David Fairen-Jimenez

List of Publications by Year in Descending Order

116 papers	7,701 citations	45 h-index	86 g-index
131 ext. papers	9,242 ext. citations	9.3 avg, IF	6.25 L-index

#	Paper	IF	Citations
116	Lanthanide metal–organic frameworks for the fixation of CO2 under aqueous-rich and mixed-gas conditions. *Journal of Materials Chemistry A*, **2022**, 10, 1442-1450	13	1
115	Insights into the Ultra-High Volumetric Capacity in a Robust Metal–Organic Framework for Efficient C2H2/CO2 Separation. *Chemistry of Materials*, **2022**, 34, 2708-2716	9.6	2
114	An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles. *Nature Energy*, **2022**, 7, 107-115	62.3	26
113	Modulated self-assembly of an interpenetrated MIL-53 Sc metal–organic framework with excellent volumetric H2 storage and working capacity. *Materials Today Chemistry*, **2022**, 24, 100887	6.2	
112	The launch of a freely accessible MOF CIF collection from the CSD. *Matter*, **2021**, 4, 1105-1106	12.7	6
111	25 Jahre retikuläre Chemie. *Angewandte Chemie*, **2021**, 133, 24142	3.6	0
110	Metal-Organic Framework Composites for Theragnostics and Drug Delivery Applications. *Biotechnology Journal*, **2021**, 16, e2000005	5.6	39
109	Monolithic metal-organic frameworks for carbon dioxide separation. *Faraday Discussions*, **2021**, 231, 51-65	3.6	0
108	Insights into the electric double-layer capacitance of two-dimensional electrically conductive metal-organic frameworks. *Journal of Materials Chemistry A*, **2021**, 9, 16006-16015	13	6
107	The development of a comprehensive toolbox based on multi-level, high-throughput screening of MOFs for CO/N separations. *Chemical Science*, **2021**, 12, 12068-12081	9.4	2
106	Molecular Sieving Properties of Nanoporous Mixed-Linker ZIF-62: Associated Structural Changes upon Gas Adsorption Application. *ACS Applied Nano Materials*, **2021**, 4, 3519-3528	5.6	0
105	Biological basis for novel mesothelioma therapies. *British Journal of Cancer*, **2021**, 125, 1039-1055	8.7	5
104	25 Years of Reticular Chemistry. *Angewandte Chemie - International Edition*, **2021**, 60, 23946-23974	16.4	50
103	Formulation of Metal-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	16.4	15
102	Structural heterogeneity and dynamics in flexible metal-organic frameworks. *Cell Reports Physical Science*, **2021**, 2, 100544	6.1	3
101	Metal-Organic Frameworks as Delivery Systems of Small Drugs and Biological Gases **2021**, 349-378		1
100	Enabling efficient exploration of metal–organic frameworks in the Cambridge Structural Database. *CrystEngComm*, **2020**, 22, 7152-7161	3.3	23

99	Targeted classification of metal-organic frameworks in the Cambridge structural database (CSD). *Chemical Science*, **2020**, 11, 8373-8387	9.4	61
98	Design of a Functionalized Metal-Organic Framework System for Enhanced Targeted Delivery to Mitochondria. *Journal of the American Chemical Society*, **2020**, 142, 6661-6674	16.4	53
97	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. *Angewandte Chemie - International Edition*, **2020**, 59, 17600-17606	16.4	14
96	Biocompatible, Crystalline, and Amorphous Bismuth-Based Metal-Organic Frameworks for Drug Delivery. *ACS Applied Materials & Interfaces*, **2020**, 12, 5633-5641	9.5	35
95	A general approach for hysteresis-free, operationally stable metal halide perovskite field-effect transistors. *Science Advances*, **2020**, 6, eaaz4948	14.3	73
94	Shaping the Future of Fuel: Monolithic Metal-Organic Frameworks for High-Density Gas Storage. *Journal of the American Chemical Society*, **2020**, 142, 8541-8549	16.4	82
93	Wiz: A Web-Based Tool for Interactive Visualization of Big Data. *Patterns*, **2020**, 1, 100107	5.1	2
92	Identifying Differing Intracellular Cargo Release Mechanisms by Monitoring Drug Delivery from MOFs in Real Time. *Cell Reports Physical Science*, **2020**, 1, 100254	6.1	5
91	Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database. *Chemistry of Materials*, **2020**, 32, 9849-9867	9.6	37
90	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. *Angewandte Chemie*, **2020**, 132, 17753-17759	3.6	8
89	Screening Metal□rganic Frameworks for Dynamic CO/N2 Separation Using Complementary Adsorption Measurement Techniques. *Industrial & Engineering Chemistry Research*, **2019**, 58, 18336-18344	3.9	9
88	Core-Shell Gold Nanorod@Zirconium-Based Metal-Organic Framework Composites as in Situ Size-Selective Raman Probes. *Journal of the American Chemical Society*, **2019**, 141, 3893-3900	16.4	73
87	Tuning porosity in macroscopic monolithic metal-organic frameworks for exceptional natural gas storage. *Nature Communications*, **2019**, 10, 2345	17.4	100
86	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. *Matter*, **2019**, 1, 219-234	12.7	99
85	Reverse Hierarchy of Alkane Adsorption in Metal□rganic Frameworks (MOFs) Revealed by Immersion Calorimetry. *Journal of Physical Chemistry C*, **2019**, 123, 11699-11706	3.8	8
84	A Highly Porous Metal-Organic Framework System to Deliver Payloads for Gene Knockdown. *CheM*, **2019**, 5, 2926-2941	16.2	34
83	Structural dynamics of a metal-organic framework induced by CO migration in its non-uniform porous structure. *Nature Communications*, **2019**, 10, 999	17.4	36
82	Engineering new defective phases of UiO family metal□rganic frameworks with water. *Journal of Materials Chemistry A*, **2019**, 7, 7459-7469	13	37

81	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. *Nature Communications*, **2018**, 9, 1378	17.4	100
80	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	9.5	56
79	Sol□Gel Synthesis of Robust Metal□Organic Frameworks for Nanoparticle Encapsulation. *Advanced Functional Materials*, **2018**, 28, 1705588	15.6	43
78	Nitro-functionalized Bis(pyrazolate) Metal-Organic Frameworks as Carbon Dioxide Capture Materials under Ambient Conditions. *Chemistry - A European Journal*, **2018**, 24, 13170-13180	4.8	19
77	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	9.5	67
76	Modulation of pore shape and adsorption selectivity by ligand functionalization in a series of □ob□like flexible metal□organic frameworks. *Journal of Materials Chemistry A*, **2018**, 6, 17409-17416	13	10
75	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. *Chemistry of Materials*, **2018**, 30, 4571-4579	9.6	43
74	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 382-387	16.4	37
73	A sol-gel monolithic metal-organic framework with enhanced methane uptake. *Nature Materials*, **2018**, 17, 174-179	27	257
72	Controlling interpenetration through linker conformation in the modulated synthesis of Sc metal□rganic frameworks. *Journal of Materials Chemistry A*, **2018**, 6, 1181-1187	13	30
71	Probing the Mechanochemistry of Metal□Organic Frameworks with Low-Frequency Vibrational Spectroscopy. *Journal of Physical Chemistry C*, **2018**, 122, 27442-27450	3.8	25
70	Advances in the Synthesis and Long-Term Protection of Zero-Valent Iron Nanoparticles. *Particle and Particle Systems Characterization*, **2018**, 35, 1800120	3.1	8
69	From synthesis to applications: Metal□rganic frameworks for an environmentally sustainable future. *Current Opinion in Green and Sustainable Chemistry*, **2018**, 12, 47-56	7.9	27
68	A comparison of copper and acid site zeolites for the production of nitric oxide for biomedical applications. *Dalton Transactions*, **2017**, 46, 3915-3920	4.3	7
67	Selective Surface PEGylation of UiO-66 Nanoparticles for Enhanced Stability, Cell Uptake, and pH-Responsive Drug Delivery. *CheM*, **2017**, 2, 561-578	16.2	183
66	Temperature Treatment of Highly Porous Zirconium-Containing Metal-Organic Frameworks Extends Drug Delivery Release. *Journal of the American Chemical Society*, **2017**, 139, 7522-7532	16.4	216
65	Metal-Organic Nanosheets Formed via Defect-Mediated Transformation of a Hafnium Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 5397-5404	16.4	165
64	Development of a Cambridge Structural Database Subset: A Collection of Metal□Organic Frameworks for Past, Present, and Future. *Chemistry of Materials*, **2017**, 29, 2618-2625	9.6	499

63	"Explosive" synthesis of metal-formate frameworks for methane capture: an experimental and computational study. *Chemical Communications*, **2017**, 53, 11437-11440	5.8	14
62	Tuning the Endocytosis Mechanism of Zr-Based Metal-Organic Frameworks through Linker Functionalization. *ACS Applied Materials & Interfaces*, **2017**, 9, 35516-35525	9.5	31
61	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
60	Metal-organic frameworks as biosensors for luminescence-based detection and imaging. *Interface Focus*, **2016**, 6, 20160027	3.9	109
59	Endocytosis Mechanism of Nano Metal-Organic Frameworks for Drug Delivery. *Advanced Healthcare Materials*, **2016**, 5, 2261-70	10.1	59
58	Drug delivery and controlled release from biocompatible metal-organic frameworks using mechanical amorphization. *Journal of Materials Chemistry B*, **2016**, 4, 7697-7707	7.3	100
57	Trinuclear Cage-Like Zn(II) Macrocyclic Complexes: Enantiomeric Recognition and Gas Adsorption Properties. *Chemistry - A European Journal*, **2016**, 22, 598-609	4.8	45
56	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. *Chemical Communications*, **2016**, 52, 3639-42	5.8	77
55	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. *Journal of Materials Chemistry A*, **2016**, 4, 529-536	13	71
54	Highly Active Anti-Diabetic Metal□rganic Framework. *Crystal Growth and Design*, **2016**, 16, 537-540	3.5	20
53	Rare earth anthracenedicarboxylate metal-organic frameworks: slow relaxation of magnetization of Nd(3+), Gd(3+), Dy(3+), Er(3+) and Yb(3+) based materials. *Dalton Transactions*, **2016**, 45, 591-8	4.3	55
52	Luminescence and Magnetic Properties of Two Three-Dimensional Terbium and Dysprosium MOFs Based on Azobenzene-4,4′-Dicarboxylic Linker. *Polymers*, **2016**, 8,	4.5	7
51	Role of crystal size on swing-effect and adsorption induced structure transition of ZIF-8. *Dalton Transactions*, **2016**, 45, 6893-900	4.3	45
50	Amorphous metal-organic frameworks for drug delivery. *Chemical Communications*, **2015**, 51, 13878-81	5.8	247
49	Towards a potential 4,4?-(1,2,4,5-tetrazine-3,6-diyl) dibenzoic spacer to construct metal□rganic frameworks. *New Journal of Chemistry*, **2015**, 39, 6453-6458	3.6	9
48	Computational Screening of Metal Catecholates for Ammonia Capture in Metal□rganic Frameworks. *Industrial & Engineering Chemistry Research*, **2015**, 54, 3257-3267	3.9	26
47	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, 18970-82	4.3	20
46	Investigation of the terahertz vibrational modes of ZIF-8 and ZIF-90 with terahertz time-domain spectroscopy. *Chemical Communications*, **2015**, 51, 16037-40	5.8	39

45	Structure-directing factors when introducing hydrogen bond functionality to metal–organic frameworks. *CrystEngComm*, **2015**, 17, 299-306	3.3	31
44	2D-cadmium MOF and gismondine-like zinc coordination network based on the N-(2-tetrazolethyl)-4?-glycine linker. *New Journal of Chemistry*, **2015**, 39, 3982-3986	3.6	2
43	Mechanically and chemically robust ZIF-8 monoliths with high volumetric adsorption capacity. *Journal of Materials Chemistry A*, **2015**, 3, 2999-3005	13	71
42	A mechanochemical strategy for IRMOF assembly based on pre-designed oxo-zinc precursors. *Chemical Communications*, **2015**, 51, 4032-5	5.8	94
41	Long lifetime photoluminescence emission of 3D cadmium metal–organic frameworks based on the 5-(4-pyridyl)tetrazole ligand. *Inorganica Chimica Acta*, **2015**, 427, 131-137	2.7	15
40	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
39	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
38	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	3.8	9
37	Enhanced gas sorption properties and unique behavior toward liquid water in a pillared-paddlewheel metal-organic framework transmetalated with Ni(II). *Inorganic Chemistry*, **2014**, 53, 10432-6	5.1	22
36	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
35	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
34	Graphene-wrapped sulfur/metal organic framework-derived microporous carbon composite for lithium sulfur batteries. *APL Materials*, **2014**, 2, 124109	5.7	66
33	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
32	Metal–Organic Framework Thin Films Composed of Free-Standing Acicular Nanorods Exhibiting Reversible Electrochromism. *Chemistry of Materials*, **2013**, 25, 5012-5017	9.6	194
31	Novel 3D lanthanum oxalate metal-organic-framework: Synthetic, structural, luminescence and adsorption properties. *Polyhedron*, **2013**, 52, 315-320	2.7	20
30	Permanent porosity derived from the self-assembly of highly luminescent molecular zinc carbonate nanoclusters. *Angewandte Chemie - International Edition*, **2013**, 52, 13414-8	16.4	37
29	Modular structure of a robust microporous MOF based on Cu2 paddle-wheels with high CO2 selectivity. *Chemical Communications*, **2013**, 49, 11329-31	5.8	30
28	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

27	First examples of metal-organic frameworks with the novel 3,3'-(1,2,4,5-tetrazine-3,6-diyl)dibenzoic spacer. Luminescence and adsorption properties. *Inorganic Chemistry*, **2013**, 52, 546-8	5.1	26
26	Elucidating the breathing of the metal-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, 15763-73	16.4	154
25	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
24	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. *Journal of Physical Chemistry C*, **2013**, 117, 20116-20126	3.8	80
23	Permanent Porosity Derived From the Self-Assembly of Highly Luminescent Molecular Zinc Carbonate Nanoclusters. *Angewandte Chemie*, **2013**, 125, 13656-13660	3.6	8
22	Novel metal□organic frameworks based on 5-bromonicotinic acid: Multifunctional materials with H2 purification capabilities. *CrystEngComm*, **2012**, 14, 6390	3.3	13
21	A novel structural form of MIL-53 observed for the scandium analogue and its response to temperature variation and CO2 adsorption. *Dalton Transactions*, **2012**, 41, 3937-41	4.3	87
20	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	5.8	27
19	Understanding excess uptake maxima for hydrogen adsorption isotherms in frameworks with rht topology. *Chemical Communications*, **2012**, 48, 10496-8	5.8	46
18	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
17	Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. *Dalton Transactions*, **2012**, 41, 10752-62	4.3	150
16	Opening the gate: framework flexibility in ZIF-8 explored by experiments and simulations. *Journal of the American Chemical Society*, **2011**, 133, 8900-2	16.4	773
15	Structural chemistry, monoclinic-to-orthorhombic phase transition, and CO2 adsorption behavior of the small pore scandium terephthalate, Sc2(O2CC6H4)CO2)3, and its nitro- and amino-functionalized derivatives. *Inorganic Chemistry*, **2011**, 50, 10844-58	5.1	66
14	Hydrogen uptake by {H[Mg(HCOO)3]?NHMe2}□and determination of its H2 adsorption sites through Monte Carlo simulations. *Langmuir*, **2011**, 27, 10124-31	4	19
13	Unusual adsorption behavior on metal-organic frameworks. *Langmuir*, **2010**, 26, 14694-9	4	48
12	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	5.3	117
11	Carbon aerogels from gallic acid□resorcinol mixtures as adsorbents of benzene, toluene and xylenes from dry and wet air under dynamic conditions. *Carbon*, **2009**, 47, 463-469	10.4	44
10	Inter- and intra-primary-particle structure of monolithic carbon aerogels obtained with varying solvents. *Langmuir*, **2008**, 24, 2820-5	4	20

9	Adsorption of benzene, toluene, and xylenes on monolithic carbon aerogels from dry air flows. *Langmuir*, **2007**, 23, 10095-101	4	62
8	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, 8681-8	3.4	39
7	Porosity and surface area of monolithic carbon aerogels prepared using alkaline carbonates and organic acids as polymerization catalysts. *Carbon*, **2006**, 44, 2301-2307	10.4	89
6	Granular and monolithic activated carbons from KOH-activation of olive stones. *Microporous and Mesoporous Materials*, **2006**, 92, 64-70	5.3	100
5	Nanoporous carbon materials: Comparison between information obtained by SAXS and WAXS and by gas adsorption. *Carbon*, **2005**, 43, 3009-3012	10.4	16
4	Material Informatics with PoreBlazer v4.0 and CSD MOF Database		2
3	How Reproducible Are Surface Areas Calculated from the BET Equation?		5
2	Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. *Journal of Materials Chemistry C*,	7.1	0
1	How Reproducible are Surface Areas Calculated from the BET Equation?. *Advanced Materials*,2201502	24	12