Zhiwei Qiao

List of Publications by Citations

126 papers	4,245 citations	37 h-index	60 g-index
136 ext. papers	5,466 ext. citations	7.9 avg, IF	5.92 L-index

#	Paper	IF	Citations
126	Topologically guided tuning of Zr-MOF pore structures for highly selective separation of C6 alkane isomers. *Nature Communications*, **2018**, 9, 1745	17.4	166
125	A novel MOF/graphene oxide composite GrO@MIL-101 with high adsorption capacity for acetone. *Journal of Materials Chemistry A*, **2014**, 2, 4722-4730	13	165
124	A new MOF-505@GO composite with high selectivity for CO 2 /CH 4 and CO 2 /N 2 separation. *Chemical Engineering Journal*, **2017**, 308, 1065-1072	14.7	163
123	Enhancement of CO2 Adsorption and CO2/N2 Selectivity on ZIF-8 via Postsynthetic Modification. *AICHE Journal*, **2013**, 59, 2195-2206	3.6	137
122	An ethane-trapping MOF PCN-250 for highly selective adsorption of ethane over ethylene. *Chemical Engineering Science*, **2018**, 175, 110-117	4.4	125
121	Adsorption and Diffusion of Benzene on Chromium-Based Metal Organic Framework MIL-101 Synthesized by Microwave Irradiation. *Industrial & Engineering Chemistry Research*, **2011**, 50, 2254-2261	3.9	109
120	A new anti-biofilm strategy of enabling arbitrary surfaces of materials and devices with robust bacterial anti-adhesion via a spraying modified microsphere method. *Journal of Materials Chemistry A*, **2019**, 7, 26039-26052	13	104
119	Adsorption of Benzothiophene and Dibenzothiophene on Ion-Impregnated Activated Carbons and Ion-Exchanged Y Zeolites. *Energy & Fuels*, **2008**, 22, 3858-3863	4.1	103
118	Preparation and Adsorption Performance of for Separation of CO2/CH4. *Industrial & Engineering Chemistry Research*, **2014**, 53, 11176-11184	3.9	101
117	Ethane selective adsorbent Ni(bdc)(ted)0.5 with high uptake and its significance in adsorption separation of ethane and ethylene. *Chemical Engineering Science*, **2016**, 148, 275-281	4.4	98
116	Adsorption of CO2 on Zeolite 13X and Activated Carbon with Higher Surface Area. *Separation Science and Technology*, **2010**, 45, 710-719	2.5	91
115	A novel bimetallic MIL-101(Cr, Mg) with high CO2 adsorption capacity and CO2/N2 selectivity. *Chemical Engineering Science*, **2016**, 147, 109-117	4.4	86
114	Experimental and molecular simulation studies of CO2 adsorption on zeolitic imidazolate frameworks: ZIF-8 and amine-modified ZIF-8. *Adsorption*, **2013**, 19, 25-37	2.6	85
113	In silico screening of 4764 computation-ready, experimental metal–organic frameworks for CO2 separation. *Journal of Materials Chemistry A*, **2016**, 4, 2105-2114	13	84
112	Polydopamine-based synthesis of a zeolite imidazolate framework ZIF-100 membrane with high H2/CO2 selectivity. *Journal of Materials Chemistry A*, **2015**, 3, 4722-4728	13	82
111	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
110	Highly enhanced and weakened adsorption properties of two MOFs by water vapor for separation of CO2/CH4 and CO2/N2 binary mixtures. *Chemical Engineering Journal*, **2015**, 270, 385-392	14.7	77

109	Selective Adsorption of Ethane over Ethylene in PCN-245: Impacts of Interpenetrated Adsorbent. *ACS Applied Materials & Interfaces*, **2018**, 10, 8366-8373	9.5	77
108	Competitive adsorption of water vapor with VOCs dichloroethane, ethyl acetate and benzene on MIL-101(Cr) in humid atmosphere. *RSC Advances*, **2015**, 5, 1827-1834	3.7	73
107	High-throughput computational screening of 137953 metal–organic frameworks for membrane separation of a CO2/N2/CH4 mixture. *Journal of Materials Chemistry A*, **2016**, 4, 15904-15912	13	70
106	Efficient Mechanochemical Synthesis of MOF-5 for Linear Alkanes Adsorption. *Journal of Chemical & Engineering Data*, **2017**, 62, 2030-2036	2.8	64
105	Design of amine-functionalized metal-organic frameworks for CO2 separation: the more amine, the better?. *Chemical Communications*, **2016**, 52, 974-7	5.8	62
104	Highly Adsorptive Separation of Ethane/Ethylene by An Ethane-Selective MOF MIL-142A. *Industrial & Engineering Chemistry Research*, **2018**, 57, 4063-4069	3.9	61
103	Selective gas diffusion in two-dimensional MXene lamellar membranes: insights from molecular dynamics simulations. *Journal of Materials Chemistry A*, **2018**, 6, 11734-11742	13	61
102	Self-Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Live-Cell Imaging. *Angewandte Chemie - International Edition*, **2020**, 59, 10151-10159	16.4	55
101	Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study. *ACS Applied Materials & Interfaces*, **2016**, 8, 13392-9	9.5	54
100	High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas. *Journal of Membrane Science*, **2018**, 551, 47-54	9.6	53
99	Computational screening of hydrophobic metal–organic frameworks for the separation of H2S and CO2 from natural gas. *Journal of Materials Chemistry A*, **2018**, 6, 18898-18905	13	52
98	Formation of willow leaf-like structures composed of NH2-MIL68(In) on a multifunctional multiwalled carbon nanotube backbone for enhanced photocatalytic reduction of Cr(VI). *Nano Research*, **2017**, 10, 3543-3556	10	51
97	Design and self-assembly of hexahedral coordination cages for cascade reactions. *Nature Communications*, **2018**, 9, 4423	17.4	49
96	Liquid-Assisted Mechanochemical Synthesis of Copper Based MOF-505 for the Separation of CO2 over CH4 or N2. *Industrial & Engineering Chemistry Research*, **2018**, 57, 703-709	3.9	48
95	Highly efficient mechanochemical synthesis of an indium based metal-organic framework with excellent water stability. *Chemical Engineering Science*, **2017**, 158, 539-544	4.4	47
94	Efficient adsorptive separation of C3H6 over C3H8 on flexible and thermoresponsive CPL-1. *Chemical Engineering Journal*, **2017**, 328, 360-367	14.7	45
93	Structural Diversity of Zirconium Metal-Organic Frameworks and Effect on Adsorption of Toxic Chemicals. *Journal of the American Chemical Society*, **2020**, 142, 21428-21438	16.4	44
92	Adsorption performance of a MIL-101(Cr)/graphite oxide composite for a series of n-alkanes. *RSC Advances*, **2014**, 4, 56216-56223	3.7	41

91	Adsorption Isotherms, Kinetics, and Desorption of 1,2-Dichloroethane on Chromium-Based Metal Organic Framework MIL-101. *Separation Science and Technology*, **2013**, 48, 1479-1489	2.5	41
90	Zirconium-Based Metal□Organic Framework with 9-Connected Nodes for Ammonia Capture. *ACS Applied Nano Materials*, **2019**, 2, 6098-6102	5.6	37
89	Decomposition of Toluene in a Plasma Catalysis System with NiO, MnO2, CeO2, Fe2O3, and CuO Catalysts. *Plasma Chemistry and Plasma Processing*, **2013**, 33, 1073-1082	3.6	37
88	Machine-learning-assisted high-throughput computational screening of high performance metal□rganic frameworks. *Molecular Systems Design and Engineering*, **2020**, 5, 725-742	4.6	37
87	Selective Adsorption of Light Alkanes on a Highly Robust Indium Based Metal□Organic Framework. *Industrial & Engineering Chemistry Research*, **2017**, 56, 4488-4495	3.9	36
86	Highly selective adsorption separation of light hydrocarbons with a porphyrinic zirconium metal-organic framework PCN-224. *Separation and Purification Technology*, **2018**, 207, 262-268	8.3	33
85	Novel glucosamine-based carbon adsorbents with high capacity and its enhanced mechanism of preferential adsorption of C2H6 over C2H4. *Chemical Engineering Journal*, **2019**, 358, 1114-1125	14.7	33
84	Unusual Moisture-Enhanced CO Capture within Microporous PCN-250 Frameworks. *ACS Applied Materials & Interfaces*, **2018**, 10, 38638-38647	9.5	33
83	Protein Translocation through a MoS2 Nanopore:A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2018**, 122, 2070-2080	3.8	32
82	An indium-based ethane-trapping MOF for efficient selective separation of C2H6/C2H4 mixture. *Separation and Purification Technology*, **2019**, 212, 51-56	8.3	32
81	Effects of loading different metal ions on an activated carbon on the desorption activation energy of dichloromethane/trichloromethane. *Journal of Hazardous Materials*, **2010**, 179, 790-4	12.8	31
80	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal-Organic Polyhedra. *Angewandte Chemie - International Edition*, **2019**, 58, 1041-1045	16.4	31
79	Molecular dynamics simulations on the melting of gold nanoparticles. *Phase Transitions*, **2014**, 87, 59-70	1.3	30
78	Generation of novel patient-derived CIC- DUX4 sarcoma xenografts and cell lines. *Scientific Reports*, **2017**, 7, 4712	4.9	29
77	Molecular simulation study of wet flue gas adsorption on zeolite 13X. *Microporous and Mesoporous Materials*, **2018**, 261, 181-197	5.3	29
76	Selective Adsorptive Separation of CO2/CH4 and CO2/N2 by a Water Resistant Zirconium□Porphyrin Metal□Organic Framework. *Industrial & Engineering Chemistry Research*, **2018**, 57, 12215-12224	3.9	28
75	Iron-Based Metal-Organic Framework with Hydrophobic Quadrilateral Channels for Highly Selective Separation of Hexane Isomers. *ACS Applied Materials & Interfaces*, **2018**, 10, 6031-6038	9.5	27
74	Ultrahigh CO2/CH4 and CO2/N2 adsorption selectivities on a cost-effectively L-aspartic acid based metal-organic framework. *Chemical Engineering Journal*, **2019**, 375, 122074	14.7	26

73	Adsorption and Diffusion of Ethyl Acetate on the Chromium-Based Metal−Organic Framework MIL-101. *Journal of Chemical & Engineering Data*, **2011**, 56, 3419-3425	2.8	26
72	Machine learning and in silico discovery of metal-organic frameworks: Methanol as a working fluid in adsorption-driven heat pumps and chillers. *Chemical Engineering Science*, **2020**, 214, 115430	4.4	26
71	Highly rapid mechanochemical synthesis of a pillar-layer metal-organic framework for efficient CH4/N2 separation. *Chemical Engineering Journal*, **2020**, 385, 123836	14.7	26
70	Molecular Design of Zirconium Tetrazolate Metal−Organic Frameworks for CO2 Capture. *Crystal Growth and Design*, **2017**, 17, 543-549	3.5	25
69	High-Throughput Computational Screening of Metal−Organic Frameworks for Thiol Capture. *Journal of Physical Chemistry C*, **2017**, 121, 22208-22215	3.8	25
68	Large-Scale Screening and Machine Learning to Predict the Computation-Ready, Experimental Metal-Organic Frameworks for CO2 Capture from Air. *Applied Sciences (Switzerland)*, **2020**, 10, 569	2.6	23
67	Amino Acid Imprinted UiO-66s for Highly Recognized Adsorption of Small Angiotensin-Converting-Enzyme-Inhibitory Peptides. *ACS Applied Materials & Interfaces*, **2019**, 11, 23039-23049	9.5	22
66	Adsorption and separation of propane/propylene on various ZIF-8 polymorphs: Insights from GCMC simulations and the ideal adsorbed solution theory (IAST). *Chemical Engineering Journal*, **2020**, 386, 123945	14.7	21
65	Moisture stability of ethane-selective Ni(II), Fe(III), Zr(IV)-based metal−organic frameworks. *AICHE Journal*, **2019**, 65, e16616	3.6	20
64	Estimation of Activation Energy of Desorption of n-Hexanol from Activated Carbons by the TPD Technique. *Adsorption Science and Technology*, **2003**, 21, 125-133	3.6	20
63	A pillar-layer metal-organic framework for efficient adsorption separation of propylene over propane. *Separation and Purification Technology*, **2018**, 204, 75-80	8.3	19
62	Molecular simulation on the separation of water/ethanol azeotropic mixture by poly(vinyl alcohol) membrane. *Fluid Phase Equilibria*, **2011**, 302, 14-20	2.5	19
61	Implanting polyethylene glycol into MIL-101(Cr) as hydrophobic barrier for enhancing toluene adsorption under highly humid environment. *Chemical Engineering Journal*, **2021**, 404, 126562	14.7	19
60	Chiral metal-organic frameworks with tunable catalytic selectivity in asymmetric transfer hydrogenation reactions. *Nano Research*, **2021**, 14, 466-472	10	18
59	Encapsulation and Protection of Ultrathin Two-Dimensional Porous Organic Nanosheets within Biocompatible Metal−Organic Frameworks for Live-Cell Imaging. *Chemistry of Materials*, **2019**, 31, 4897-4912	9.6	17
58	Insights into the Structure-Activity Relationship in Aerobic Alcohol Oxidation over a Metal-Organic-Framework-Supported Molybdenum(VI) Catalyst. *Journal of the American Chemical Society*, **2021**, 143, 4302-4310	16.4	17
57	Mn3O4@C Nanoparticles Supported on Porous Carbon as Bifunctional Oxygen Electrodes and their Electrocatalytic Mechanism. *ChemElectroChem*, **2019**, 6, 359-368	4.3	17
56	Improving CH4/N2 selectivity within isomeric Al-based MOFs for the highly selective capture of coal-mine methane. *AICHE Journal*, **2020**, 66, e16287	3.6	16

55	Efficient adsorptive separation of propene over propane through a pillar-layer cobalt-based metal□organic framework. *AICHE Journal*, **2020**, 66, e16858	3.6	16
54	A gemini-type superspreader: Synthesis, spreading behavior and superspreading mechanism. *Chemical Engineering Journal*, **2017**, 315, 262-273	14.7	14
53	Machine learning and high-throughput computational screening of hydrophobic metal□organic frameworks for capture of formaldehyde from air. *Green Energy and Environment*, **2020**,	5.7	14
52	An Ultramicroporous Nickel-Based Metal□Organic Framework for Adsorption Separation of CO2 over N2 or CH4. *Energy & Fuels*, **2018**, 32, 8676-8682	4.1	14
51	Free-standing homochiral 2D monolayers by exfoliation of molecular crystals.. *Nature*, **2022**, 602, 606-611	50.4	14
50	Computational Screening of Metal?Organic Framework Membranes for the Separation of 15 Gas Mixtures. *Nanomaterials*, **2019**, 9,	5.4	13
49	Designing new amine functionalized metal-organic frameworks for carbon dioxide/methane separation. *Fluid Phase Equilibria*, **2014**, 362, 342-348	2.5	13
48	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
47	Novel Hierarchical Fe(III)-Doped Cu-MOFs With Enhanced Adsorption of Benzene Vapor. *Frontiers in Chemistry*, **2019**, 7, 652	5	12
46	Superoxide Decay Pathways in Oxygen Reduction Reaction on Carbon-Based Catalysts Evidenced by Theoretical Calculations. *ChemSusChem*, **2019**, 12, 1133-1138	8.3	12
45	Combining large-scale screening and machine learning to predict the metal-organic frameworks for organosulfurs removal from high-sour natural gas. *APL Materials*, **2019**, 7, 091101	5.7	11
44	Molecular Understanding and Design of Porous Polyurethane Hydrogels with Ultralow-Oil-Adhesion for Oil-Water Separation. *ACS Applied Materials & Interfaces*, **2020**, 12, 56530-56540	9.5	11
43	Enhanced Adsorption Performance of Aromatics on a Novel Chromium-Based [email□protected] Oxide Composite. *Energy & Fuels*, **2017**, 31, 13985-13990	4.1	11
42	Recent advances in adsorptive separation of ethane and ethylene by C2H6-selective MOFs and other adsorbents. *Chemical Engineering Journal*, **2021**, 431, 133208	14.7	11
41	Establishment and characterization of novel patient-derived osteosarcoma xenograft and cell line. *In Vitro Cellular and Developmental Biology - Animal*, **2018**, 54, 528-536	2.6	11
40	Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: A molecular simulation study. *Chemical Engineering Journal*, **2019**, 356, 737-745	14.7	10
39	Proteomic approach toward determining the molecular background of pazopanib resistance in synovial sarcoma. *Oncotarget*, **2017**, 8, 109587-109595	3.3	10
38	High-Throughput Screening of Metal-Organic Frameworks for the Separation of Hydrogen Sulfide and Carbon Dioxide from Natural Gas. *Acta Chimica Sinica*, **2018**, 76, 785	3.3	10

37	Tuning the Structural Flexibility for Multi-Responsive Gas Sorption in Isonicotinate-Based Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2021**, 13, 16820-16827	9.5	10
36	Ethane-Selective Behavior Achieved on a Nickel-Based Metal–Organic Framework: Impact of Pore Effect and Hydrogen Bonds. *Industrial & Engineering Chemistry Research*, **2019**, 58, 10516-10523	3.9	9
35	Selective extraction of methane from C1/C2/C3 on moisture-resistant MIL-142A with interpenetrated networks. *Chemical Engineering Journal*, **2020**, 395, 125057	14.7	9
34	Machine Learning and High-throughput Computational Screening of Metal-organic Framework for Separation of Methane/ethane/propane. *Acta Chimica Sinica*, **2020**, 78, 427	3.3	9
33	Tuning the Atrazine Binding Sites in an Indium-Based Flexible Metal-Organic Framework. *ACS Applied Materials & Interfaces*, **2020**, 12, 44762-44768	9.5	9
32	A novel fructose-based adsorbent with high capacity and its ethane-selective adsorption property. *Journal of Solid State Chemistry*, **2018**, 268, 190-197	3.3	9
31	Machine learning and in-silico screening of metal–organic frameworks for O2/N2 dynamic adsorption and separation. *Chemical Engineering Journal*, **2022**, 427, 131604	14.7	9
30	Rapid room temperature conversion of hydroxy double salt to MOF-505 for CO2 capture. *CrystEngComm*, **2019**, 21, 165-171	3.3	8
29	Self-Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Live-Cell Imaging. *Angewandte Chemie*, **2020**, 132, 10237-10245	3.6	8
28	Solution-Processable Metal-Organic Framework Nanosheets with Variable Functionalities. *Advanced Materials*, **2021**, 33, e2101257	24	8
27	Identifying the best metal–organic frameworks and unravelling different mechanisms for the separation of pentane isomers. *Molecular Systems Design and Engineering*, **2019**, 4, 609-615	4.6	7
26	Cerium Doped Pt/TiO2 for Catalytic Oxidation of Low Concentration Formaldehyde at Room Temperature. *Catalysis Letters*, **2019**, 149, 1319-1325	2.8	7
25	Development of Iron Encapsulated Hollow Beta Zeolites for Ammonia Selective Catalytic Reduction. *Industrial & Engineering Chemistry Research*, **2019**, 58, 2914-2923	3.9	7
24	Role of Temperature in the Structure of Zn(II)-1,4,-BDC Metal-Organic Frameworks and their Adsorption and Diffusion Properties for Carbon Dioxide. *Separation Science and Technology*, **2011**, 46, 1337-1345	2.5	7
23	Pore Distortion in a Metal-Organic Framework for Regulated Separation of Propane and Propylene. *Journal of the American Chemical Society*, **2021**, 143, 19300-19305	16.4	7
22	Highly Efficient Capture of Postcombustion Generated CO2 through a Copper-Based Metal–Organic Framework. *Energy & Fuels*, **2021**, 35, 610-617	4.1	7
21	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal–Organic Polyhedra. *Angewandte Chemie*, **2019**, 131, 1053-1057	3.6	7
20	Techno-economic analysis of metal–organic frameworks for adsorption heat pumps/chillers: from directional computational screening, machine learning to experiment. *Journal of Materials Chemistry A*, **2021**, 9, 7656-7666	13	7

19	Room-Temperature Synthesis of Pyr1/3@CuBTC with Enhanced Stability and Its Excellent Performance for Separation of Propylene/Propane. *Industrial & Engineering Chemistry Research*, **2020**, 59, 6202-6209	3.9	6
18	Metal□Organic Frameworks for Xylene Separation: From Computational Screening to Machine Learning. *Journal of Physical Chemistry C*, **2021**, 125, 7839-7848	3.8	6
17	Adsorption behavior of metal-organic frameworks: From single simulation, high-throughput computational screening to machine learning. *Computational Materials Science*, **2021**, 193, 110383	3.2	6
16	Preferential adsorption of ethane over ethylene on a Zr-based metal□organic framework: impacts of C□H?N hydrogen bonding. *New Journal of Chemistry*, **2021**, 45, 8045-8053	3.6	6
15	Establishment and characterization of a novel dedifferentiated chondrosarcoma cell line, NCC-dCS1-C1. *Human Cell*, **2019**, 32, 202-213	4.5	5
14	Fe-Encapsulated ZSM-5 Zeolite with Nanosheet-Assembled Structure for the Selective Catalytic Reduction of NOx with NH3. *Industrial & Engineering Chemistry Research*, **2020**, 59, 8592-8600	3.9	5
13	Synthesis and Adsorption Performance of Ag/□Al2O3 with High Adsorption Capacities for Dibenzyl Disulfide. *Industrial & Engineering Chemistry Research*, **2020**, 59, 6164-6171	3.9	3
12	A Ni-based metal-organic framework with super-high C3H8 uptake for adsorptive separation of light alkanes. *Separation and Purification Technology*, **2021**, 266, 118198	8.3	3
11	The modulation of ethane-selective adsorption performance in series of bimetal PCN-250 metal□organic frameworks: Impact of metal composition. *AICHE Journal*,e17385	3.6	3
10	Effect of textural property of coconut shell-based activated carbon on desorption activation energy of benzothiophene. *Frontiers of Chemical Engineering in China*, **2008**, 2, 269-275		2
9	Molecular fingerprint and machine learning to accelerate design of high-performance homochiral metal□organic frameworks. *AICHE Journal*, **2021**, 67, e17352	3.6	2
8	Molecular-fingerprint machine-learning-assisted design and prediction for high-performance MOFs for capture of NMHCs from air **2022**, 1, 100026		2
7	Kinome profiling analysis identified Src pathway as a novel therapeutic target in combination with histone deacetylase inhibitors for cutaneous T-cell lymphoma. *Journal of Dermatological Science*, **2021**, 101, 194-201	4.3	1
6	Pazopanib-induced changes in protein expression signatures of extracellular vesicles in synovial sarcoma. *Biochemical and Biophysical Research Communications*, **2018**, 506, 723-730	3.4	1
5	Predicting adsorption and separation performance indicators of Xe/Kr in metal-organic frameworks via a precursor-based neural network model. *Chemical Engineering Science*, **2021**, 243, 116772	4.4	1
4	Machine-Learning-Assisted High-Throughput Computational Screening of Metal□Organic Framework Membranes for Hydrogen Separation. *Chemical Engineering Journal*, **2022**, 136783	14.7	1
3	Mechanochemical synthesis of a robust cobalt-based metal□organic framework for adsorption separation methane from nitrogen. *Chemical Engineering Journal*, **2021**, 133876	14.7	0
2	Separation of propylene and propane with pillar-layer metal-organic frameworks by exploiting thermodynamic-kinetic synergetic effect. *Chemical Engineering Journal*, **2021**, 133284	14.7	0

1	Metal-Organic Frameworks: Solution-Processable Metal–Organic Framework Nanosheets with Variable Functionalities (Adv. Mater. 29/2021). *Advanced Materials*, **2021**, 33, 2170228	24	0