Krista S Walton

List of Publications by Citations

129 papers	12,860 citations	50 h-index	113 g-index
133 ext. papers	14,579 ext. citations	7.9 avg, IF	6.91 L-index

#	Paper	IF	Citations
129	Water stability and adsorption in metal-organic frameworks. *Chemical Reviews*, **2014**, 114, 10575-612	68.1	1513
128	Highly efficient separation of carbon dioxide by a metal-organic framework replete with open metal sites. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 20637-40	11.5	950
127	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
126	Exceptional ammonia uptake by a covalent organic framework. *Nature Chemistry*, **2010**, 2, 235-8	17.6	675
125	Stability and degradation mechanisms of metal□rganic frameworks containing the Zr6O4(OH)4 secondary building unit. *Journal of Materials Chemistry A*, **2013**, 1, 5642	13	469
124	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
123	Calculating Geometric Surface Areas as a Characterization Tool for Metal□rganic Frameworks. *Journal of Physical Chemistry C*, **2007**, 111, 15350-15356	3.8	446
122	MOF-74 building unit has a direct impact on toxic gas adsorption. *Chemical Engineering Science*, **2011**, 66, 163-170	4.4	438
121	Effect of Water Adsorption on Retention of Structure and Surface Area of Metal□rganic Frameworks. *Industrial & Engineering Chemistry Research*, **2012**, 51, 6513-6519	3.9	393
120	Tuning the adsorption properties of UiO-66 via ligand functionalization. *Langmuir*, **2012**, 28, 15606-13	4	388
119	CO2 adsorption in Y and X zeolites modified by alkali metal cation exchange. *Microporous and Mesoporous Materials*, **2006**, 91, 78-84	5.3	359
118	Exceptional negative thermal expansion in isoreticular metal-organic frameworks. *Angewandte Chemie - International Edition*, **2007**, 46, 4496-9	16.4	260
117	On the inner workings of Monte Carlo codes. *Molecular Simulation*, **2013**, 39, 1253-1292	2	238
116	Nickel-based pillared MOFs for high-performance supercapacitors: Design, synthesis and stability study. *Nano Energy*, **2016**, 26, 66-73	17.1	238
115	Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory. *AICHE Journal*, **2015**, 61, 2757-2762	3.6	219
114	Effect of open metal sites on adsorption of polar and nonpolar molecules in metal-organic framework Cu-BTC. *Langmuir*, **2008**, 24, 8620-6	4	190
113	Molecular Simulations and Experimental Studies of CO2, CO, and N2 Adsorption in Metal□rganic Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 15735-15740	3.8	154

112	Rapid Cycling and Exceptional Yield in a Metal-Organic Framework Water Harvester. *ACS Central Science*, **2019**, 5, 1699-1706	16.8	150
111	Fabrication of metal-organic framework-containing silica-colloidal crystals for vapor sensing. *Advanced Materials*, **2011**, 23, 4449-52	24	148
110	Gas Adsorption Study on Mesoporous Metal□Organic Framework UMCM-1. *Journal of Physical Chemistry C*, **2010**, 114, 6464-6471	3.8	148
109	Evaluation of MOFs for air purification and air quality control applications: Ammonia removal from air. *Chemical Engineering Science*, **2015**, 124, 118-124	4.4	144
108	Adjusting the stability of metal-organic frameworks under humid conditions by ligand functionalization. *Langmuir*, **2012**, 28, 16874-80	4	143
107	A novel metal-organic coordination polymer for selective adsorption of CO2 over CH4. *Chemical Communications*, **2009**, 2493-5	5.8	143
106	Kinetic water stability of an isostructural family of zinc-based pillared metal-organic frameworks. *Langmuir*, **2013**, 29, 633-42	4	138
105	Direct Air Capture of CO2 Using Amine Functionalized MIL-101(Cr). *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 5761-5768	8.3	131
104	Functionalized Bimetallic Hydroxides Derived from Metal□Organic Frameworks for High-Performance Hybrid Supercapacitor with Exceptional Cycling Stability. *ACS Energy Letters*, **2017**, 2, 1263-1269	20.1	128
103	Rational Tuning of Water Vapor and CO2Adsorption in Highly Stable Zr-Based MOFs. *Journal of Physical Chemistry C*, **2012**, 116, 23526-23532	3.8	121
102	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
101	Effects of pelletization pressure on the physical and chemical properties of the metal□organic frameworks Cu3(BTC)2 and UiO-66. *Microporous and Mesoporous Materials*, **2013**, 179, 48-53	5.3	115
100	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
99	Structure and mobility of metal clusters in MOFs: Au, Pd, and AuPd clusters in MOF-74. *Journal of the American Chemical Society*, **2012**, 134, 12807-16	16.4	109
98	Tuning the Kinetic Water Stability and Adsorption Interactions of Mg-MOF-74 by Partial Substitution with Co or Ni. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12408-12414	3.9	108
97	Thermal Analysis and Heat Capacity Study of Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2011**, 115, 22748-22754	3.8	107
96	Effect of catenation and basicity of pillared ligands on the water stability of MOFs. *Dalton Transactions*, **2013**, 42, 15421-6	4.3	96
95	High-throughput screening of metal-organic frameworks for CO2 separation. *ACS Combinatorial Science*, **2012**, 14, 263-7	3.9	91

94	CO2 capture via adsorption in amine-functionalized sorbents. *Current Opinion in Chemical Engineering*, **2016**, 12, 82-90	5.4	84
93	Molecular-level insight into unusual low pressure CO2 affinity in pillared metal-organic frameworks. *Journal of the American Chemical Society*, **2013**, 135, 7172-80	16.4	82
92	MOF stability and gas adsorption as a function of exposure to water, humid air, SO2, and NO2. *Microporous and Mesoporous Materials*, **2013**, 173, 86-91	5.3	81
91	Modulating adsorption and stability properties in pillared metal-organic frameworks: a model system for understanding ligand effects. *Accounts of Chemical Research*, **2015**, 48, 2850-7	24.3	72
90	Interactions of SO2-Containing Acid Gases with ZIF-8: Structural Changes and Mechanistic Investigations. *Journal of Physical Chemistry C*, **2016**, 120, 27221-27229	3.8	71
89	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
88	Effect of synthesis solvent on the breathing behavior of MIL-53(Al). *Journal of Colloid and Interface Science*, **2015**, 447, 33-9	9.3	63
87	Breathing effects of CO2 adsorption on a flexible 3D lanthanide metal□organic framework. *Journal of Materials Chemistry*, **2012**, 22, 10172		61
86	A porous flexible homochiral SrSi2 array of single-stranded helical nanotubes exhibiting single-crystal-to-single-crystal oxidation transformation. *Angewandte Chemie - International Edition*, **2011**, 50, 436-40	16.4	61
85	Impact of Alkyl-Functionalized BTC on Properties of Copper-Based Metal□Organic Frameworks. *Crystal Growth and Design*, **2012**, 12, 3709-3713	3.5	59
84	Synergistic Effects of Water and SO2 on Degradation of MIL-125 in the Presence of Acid Gases. *Journal of Physical Chemistry C*, **2016**, 120, 27230-27240	3.8	59
83	Synthesis of cobalt-, nickel-, copper-, and zinc-based, water-stable, pillared metal-organic frameworks. *Langmuir*, **2014**, 30, 14300-7	4	58
82	Experimental Study of CO2, CH4, and Water Vapor Adsorption on a Dimethyl-Functionalized UiO-66 Framework. *Journal of Physical Chemistry C*, **2013**, 117, 7062-7068	3.8	56
81	Monolith-Supported Amine-Functionalized Mg(dobpdc) Adsorbents for CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 17042-17050	9.5	53
80	Kinetics study and crystallization process design for scale-up of UiO-66-NH2 synthesis. *AICHE Journal*, **2013**, 59, 1255-1262	3.6	51
79	Adsorption study of CO2, CH4, N2, and H2O on an interwoven copper carboxylate metal-organic framework (MOF-14). *Journal of Colloid and Interface Science*, **2013**, 392, 331-336	9.3	50
78	CO2 Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites. *Journal of Physical Chemistry C*, **2017**, 121, 25778-25787	3.8	49
77	Acid Gas Stability of Zeolitic Imidazolate Frameworks: Generalized Kinetic and Thermodynamic Characteristics. *Chemistry of Materials*, **2018**, 30, 4089-4101	9.6	49

76	Synthesis and Characterization of UiO-66-NH2 Metal Organic Framework Cotton Composite Textiles. *Industrial & Engineering Chemistry Research*, **2018**, 57, 9151-9161	3.9	47
75	Impact of MOF defects on the binary adsorption of CO2 and water in UiO-66. *Chemical Engineering Science*, **2019**, 203, 346-357	4.4	46
74	Control of Metal Organic Framework Crystal Topology by Ligand Functionalization: Functionalized HKUST-1 Derivatives. *Crystal Growth and Design*, **2014**, 14, 6122-6128	3.5	43
73	Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies. *Journal of Physical Chemistry C*, **2017**, 121, 23471-23479	3.8	42
72	Synthesis, Characterization, and Adsorption Studies of Nickel(II), Zinc(II), and Magnesium(II) Coordination Frameworks of BTTB. *Crystal Growth and Design*, **2013**, 13, 1075-1081	3.5	39
71	Probing Metal-Organic Framework Design for Adsorptive Natural Gas Purification. *Langmuir*, **2018**, 34, 8443-8450	4	39
70	Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74. *Journal of Physical Chemistry C*, **2017**, 121, 627-635	3.8	37
69	Liquid-Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents. *Journal of Physical Chemistry C*, **2018**, 122, 386-397	3.8	36
68	CO2 hydrogenation to methanol on Pd Cu bimetallic catalysts with lower metal loadings. *Catalysis Communications*, **2019**, 118, 10-14	3.2	36
67	A combined experimental and DFT study of H2O effect on In2O3/ZrO2 catalyst for CO2 hydrogenation to methanol. *Journal of Catalysis*, **2020**, 383, 283-296	7.3	35
66	DMOF-1 as a Representative MOF for SO2 Adsorption in Both Humid and Dry Conditions. *Journal of Physical Chemistry C*, **2018**, 122, 23493-23500	3.8	35
65	An alternative UiO-66 synthesis for HCl-sensitive nanoparticle encapsulation. *RSC Advances*, **2014**, 4, 51080-51083	3.7	30
64	Understanding DABCO Nanorotor Dynamics in Isostructural Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2015**, 6, 812-6	6.4	30
63	In situ visualization of loading-dependent water effects in a stable metal-organic framework. *Nature Chemistry*, **2020**, 12, 186-192	17.6	30
62	Moving Beyond Adsorption Capacity in Design of Adsorbents for CO2 Capture from Ultradilute Feeds: Kinetics of CO2 Adsorption in Materials with Stepped Isotherms. *Industrial & Engineering Chemistry Research*, **2019**, 58, 366-377	3.9	30
61	Effect of Surface Structure of TiO2 Nanoparticles on CO2 Adsorption and SO2 Resistance. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 9295-9306	8.3	29
60	Prediction of water stability of metal organic frameworks using machine learning. *Nature Machine Intelligence*, **2020**, 2, 704-710	22.5	29
59	Research Challenges in Avoiding Showstoppers In Developing Materials for Large-Scale Energy Applications. *Joule*, **2017**, 1, 208-211	27.8	28

58	Structured Growth of Metal-Organic Framework MIL-53(Al) from Solid Aluminum Carbide Precursor. *Journal of the American Chemical Society*, **2018**, 140, 9148-9153	16.4	28
57	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. *Advanced Theory and Simulations*, **2019**, 2, 1900135	3.5	27
56	Natural gas storage cycles: Influence of nonisothermal effects and heavy alkanes. *Adsorption*, **2006**, 12, 227-235	2.6	25
55	Adsorption Equilibrium of Alkanes on a High Surface Area Activated Carbon Prepared from Brazilian Coconut Shells. *Adsorption*, **2005**, 11, 107-111	2.6	25
54	High-Performance Electrodes for a Hybrid Supercapacitor Derived from a Metal□Organic Framework/Graphene Composite. *ACS Applied Energy Materials*, **2019**, 2, 5029-5038	6.1	24
53	Role of defects and metal coordination on adsorption of acid gases in MOFs and metal oxides: An in situ IR spectroscopic study. *Microporous and Mesoporous Materials*, **2016**, 227, 65-75	5.3	24
52	A Novel Adsorption Cycle for CO2 Recovery: Experimental and Theoretical Investigations of a Temperature Swing Compression Process. *Separation Science and Technology*, **2006**, 41, 485-500	2.5	24
51	Engineering Copper Carboxylate Functionalities on Water Stable Metal□Organic Frameworks for Enhancement of Ammonia Removal Capacities. *Journal of Physical Chemistry C*, **2017**, 121, 3310-3319	3.8	22
50	Computational Screening of Functionalized UiO-66 Materials for Selective Contaminant Removal from Air. *Journal of Physical Chemistry C*, **2017**, 121, 20396-20406	3.8	22
49	A metal□organic framework with coordinatively unsaturated metal centers and microporous structure. *CrystEngComm*, **2010**, 12, 2347	3.3	22
48	A Collection of More than 900 Gas Mixture Adsorption Experiments in Porous Materials from Literature Meta-Analysis. *Industrial & Engineering Chemistry Research*, **2021**, 60, 639-651	3.9	22
47	Stability of Zeolitic Imidazolate Frameworks in NO2. *Journal of Physical Chemistry C*, **2019**, 123, 2336-2346	3.8	22
46	Structural stability of BTTB-based metal□organic frameworks under humid conditions. *Journal of Materials Chemistry A*, **2015**, 3, 1624-1631	13	19
45	Tuning the Structures of Metal□Organic Frameworks via a Mixed-Linker Strategy for Ethylene/Ethane Kinetic Separation. *Chemistry of Materials*, **2020**, 32, 3715-3722	9.6	19
44	Kinetics of Water Adsorption in UiO-66 MOF. *Industrial & Engineering Chemistry Research*, **2019**, 58, 10550-10558	3.9	18
43	Adsorption equilibrium of methane and carbon dioxide on porous metal-organic framework Zn-BTB. *Adsorption*, **2011**, 17, 777-782	2.6	18
42	Consistency of Energy and Material Balances for Bidisperse Particles in Fixed-Bed Adsorption and Related Applications. *Industrial & Engineering Chemistry Research*, **2003**, 42, 6938-6948	3.9	18
41	Synergistic Effect of Mixed Oxide on the Adsorption of Ammonia with Metal□Organic Frameworks. *Industrial & Engineering Chemistry Research*, **2016**, 55, 6492-6500	3.9	16

40	Synthesis of embedded iron nanoparticles in Fe3C-derived carbons. *Carbon*, **2014**, 79, 74-84	10.4	16
39	Synthesis and characterization of aluminum carbide-derived carbon with residual aluminum-based nanoparticles. *Carbon*, **2017**, 114, 482-495	10.4	15
38	Tuning the Wettability of Metal-Organic Frameworks via Defect Engineering for Efficient Oil/Water Separation. *ACS Applied Materials & Interfaces*, **2020**, 12, 34413-34422	9.5	15
37	High-Pressure Adsorption Equilibrium of CO2, CH4, and CO on an Impregnated Activated Carbon. *Journal of Chemical & Engineering Data*, **2011**, 56, 390-397	2.8	15
36	Carbon Dioxide Capture Chemistry of Amino Acid Functionalized Metal-Organic Frameworks in Humid Flue Gas.. *Journal of the American Chemical Society*, **2022**,	16.4	15
35	Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC. *Journal of Physical Chemistry C*, **2016**, 120, 9148-9159	3.8	15
34	Does Chemical Engineering Research Have a Reproducibility Problem?. *Annual Review of Chemical and Biomolecular Engineering*, **2019**, 10, 43-57	8.9	14
33	A Porous Flexible Homochiral SrSi2 Array of Single-Stranded Helical Nanotubes Exhibiting Single-Crystal-to-Single-Crystal Oxidation Transformation. *Angewandte Chemie*, **2011**, 123, 456-460	3.6	13
32	How Reproducible are Surface Areas Calculated from the BET Equation?. *Advanced Materials*,2201502	24	12
31	Membrane-Coated UiO-66 MOF Adsorbents. *Industrial & Engineering Chemistry Research*, **2019**, 58, 1352-1362	3.9	11
30	Room-Temperature Synthesis of Metal-Organic Framework Isomers in the Tetragonal and Kagome Crystal Structure. *Inorganic Chemistry*, **2019**, 58, 7690-7697	5.1	11
29	Flexible Force Field Parameterization through Fitting on the Ab Initio-Derived Elastic Tensor. *Journal of Chemical Theory and Computation*, **2017**, 13, 3722-3730	6.4	11
28	Adsorbed-Phase Heat Capacities: Thermodynamically Consistent Values Determined from Temperature-Dependent Equilibrium Models. *Industrial & Engineering Chemistry Research*, **2005**, 44, 178-182	3.9	11
27	Investigating water and framework dynamics in pillared MOFs. *Molecular Simulation*, **2015**, 41, 1379-1387	2	10
26	Tailored Fe3C-derived carbons with embedded Fe nanoparticles for ammonia adsorption. *Carbon*, **2015**, 95, 208-219	10.4	10
25	Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory. *Chemistry - A European Journal*, **2016**, 22, 18045-18050	4.8	10
24	Effect of Energy Balance Approximations on Simulation of Fixed-Bed Adsorption. *Industrial & Engineering Chemistry Research*, **2005**, 44, 7474-7480	3.9	10
23	Production of metal-organic framework-bearing polystyrene fibers by solution blow spinning. *Chemical Engineering Science*, **2019**, 203, 220-227	4.4	9

22	Computational investigation on CO2 adsorption in titanium carbide-derived carbons with residual titanium. *Carbon*, **2017**, 111, 741-751	10.4	9
21	Simple group contribution theory for adsorption of alkanes in nanoporous carbons. *Chemical Engineering Science*, **2004**, 59, 4425-4432	4.4	9
20	Enhanced Sulfur Dioxide Adsorption in UiO-66 Through Crystal Engineering and Chalcogen Bonding. *Crystal Growth and Design*, **2020**, 20, 6139-6146	3.5	9
19	Superhydrophobic Functionalization of Cotton Fabric via Reactive Dye Chemistry and a Thiol□ene Click Reaction. *Industrial & Engineering Chemistry Research*, **2019**, 58, 22534-22540	3.9	8
18	110th Anniversary: Commentary: Perspectives on Adsorption of Complex Mixtures. *Industrial & Engineering Chemistry Research*, **2019**, 58, 17100-17105	3.9	7
17	Household Aluminum Products as Insoluble Precursors for Directed Growth of Metal□Organic Frameworks. *Crystal Growth and Design*, **2019**, 19, 5097-5104	3.5	7
16	Tuning residual metal in partially etched carbide-derived carbons for enhanced acid gas adsorption. *Carbon*, **2020**, 158, 481-493	10.4	6
15	Humid Ethylene/Ethane Separation on Ethylene-Selective Materials. *Industrial & Engineering Chemistry Research*, **2021**, 60, 9940-9947	3.9	6
14	The effects of reactor design on the synthesis of titanium carbide-derived carbon. *Chemical Engineering Science*, **2017**, 160, 191-199	4.4	5
13	How Reproducible Are Surface Areas Calculated from the BET Equation?		5
12	Modulation and Tuning of UiO-66 for Lewis Acid Catalyzed Carbohydrate Conversion: Conversion of Unprotected Aldose Sugars to Polyhydroxyalkyl and C-Glycosyl Furans. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 11581-11595	8.3	4
11	Opening the Toolbox: 18 Experimental Techniques for Measurement of Mixed Gas Adsorption. *Industrial & Engineering Chemistry Research*,	3.9	3
10	Water Bridges Substitute for Defects in Amine-Functionalized UiO-66, Boosting CO Adsorption. *Langmuir*, **2021**, 37, 10439-10449	4	3
9	Inorganic chemistry: Movies of a growth mechanism. *Nature*, **2015**, 523, 535-6	50.4	2
8	An automated multi-component gas adsorption system (MC GAS). *Review of Scientific Instruments*, **2021**, 92, 054102	1.7	2
7	NMR Crystallography of Aluminum Carbide: Impurities in the Reagent and Improved 27Al NMR Tensors. *Journal of Physical Chemistry C*, **2020**, 124, 7238-7243	3.8	1
6	Anisotropic Thermal Expansion in an Anionic Framework Showing Guest-Dependent Phases. *Frontiers in Chemistry*, **2020**, 8, 506	5	1
5	Steric and Electronic Effects on the Interaction of Xe and Kr with Functionalized Zirconia Metal□Organic Frameworks **2021**, 3, 504-510		1

4	Structural similarity, synthesis, and adsorption properties of aluminum-based metal-organic frameworks. *Adsorption*, **2021**, 27, 227-236	2.6	1
3	Effect of Loading on the Water Stability of the Metal−Organic Framework DMOF-1 [Zn(bdc)(dabco)0.5]. *Journal of Physical Chemistry Letters*,4891-4896	6.4	1
2	Development of Energy Balances for Fixed-Bed Adsorption Processes: Thermodynamic Paths, Heat Capacities and Isosteric Heats. *Adsorption*, **2005**, 11, 555-559	2.6	0
1	Discrepancy quantification between experimental and simulated data of CO2 adsorption isotherm using hierarchical Bayesian estimation. *Separation and Purification Technology*, **2022**, 121371	8.3	0