311	High propene/propane selectivity in isostructural metal-organic frameworks with high densities of open metal sites. *Angewandte Chemie - International Edition*, **2012**, 51, 1857-60	16.4	348
310	Enhancement of CO2/N2 selectivity in a metal-organic framework by cavity modification. *Journal of Materials Chemistry*, **2009**, 19, 2131		346
309	Object-oriented Programming Paradigms for Molecular Modeling. *Molecular Simulation*, **2003**, 29, 29-46	2	338
308	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. *The Journal of Physical Chemistry*, **1993**, 97, 13742-13752		336
307	Carborane-based metal-organic frameworks as highly selective sorbents for CO(2) over methane. *Chemical Communications*, **2008**, 4135-7	5.8	319
306	Structure□roperty relationships of porous materials for carbon dioxide separation and capture. *Energy and Environmental Science*, **2012**, 5, 9849	35.4	290
305	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
304	Highly selective carbon dioxide uptake by [Cu(bpy-n)2(SiF6)] (bpy-1 = 4,4'-bipyridine; bpy-2 = 1,2-bis(4-pyridyl)ethene). *Journal of the American Chemical Society*, **2012**, 134, 3663-6	16.4	263
303	Exceptional negative thermal expansion in isoreticular metal-organic frameworks. *Angewandte Chemie - International Edition*, **2007**, 46, 4496-9	16.4	260
302	Synthesis, Properties, and Gas Separation Studies of a Robust Diimide-Based Microporous Organic Polymer. *Chemistry of Materials*, **2009**, 21, 3033-3035	9.6	252
301	High-throughput computational screening of metal-organic frameworks. *Chemical Society Reviews*, **2014**, 43, 5735-49	58.5	251
300	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

299	Prospects for nanoporous metal-organic materials in advanced separations processes. *AICHE Journal*, **2004**, 50, 1090-1095	3.6	241
298	Toward Design Rules for Enzyme Immobilization in Hierarchical Mesoporous Metal-Organic Frameworks. *CheM*, **2016**, 1, 154-169	16.2	217
297	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. *Journal of the American Chemical Society*, **2011**, 133, 5228-31	16.4	211
296	Incorporation of an A1/A2-difunctionalized pillar[5]arene into a metal-organic framework. *Journal of the American Chemical Society*, **2012**, 134, 17436-9	16.4	209
295	Molecular modeling and experimental studies of the thermodynamic and transport properties of pyridinium-based ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 2821-32	3.4	209
294	Nanoporous carbohydrate metal-organic frameworks. *Journal of the American Chemical Society*, **2012**, 134, 406-17	16.4	208
293	CD-MOF: A Versatile Separation Medium. *Journal of the American Chemical Society*, **2016**, 138, 2292-301	16.4	203
292	Gram-scale, high-yield synthesis of a robust metal□rganic framework for storing methane and other gases. *Energy and Environmental Science*, **2013**, 6, 1158	35.4	203
291	Evaluation of the BET method for determining surface areas of MOFs and zeolites that contain ultra-micropores. *Langmuir*, **2010**, 26, 5475-83	4	193
290	Thermodynamic analysis of Xe/Kr selectivity in over 137 000 hypothetical metal□rganic frameworks. *Chemical Science*, **2012**, 3, 2217	9.4	190
289	Monomolecular cracking of n-hexane on Y, MOR, and ZSM-5 zeolites. *Applied Catalysis A: General*, **1999**, 179, 71-86	5.1	187
288	An Extended Charge Equilibration Method. *Journal of Physical Chemistry Letters*, **2012**, 3, 2506-11	6.4	184
287	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal□rganic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*, **2019**, 64, 5985-5998	2.8	183
286	Heats of adsorption for seven gases in three metal-organic frameworks: systematic comparison of experiment and simulation. *Langmuir*, **2009**, 25, 7383-8	4	183
285	Water adsorption in UiO-66: the importance of defects. *Chemical Communications*, **2014**, 50, 11329-31	5.8	175
284	Design Requirements for Metal-Organic Frameworks as Hydrogen Storage Materials. *Journal of Physical Chemistry C*, **2007**, 111, 18794-18803	3.8	172
283	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
282	Designing higher surface area metal-organic frameworks: are triple bonds better than phenyls?. *Journal of the American Chemical Society*, **2012**, 134, 9860-3	16.4	170

281	In silico discovery of metal-organic frameworks for precombustion CO capture using a genetic algorithm. *Science Advances*, **2016**, 2, e1600909	14.3	164
280	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
279	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	3.4	158
278	Nanosizing a Metal-Organic Framework Enzyme Carrier for Accelerating Nerve Agent Hydrolysis. *ACS Nano*, **2016**, 10, 9174-9182	16.7	157
277	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
276	Evaluating topologically diverse metal−organic frameworks for cryo-adsorbed hydrogen storage. *Energy and Environmental Science*, **2016**, 9, 3279-3289	35.4	151
275	Molecular Simulations and NMR Measurements of Binary Diffusion in Zeolites. *Journal of Physical Chemistry B*, **1997**, 101, 6469-6473	3.4	146
274	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
273	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
272	Recent developments in the molecular modeling of diffusion in nanoporous materials. *Molecular Simulation*, **2007**, 33, 305-325	2	141
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270	Large-Scale Quantitative Structure−Property Relationship (QSPR) Analysis of Methane Storage in Metal−Organic Frameworks. *Journal of Physical Chemistry C*, **2013**, 117, 7681-7689	3.8	131
269	Separation of gas mixtures using Co(II) carborane-based porous coordination polymers. *Chemical Communications*, **2010**, 46, 3478-80	5.8	128
268	Adsorption of CH4−CF4 Mixtures in Silicalite: Simulation, Experiment, and Theory. *Langmuir*, **1997**, 13, 6795-6804	4	128
267	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	5.1	128
266	Simultaneously high gravimetric and volumetric methane uptake characteristics of the metal-organic framework NU-111. *Chemical Communications*, **2013**, 49, 2992-4	5.8	127
265	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
264	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

263	Control over Catenation in Pillared Paddlewheel Metal–Organic Framework Materials via Solvent-Assisted Linker Exchange. *Chemistry of Materials*, **2013**, 25, 739-744	9.6	120
262	Molecular simulation of adsorption sites of light gases in the metal-organic framework IRMOF-1. *Fluid Phase Equilibria*, **2007**, 261, 152-161	2.5	120
261	Molecular modelling of adsorption in novel nanoporous metal–organic materials. *Molecular Physics*, **2004**, 102, 211-221	1.7	120
260	Computational screening of metal-organic frameworks for xenon/krypton separation. *AICHE Journal*, **2011**, 57, 1759-1766	3.6	118
259	Enhancement of CO2/CH4 selectivity in metal-organic frameworks containing lithium cations. *Microporous and Mesoporous Materials*, **2011**, 141, 231-235	5.3	117
258	Optimal isosteric heat of adsorption for hydrogen storage and delivery using metal–organic frameworks. *Microporous and Mesoporous Materials*, **2010**, 132, 300-303	5.3	116
257	Towards rapid computational screening of metal-organic frameworks for carbon dioxide capture: Calculation of framework charges via charge equilibration. *Chemical Engineering Journal*, **2011**, 171, 775-781	14.7	111
256	Separation and molecular-level segregation of complex alkane mixtures in metal-organic frameworks. *Journal of the American Chemical Society*, **2008**, 130, 10884-5	16.4	111
255	Energy-based descriptors to rapidly predict hydrogen storage in metal–organic frameworks. *Molecular Systems Design and Engineering*, **2019**, 4, 162-174	4.6	100
254	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. *Nature Communications*, **2018**, 9, 1378	17.4	100
253	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
252	Metal Alkoxide Functionalization in Metal–Organic Frameworks for Enhanced Ambient-Temperature Hydrogen Storage. *Journal of Physical Chemistry C*, **2011**, 115, 2066-2075	3.8	99
251	Carborane-Based Metal–Organic Framework with High Methane and Hydrogen Storage Capacities. *Chemistry of Materials*, **2013**, 25, 3539-3543	9.6	98
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249	Carbohydrate-mediated purification of petrochemicals. *Journal of the American Chemical Society*, **2015**, 137, 5706-19	16.4	95
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245	Nonequilibrium Molecular Dynamics Simulations of Diffusion of Binary Mixtures Containing Short n-Alkanes in Faujasite. *Journal of Physical Chemistry B*, **2004**, 108, 13481-13491	3.4	93
244	Porö e Materialien zur CO2-Abtrennung und -Abscheidung Ü Entwicklung und Bewertung. *Angewandte Chemie*, **2011**, 123, 11790-11801	3.6	88
243	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. *The Journal of Physical Chemistry*, **1994**, 98, 11948-11961		88
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239	Molecular mechanisms of liquid slip. *Journal of Fluid Mechanics*, **2008**, 600, 257-269	3.7	81
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234	Water adsorption in hydrophobic nanopores: Monte Carlo simulations of water in silicalite. *Microporous and Mesoporous Materials*, **2006**, 90, 293-298	5.3	77
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232	Water stabilization of Zr-based metal-organic frameworks solvent-assisted ligand incorporation. *Chemical Science*, **2015**, 6, 5172-5176	9.4	75
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229	Large-Scale Refinement of Metall Organic Framework Structures Using Density Functional Theory. *Chemistry of Materials*, **2017**, 29, 2521-2528	9.6	74
228	Understanding Volumetric and Gravimetric Hydrogen Adsorption Trade-off in Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2017**, 9, 33419-33428	9.5	73

227	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. *Journal of Physical Chemistry C*, **2010**, 114, 10527-10534	3.8	73
226	Is catenation beneficial for hydrogen storage in metal-organic frameworks?. *Chemical Communications*, **2008**, 4132-4	5.8	73
225	G-quadruplex organic frameworks. *Nature Chemistry*, **2017**, 9, 466-472	17.6	72
224	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
223	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. *Journal of Materials Chemistry A*, **2016**, 4, 529-536	13	71
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220	Predicting membrane flux of CH4 and CF4 mixtures in Faujasite from molecular simulations. *AICHE Journal*, **2001**, 47, 2032-2041	3.6	70
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215	A new perspective on the order-n algorithm for computing correlation functions. *Molecular Simulation*, **2009**, 35, 1084-1097	2	66
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212	Strategies for Characterization of Large-Pore Metal-Organic Frameworks by Combined Experimental and Computational Methods. *Chemistry of Materials*, **2009**, 21, 4768-4777	9.6	64
211	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
210	Structure□Activity Relationships That Identify Metal□rganic Framework Catalysts for Methane Activation. *ACS Catalysis*, **2019**, 9, 3576-3587	13.1	63

209	Adsorption of liquid-phase alkane mixtures in silicalite: simulations and experiment. *Langmuir*, **2004**, 20, 150-6	4	63
208	Siting and Segregation Effects of Simple Molecules in Zeolites MFI, MOR, and BOG. *Journal of Physical Chemistry B*, **1998**, 102, 6720-6731	3.4	62
207	Hierarchically porous organic polymers: highly enhanced gas uptake and transport through templated synthesis. *Chemical Science*, **2015**, 6, 384-389	9.4	61
206	Monte Carlo simulation of n-alkane adsorption isotherms in carbon slit pores. *Journal of Chemical Physics*, **2007**, 126, 134708	3.9	61
205	Identification Schemes for Metal□Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
204	High Propene/Propane Selectivity in Isostructural Metal□Organic Frameworks with High Densities of Open Metal Sites. *Angewandte Chemie*, **2012**, 124, 1893-1896	3.6	59
203	Inverse design of nanoporous crystalline reticular materials with deep generative models. *Nature Machine Intelligence*, **2021**, 3, 76-86	22.5	58
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200	Adsorption isotherm sensitivity to small changes in zeolite structure. *Chemical Physics Letters*, **1999**, 308, 155-159	2.5	55
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194	Molecular Squares as Molecular Sieves: Size-Selective Transport Through Porous-Membrane-Supported Thin-Film Materials. *Advanced Materials*, **2001**, 13, 1895	24	51
193	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
192	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

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189	Packing Effects in the Liquid-Phase Adsorption of C5-C22n-Alkanes on ZSM-5. *Journal of Physical Chemistry B*, **2003**, 107, 10760-10766	3.4	48
188	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
187	Computational Screening of Nanoporous Materials for Hexane and Heptane Isomer Separation. *Chemistry of Materials*, **2017**, 29, 6315-6328	9.6	46
186	Understanding excess uptake maxima for hydrogen adsorption isotherms in frameworks with rht topology. *Chemical Communications*, **2012**, 48, 10496-8	5.8	46
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183	Machine learning the quantum-chemical properties of metal–organic frameworks for accelerated materials discovery. *Matter*, **2021**, 4, 1578-1597	12.7	43
182	Boundary effects of molecular diffusion in nanoporous materials: a pulsed field gradient nuclear magnetic resonance study. *Journal of Chemical Physics*, **2004**, 120, 367-73	3.9	42
181	Diffusion mechanisms of normal alkanes in faujasite zeolites. *Journal of Chemical Physics*, **1999**, 111, 1209-1222	3.9	42
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179	The effect of pyridine modification of Ni-DOBDC on CO2 capture under humid conditions. *Chemical Communications*, **2014**, 50, 3296-8	5.8	41
178	Computational screening of functional groups for ammonia capture in metal-organic frameworks. *Langmuir*, **2013**, 29, 1446-56	4	41
177	Screening CO2/N2 selectivity in metal-organic frameworks using Monte Carlo simulations and ideal adsorbed solution theory. *Canadian Journal of Chemical Engineering*, **2012**, 90, 825-832	2.3	41
176	Investigation of particle damping mechanism via particle dynamics simulations. *Granular Matter*, **2009**, 11, 417-429	2.6	41
175	Multiscale modeling of transport and residence times in nanostructured membranes. *AICHE Journal* , **2006**, 52, 3679-3687	3.6	41
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170	Evidence of different reaction mechanisms during the cracking of n-hexane on H-USY zeolite. *Applied Catalysis A: General*, **2000**, 203, 179-190	5.1	38
169	In SituPFG NMR Study of Intracrystalline Diffusion during Ethene Conversion in ZSM-5. *Journal of Catalysis*, **1996**, 163, 130-137	7.3	38
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167	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
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