David Fairen-Jimenez

List of Publications by Year
in descending order

119 papers	10,984 citations	30047 54 h-index	30894 102 g-index
131 all docs	131 docs citations	131 times ranked	11541 citing authors

#	Article	IF	Citations
1	Opening the Gate: Framework Flexibility in ZIF-8 Explored by Experiments and Simulations. Journal of the American Chemical Society, 2011, 133, 8900-8902.	6.6	947
2	Vapor-Phase Metalation by Atomic Layer Deposition in a Metalâ€"Organic Framework. Journal of the American Chemical Society, 2013, 135, 10294-10297.	6.6	821
3	Development of a Cambridge Structural Database Subset: A Collection of Metalâ€"Organic Frameworks for Past, Present, and Future. Chemistry of Materials, 2017, 29, 2618-2625.	3.2	718
4	A solâ€"gel monolithic metalâ€"organic framework with enhanced methane uptake. Nature Materials, 2018, 17, 174-179.	13.3	386
5	Amorphous metalâ€"organic frameworks for drug delivery. Chemical Communications, 2015, 51, 13878-13881.	2.2	309
6	Temperature Treatment of Highly Porous Zirconium-Containing Metalâ€"Organic Frameworks Extends Drug Delivery Release. Journal of the American Chemical Society, 2017, 139, 7522-7532.	6.6	269
7	Selective Surface PEGylation of UiO-66 Nanoparticles for Enhanced Stability, Cell Uptake, and pH-Responsive Drug Delivery. CheM, 2017, 2, 561-578.	5.8	266
8	Incorporation of an A1/A2-Difunctionalized Pillar[5]arene into a Metalâ€"Organic Framework. Journal of the American Chemical Society, 2012, 134, 17436-17439.	6.6	254
9	Metalâ€"Organic Framework Thin Films Composed of Free-Standing Acicular Nanorods Exhibiting Reversible Electrochromism. Chemistry of Materials, 2013, 25, 5012-5017.	3.2	242
10	Metalâ€"Organic Nanosheets Formed via Defect-Mediated Transformation of a Hafnium Metalâ€"Organic Framework. Journal of the American Chemical Society, 2017, 139, 5397-5404.	6.6	224
11	Screening of bio-compatible metalâ€"organic frameworks as potential drug carriers using Monte Carlo simulations. Journal of Materials Chemistry B, 2014, 2, 766-774.	2.9	215
12	25 Years of Reticular Chemistry. Angewandte Chemie - International Edition, 2021, 60, 23946-23974.	7.2	204
13	Shaping the Future of Fuel: Monolithic Metalâ€"Organic Frameworks for High-Density Gas Storage. Journal of the American Chemical Society, 2020, 142, 8541-8549.	6.6	182
14	Tuning porosity in macroscopic monolithic metal-organic frameworks for exceptional natural gas storage. Nature Communications, 2019, 10, 2345.	5.8	180
15	Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. Dalton Transactions, 2012, 41, 10752.	1.6	176
16	Elucidating the Breathing of the Metalâ€"Organic Framework MIL-53(Sc) with ab Initio Molecular Dynamics Simulations and in Situ X-ray Powder Diffraction Experiments. Journal of the American Chemical Society, 2013, 135, 15763-15773.	6.6	173
17	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. Matter, 2019, 1, 219-234.	5.0	170
18	Waterâ€Stable Zirconiumâ€Based Metalâ€"Organic Framework Material with Highâ€Surface Area and Gasâ€Storage Capacities. Chemistry - A European Journal, 2014, 20, 12389-12393.	1.7	150

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19	Metal-organic frameworks as biosensors for luminescence-based detection and imaging. Interface Focus, 2016, 6, 20160027.	1.5	142
20	Computer-aided discovery of a metalâ€“organic framework with superior oxygen uptake. Nature Communications, 2018, 9, 1378.	5.8	136
21	An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles. Nature Energy, 2022, 7, 107-115.	19.8	136
22	Control over Catenation in Pillared Paddlewheel Metalâ€“Organic Framework Materials via Solvent-Assisted Linker Exchange. Chemistry of Materials, 2013, 25, 739-744.	3.2	135
23	Methane storage mechanism in the metal-organic framework Cu3(btc)2: An in situ neutron diffraction study. Microporous and Mesoporous Materials, 2010, 136, 50-58.	2.2	132
24	Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database. Chemistry of Materials, 2020, 32, 9849-9867.	3.2	132
25	Drug delivery and controlled release from biocompatible metalâ€“organic frameworks using mechanical amorphization. Journal of Materials Chemistry B, 2016, 4, 7697-7707.	2.9	131
26	A general approach for hysteresis-free, operationally stable metal halide perovskite field-effect transistors. Science Advances, 2020, 6, eaaz4948.	4.7	129
27	Granular and monolithic activated carbons from KOH-activation of olive stones. Microporous and Mesoporous Materials, 2006, 92, 64-70.	2.2	126
28	Surface-Functionalization of Zr-Fumarate MOF for Selective Cytotoxicity and Immune System Compatibility in Nanoscale Drug Delivery. ACS Applied Materials & Interfaces, 2018, 10, 31146-31157.	4.0	121
29	Coreâ€“Shell Gold Nanorod@Zirconium-Based Metalâ€“Organic Framework Composites as <i>in Situ</i> Size-Selective Raman Probes. Journal of the American Chemical Society, 2019, 141, 3893-3900.	6.6	119
30	Targeted classification of metalâ€“organic frameworks in the Cambridge structural database (CSD). Chemical Science, 2020, 11, 8373-8387.	3.7	119
31	A mechanochemical strategy for IRMOF assembly based on pre-designed oxo-zinc precursors. Chemical Communications, 2015, 51, 4032-4035.	2.2	117
32	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. Chemical Communications, 2016, 52, 3639-3642.	2.2	106
33	Mechanically and chemically robust ZIF-8 monoliths with high volumetric adsorption capacity. Journal of Materials Chemistry A, 2015, 3, 2999-3005.	5.2	104
34	Design of a Functionalized Metalâ€“Organic Framework System for Enhanced Targeted Delivery to Mitochondria. Journal of the American Chemical Society, 2020, 142, 6661-6674.	6.6	103
35	Metalâ€“Organic Framework Composites for Theragnostics and Drug Delivery Applications. Biotechnology Journal, 2021, 16, e2000005.	1.8	101
36	Porosity and surface area of monolithic carbon aerogels prepared using alkaline carbonates and organic acids as polymerization catalysts. Carbon, 2006, 44, 2301-2307.	5.4	96

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37	A novel structural form of MIL-53 observed for the scandium analogue and its response to temperature variation and CO₂adsorption. Dalton Transactions, 2012, 41, 3937-3941.	1.6	95
38	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
39	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. Journal of Physical Chemistry C, 2013, 117, 20116-20126.	1.5	92
40	Formulation of Metalâ€“Organic Framework-Based Drug Carriers by Controlled Coordination of Methoxy PEG Phosphate: Boosting Colloidal Stability and Redispersibility. Journal of the American Chemical Society, 2021, 143, 13557-13572.	6.6	88
41	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. Journal of Physical Chemistry C, 2014, 118, 5383-5389.	1.5	84
42	Mechanistic Investigation into the Selective Anticancer Cytotoxicity and Immune System Response of Surface-Functionalized, Dichloroacetate-Loaded, UiO-66 Nanoparticles. ACS Applied Materials & Interfaces, 2018, 10, 5255-5268.	4.0	84
43	How Reproducible are Surface Areas Calculated from the BET Equation?. Advanced Materials, 2022, 34, .	11.1	82
44	Endocytosis Mechanism of Nano Metalâ€Organic Frameworks for Drug Delivery. Advanced Healthcare Materials, 2016, 5, 2261-2270.	3.9	80
45	Graphene-wrapped sulfur/metal organic framework-derived microporous carbon composite for lithium sulfur batteries. APL Materials, 2014, 2, .	2.2	76
46	Structural Chemistry, Monoclinic-to-Orthorhombic Phase Transition, and CO₂ Adsorption Behavior of the Small Pore Scandium Terephthalate, Sc₂(O₂CC₆H₄CO₂)₃, and Its Nitro- And Amino-Functionalized Derivatives. Inorganic Chemistry, 2011, 50, 10844-10858.	1.9	75
47	Adsorption of Benzene, Toluene, and Xylenes on Monolithic Carbon Aerogels from Dry Air Flows. Langmuir, 2007, 23, 10095-10101.	1.6	74
48	Role of crystal size on swing-effect and adsorption induced structure transition of ZIF-8. Dalton Transactions, 2016, 45, 6893-6900.	1.6	66
49	A Highly Porous Metal-Organic Framework System to Deliver Payloads for Gene Knockdown. CheM, 2019, 5, 2926-2941.	5.8	66
50	Trinuclear Cageâ€Like Zn^{II} Macrocyclic Complexes: Enantiomeric Recognition and Gas Adsorption Properties. Chemistry - A European Journal, 2016, 22, 598-609.	1.7	64
51	Biocompatible, Crystalline, and Amorphous Bismuth-Based Metalâ€“Organic Frameworks for Drug Delivery. ACS Applied Materials & Interfaces, 2020, 12, 5633-5641.	4.0	64
52	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. Chemistry of Materials, 2018, 30, 4571-4579.	3.2	62
53	Rare earth anthracenedicarboxylate metalâ€“organic frameworks: slow relaxation of magnetization of Nd3+, Gd3+, Dy3+, Er3+ and Yb3+ based materials. Dalton Transactions, 2016, 45, 591-598.	1.6	59
54	Solâ€“Gel Synthesis of Robust Metalâ€“Organic Frameworks for Nanoparticle Encapsulation. Advanced Functional Materials, 2018, 28, 1705588.	7.8	58

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55	Engineering new defective phases of UiO family metalâ€"organic frameworks with water. Journal of Materials Chemistry A, 2019, 7, 7459-7469.	5.2	58
56	Investigation of the terahertz vibrational modes of ZIF-8 and ZIF-90 with terahertz time-domain spectroscopy. Chemical Communications, 2015, 51, 16037-16040.	2.2	55
57	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2018, 140, 382-387.	6.6	55
58	The uptake of metalâ€"organic frameworks: a journey into the cell. Chemical Society Reviews, 2022, 51, 6065-6086.	18.7	55
59	Structural dynamics of a metalâ€"organic framework induced by CO2 migration in its non-uniform porous structure. Nature Communications, 2019, 10, 999.	5.8	54
60	Surface Area and Microporosity of Carbon Aerogels from Gas Adsorption and Small- and Wide-Angle X-ray Scattering Measurements. Journal of Physical Chemistry B, 2006, 110, 8681-8688.	1.2	53
61	Unusual Adsorption Behavior on Metalâ^'Organic Frameworks. Langmuir, 2010, 26, 14694-14699.	1.6	52
62	Understanding excess uptake maxima for hydrogen adsorption isotherms in frameworks with rht topology. Chemical Communications, 2012, 48, 10496.	2.2	50
63	Carbon aerogels from gallic acidâ€"resorcinol mixtures as adsorbents of benzene, toluene and xylenes from dry and wet air under dynamic conditions. Carbon, 2009, 47, 463-469.	5.4	46
64	Permanent Porosity Derived From the Selfâ€Assembly of Highly Luminescent Molecular Zinc Carbonate Nanoclusters. Angewandte Chemie - International Edition, 2013, 52, 13414-13418.	7.2	46
65	Tuning the Endocytosis Mechanism of Zr-Based Metalâ€"Organic Frameworks through Linker Functionalization. ACS Applied Materials & Interfaces, 2017, 9, 35516-35525.	4.0	44
66	Controlling interpenetration through linker conformation in the modulated synthesis of Sc metalâ€"organic frameworks. Journal of Materials Chemistry A, 2018, 6, 1181-1187.	5.2	44
67	Enabling efficient exploration of metalâ€"organic frameworks in the Cambridge Structural Database. CrystEngComm, 2020, 22, 7152-7161.	1.3	42
68	Modular structure of a robust microporous MOF based on Cu2 paddle-wheels with high CO2 selectivity. Chemical Communications, 2013, 49, 11329.	2.2	37
69	Probing the Mechanochemistry of Metalâ€"Organic Frameworks with Low-Frequency Vibrational Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 27442-27450.	1.5	37
70	Structure-directing factors when introducing hydrogen bond functionality to metalâ€"organic frameworks. CrystEngComm, 2015, 17, 299-306.	1.3	33
71	From synthesis to applications: Metalâ€"organic frameworks for an environmentally sustainable future. Current Opinion in Green and Sustainable Chemistry, 2018, 12, 47-56.	3.2	33
72	Synthetic control of framework zinc purinate crystallisation and properties of a large pore, decorated, mixed-linker RHO-type ZIF. Chemical Communications, 2012, 48, 6690.	2.2	31

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73	Insights into the electric double-layer capacitance of two-dimensional electrically conductive metalâ€“organic frameworks. Journal of Materials Chemistry A, 2021, 9, 16006-16015.	5.2	31
74	First Examples of Metalâ€“Organic Frameworks with the Novel 3,3â€²-(1,2,4,5-Tetrazine-3,6-diyl)dibenzoic Spacer. Luminescence and Adsorption Properties. Inorganic Chemistry, 2013, 52, 546-548.	1.9	30
75	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. Angewandte Chemie - International Edition, 2020, 59, 17600-17606.	7.2	30
76	Nitroâ€Functionalized Bis(pyrazolate) Metalâ€“Organic Frameworks as Carbon Dioxide Capture Materials under Ambient Conditions. Chemistry - A European Journal, 2018, 24, 13170-13180.	1.7	29
77	Computational Screening of Metal Catecholates for Ammonia Capture in Metalâ€“Organic Frameworks. Industrial & Engineering Chemistry Research, 2015, 54, 3257-3267.	1.8	27
78	Tuning the target composition of amine-grafted CPO-27-Mg for capture of CO2 under post-combustion and air filtering conditions: a combined experimental and computational study. Dalton Transactions, 2015, 44, 18970-18982.	1.6	26
79	Lanthanide metalâ€“organic frameworks for the fixation of CO₂ under aqueous-rich and mixed-gas conditions. Journal of Materials Chemistry A, 2022, 10, 1442-1450.	5.2	26
80	Inter- and Intra-Primary-Particle Structure of Monolithic Carbon Aerogels Obtained with Varying Solvents. Langmuir, 2008, 24, 2820-2825.	1.6	25
81	â€œExplosiveâ€•synthesis of metal-formate frameworks for methane capture: an experimental and computational study. Chemical Communications, 2017, 53, 11437-11440.	2.2	25
82	Novel 3D lanthanum oxalate metal-organic-framework: Synthetic, structural, luminescence and adsorption properties. Polyhedron, 2013, 52, 315-320.	1.0	24
83	Enhanced Gas Sorption Properties and Unique Behavior toward Liquid Water in a Pillared-Paddlewheel Metalâ€“Organic Framework Transmetalated with Ni(II). Inorganic Chemistry, 2014, 53, 10432-10436.	1.9	24
84	Insights into the Ultra-High Volumetric Capacity in a Robust Metalâ€“Organic Framework for Efficient C₂H₂/CO₂ Separation. Chemistry of Materials, 2022, 34, 2708-2716.	3.2	24
85	Highly Active Anti-Diabetic Metalâ€“Organic Framework. Crystal Growth and Design, 2016, 16, 537-540.	1.4	23
86	Hydrogen Uptake by {H[Mg(HCOO)₃]âŠƒNHMe₂}_{âˆž} and Determination of Its H₂ Adsorption Sites through Monte Carlo Simulations. Langmuir, 2011, 27, 10124-10131.	1.6	21
87	Computational Study of Propylene and Propane Binding in Metalâ€“Organic Frameworks Containing Highly Exposed Cu⁺ or Ag⁺ Cations. Journal of Physical Chemistry C, 2014, 118, 9086-9092.	1.5	21
88	Identifying Differing Intracellular Cargo Release Mechanisms by Monitoring InÂVitro Drug Delivery from MOFs in Real Time. Cell Reports Physical Science, 2020, 1, 100254.	2.8	19
89	Nanoporous carbon materials: Comparison between information obtained by SAXS and WAXS and by gas adsorption. Carbon, 2005, 43, 3009-3012.	5.4	18
90	The launch of a freely accessible MOF CIF collection from the CSD. Matter, 2021, 4, 1105-1106.	5.0	18

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91	Long lifetime photoluminescence emission of 3D cadmium metalâ€“organic frameworks based on the 5-(4-pyridyl)tetrazole ligand. Inorganica Chimica Acta, 2015, 427, 131-137.	1.2	17
92	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metalâ€organic framework. AICHE Journal, 2014, 60, 2324-2334.	1.8	14
93	Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. Journal of Materials Chemistry C, 2021, 9, 13584-13599.	2.7	14
94	Biological basis for novel mesothelioma therapies. British Journal of Cancer, 2021, 125, 1039-1055.	2.9	14
95	Structural heterogeneity and dynamics in flexible metal-organic frameworks. Cell Reports Physical Science, 2021, 2, 100544.	2.8	14
96	Novel metalâ€“organic frameworks based on 5-bromonicotinic acid: Multifunctional materials with H2 purification capabilities. CrystEngComm, 2012, 14, 6390.	1.3	13
97	Modulation of pore shape and adsorption selectivity by ligand functionalization in a series of â€œrobâ€•like flexible metalâ€“organic frameworks. Journal of Materials Chemistry A, 2018, 6, 17409-17416.	5.2	13
98	Screening Metalâ€“Organic Frameworks for Dynamic CO/N₂ Separation Using Complementary Adsorption Measurement Techniques. Industrial & Engineering Chemistry Research, 2019, 58, 18336-18344.	1.8	13
99	Advances in the Synthesis and Longâ€Term Protection of Zeroâ€Valent Iron Nanoparticles. Particle and Particle Systems Characterization, 2018, 35, 1800120.	1.2	12
100	Reverse Hierarchy of Alkane Adsorption in Metalâ€“Organic Frameworks (MOFs) Revealed by Immersion Calorimetry. Journal of Physical Chemistry C, 2019, 123, 11699-11706.	1.5	12
101	Monolithic metalâ€“organic frameworks for carbon dioxide separation. Faraday Discussions, 2021, 231, 51-65.	1.6	12
102	Towards a potential 4,4â€²-(1,2,4,5-tetrazine-3,6-diyl) dibenzoic spacer to construct metalâ€“organic frameworks. New Journal of Chemistry, 2015, 39, 6453-6458.	1.4	11
103	Pore-Network Connectivity and Molecular Sieving of Normal and Isoalkanes in the Mesoporous Silica SBA-2. Journal of Physical Chemistry C, 2014, 118, 10183-10190.	1.5	10
104	Turning Molecular Springs into Nano-Shock Absorbers: The Effect of Macroscopic Morphology and Crystal Size on the Dynamic Hysteresis of Water Intrusionâ€“Extrusion into-from Hydrophobic Nanopores. ACS Applied Materials & Interfaces, 2022, 14, 26699-26713.	4.0	10
105	Luminescence and Magnetic Properties of Two Three-Dimensional Terbium and Dysprosium MOFs Based on Azobenzene-4,4â€²-Dicarboxylic Linker. Polymers, 2016, 8, 39.	2.0	9
106	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. Angewandte Chemie, 2020, 132, 17753-17759.	1.6	9
107	A comparison of copper and acid site zeolites for the production of nitric oxide for biomedical applications. Dalton Transactions, 2017, 46, 3915-3920.	1.6	8
108	Wiz: A Web-Based Tool for Interactive Visualization of Big Data. Patterns, 2020, 1, 100107.	3.1	8

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109	The development of a comprehensive toolbox based on multi-level, high-throughput screening of MOFs for CO/N₂ separations. Chemical Science, 2021, 12, 12068-12081.	3.7	8
110	Molecular Sieving Properties of Nanoporous Mixed-Linker ZIF-62: Associated Structural Changes upon Gas Adsorption Application. ACS Applied Nano Materials, 2021, 4, 3519-3528.	2.4	8
111	From computational high-throughput screenings to the lab: taking metalâ€“organic frameworks out of the computer. Chemical Science, 2022, 13, 7990-8002.	3.7	8
112	25 Jahre retikulÃre Chemie. Angewandte Chemie, 2021, 133, 24142.	1.6	6
113	Size-tuneable and immunocompatible polymer nanocarriers for drug delivery in pancreatic cancer. Nanoscale, 2022, 14, 6656-6669.	2.8	5
114	Modulated self-assembly of an interpenetrated MIL-53 Sc metalâ€“organic framework with excellent volumetric H2 storage and working capacity. Materials Today Chemistry, 2022, 24, 100887.	1.7	4
115	2D-cadmium MOF and gismondine-like zinc coordination network based on the N-(2-tetrazolethyl)-4â€²-glycine linker. New Journal of Chemistry, 2015, 39, 3982-3986.	1.4	3
116	Investigation of the terahertz vibrational modes of ZIF-8 and ZIF-90 with terahertz time-domain spectroscopy. , 2015, , .		1
117	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
118	Metal-Organic Frameworks as Delivery Systems of Small Drugs and Biological Gases. , 2021, , 349-378.		1
119	Advances in the synthesis and long-term protection of zero-valent iron nanoparticles. , 2018, , .		0