

# Katherine A Forrest

## List of Publications by Year in descending order

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69

papers

6,196

citations

117625

34

h-index

95266

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all docs

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docs citations

71

times ranked

4682

citing authors

#	ARTICLE	IF	CITATIONS
1	Self-Adjusting Metal-Organic Framework for Efficient Capture of Trace Xenon and Krypton. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	5
2	Self-Adjusting Metal-Organic Framework for Efficient Capture of Trace Xenon and Krypton. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	47
3	Investigating H <sub>2</sub> Adsorption in Isostructural Metal-Organic Frameworks M-CUK-1 (M = Co) Tj ETQq1 1 0.784314 rgBT 14, 8126-8136.	8.0	5
4	Metal-Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. <i>Journal of the American Chemical Society</i> , 2022, 144, 1681-1689.	13.7	172
5	Pore-Nanospace Engineering of Mixed-Ligand Metal-Organic Frameworks for High Adsorption of Hydrofluorocarbons and Hydrochlorofluorocarbons. <i>Chemistry of Materials</i> , 2022, 34, 5116-5124.	6.7	11
6	A MOF-based Ultra-Strong Acetylene Nano-trap for Highly Efficient C <sub>2</sub> H <sub>2</sub> /CO <sub>2</sub> Separation. <i>Angewandte Chemie</i> , 2021, 133, 5343-5348.	2.0	49
7	Frontispiz: A MOF-based Ultra-Strong Acetylene Nano-trap for Highly Efficient C <sub>2</sub> H <sub>2</sub> /CO <sub>2</sub> Separation. <i>Angewandte Chemie</i> , 2021, 133, .	2.0	1
8	Frontispiece: A MOF-based Ultra-Strong Acetylene Nano-trap for Highly Efficient C <sub>2</sub> H <sub>2</sub> /CO <sub>2</sub> Separation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, .	13.8	0
9	A MOF-based Ultra-Strong Acetylene Nano-trap for Highly Efficient C <sub>2</sub> H <sub>2</sub> /CO <sub>2</sub> Separation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5283-5288.	13.8	172
10	Nanospace Engineering of Metal-Organic Frameworks through Dynamic Spacer Installation of Multifunctionalities for Efficient Separation of Ethane from Ethane/Ethylene Mixtures. <i>Angewandte Chemie</i> , 2021, 133, 9766-9771.	2.0	9
11	Nanospace Engineering of Metal-Organic Frameworks through Dynamic Spacer Installation of Multifunctionalities for Efficient Separation of Ethane from Ethane/Ethylene Mixtures. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9680-9685.	13.8	89
12	Amino-Functionalised Hybrid Ultramicroporous Materials that Enable Single-Step Ethylene Purification from a Ternary Mixture. <i>Angewandte Chemie</i> , 2021, 133, 10997-11004.	2.0	10
13	Amino-Functionalised Hybrid Ultramicroporous Materials that Enable Single-Step Ethylene Purification from a Ternary Mixture. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10902-10909.	13.8	56
14	Molecular Sieving of Acetylene from Ethylene in a Rigid Ultramicroporous Metal Organic Framework.. <i>Chemistry - A European Journal</i> , 2021, 27, 9446-9453.	3.3	20
15	Indium-Organic Framework with <i>soc</i> Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of $\alpha$ -aminonitriles. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 52023-52033.	8.0	28
16	Toward an Understanding of the Propensity for Crystalline Hydrate Formation by Molecular Compounds. Part 2. <i>Crystal Growth and Design</i> , 2021, 21, 4927-4939.	3.0	13
17	Breaking the trade-off between selectivity and adsorption capacity for gas separation. <i>CheM</i> , 2021, 7, 3085-3098.	11.7	68
18	Efficient propyne/propadiene separation by microporous crystalline physiadsorbents. <i>Nature Communications</i> , 2021, 12, 5768.	12.8	26

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19	Pore Engineering for One-Step Ethylene Purification from a Three-Component Hydrocarbon Mixture. <i>Journal of the American Chemical Society</i> , 2021, 143, 1485-1492.	13.7	143
20	One-step ethylene production from a four-component gas mixture by a single physisorbent. <i>Nature Communications</i> , 2021, 12, 6507.	12.8	64
21	Tuning the Selectivity between C <sub>2</sub> H <sub>2</sub> and CO <sub>2</sub> in Molecular Porous Materials. <i>Langmuir</i> , 2021, 37, 13838-13845.	3.5	9
22	Simulations of H <sub>2</sub> Sorption in an Anthracene-Functionalized <i>rht</i> -Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2020, 124, 13753-13764.	3.1	1
23	MPMC and MCMD: Free High-Performance Simulation Software for Atomistic Systems. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900113.	2.8	8
24	Synergistic sorbent separation for one-step ethylene purification from a four-component mixture. <i>Science</i> , 2019, 366, 241-246.	12.6	360
25	A Metal-Organic Framework Based Methane Nano-Trap for the Capture of Coal-Mine Methane. <i>Angewandte Chemie</i> , 2019, 131, 10244-10247.	2.0	28
26	Molecular Sieving and Direct Visualization of CO <sub>2</sub> in Binding Pockets of an Ultramicroporous Lanthanide Metal-Organic Framework Platform. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 23192-23197.	8.0	26
27	Investigating CO <sub>2</sub> Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies. <i>Crystal Growth and Design</i> , 2019, 19, 3732-3743.	3.0	35
28	A Metal-Organic Framework Based Methane Nano-Trap for the Capture of Coal-Mine Methane. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10138-10141.	13.8	181
29	Robust Microporous Metal-Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. <i>Angewandte Chemie</i> , 2019, 131, 10315-10320.	2.0	16
30	Robust Microporous Metal-Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10209-10214.	13.8	69
31	Innenräcktitelbild: A Metal-Organic Framework Based Methane Nano-Trap for the Capture of Coal-Mine Methane (Angew. Chem. 30/2019). <i>Angewandte Chemie</i> , 2019, 131, 10483-10483.	2.0	0
32	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4657-4662.	13.8	283
33	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. <i>Angewandte Chemie</i> , 2018, 130, 4747-4752.	2.0	32
34	Efficient CO <sub>2</sub> Removal for Ultra- <i>b</i> -Pure CO Production by Two Hybrid Ultramicroporous Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3332-3336.	13.8	52
35	Efficient CO <sub>2</sub> Removal for Ultra- <i>b</i> -Pure CO Production by Two Hybrid Ultramicroporous Materials. <i>Angewandte Chemie</i> , 2018, 130, 3390-3394.	2.0	12
36	Readily accessible shape-memory effect in a porous interpenetrated coordination network. <i>Science Advances</i> , 2018, 4, eaal636.	10.3	61

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37	Impact of partial interpenetration in a hybrid ultramicroporous material on C <sub>2</sub> H <sub>2</sub> /C <sub>2</sub> H <sub>4</sub> separation performance. <i>Chemical Communications</i> , 2018, 54, 3488-3491.	4.1	38
38	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. <i>Angewandte Chemie</i> , 2018, 130, 11137-11141.	2.0	85
39	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10971-10975.	13.8	365
40	Investigating C <sub>2</sub> H <sub>2</sub> Sorption in $\text{M}_3(\text{O}_2\text{CH})_6$ (M = Mg, Mn) Through Theoretical Studies. <i>Crystal Growth and Design</i> , 2018, 18, 5342-5352.	3.0	2
41	Hydrogen Adsorption in a Zeolithic Imidazolate Framework with Ita Topology. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15435-15445.	3.1	17
42	Highly Selective Separation of C <sub>2</sub> H <sub>2</sub> from CO <sub>2</sub> by a New Dichromate-Based Hybrid Ultramicroporous Material. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 33395-33400.	8.0	116
43	Comparing the mechanism and energetics of CO <sub>2</sub> sorption in the SIFSIX series. <i>CrystEngComm</i> , 2017, 19, 3338-3347.	2.6	22
44	Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. <i>Chemical Science</i> , 2017, 8, 2373-2380.	7.4	121
45	Investigating gas sorption in an rht-metal-organic framework with 1,2,3-triazole groups. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29204-29221.	2.8	8
46	Experimental and theoretical investigations of the gas adsorption sites in rht-metal-organic frameworks. <i>CrystEngComm</i> , 2017, 19, 4646-4665.	2.6	20
47	Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity. <i>Angewandte Chemie</i> , 2017, 129, 11584-11588.	2.0	33
48	Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11426-11430.	13.8	119
49	An unusual H <sub>2</sub> sorption mechanism in PCN-14: insights from molecular simulation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21421-21430.	2.8	11
50	Hybrid Ultra-Microporous Materials for Selective Xenon Adsorption and Separation. <i>Angewandte Chemie</i> , 2016, 128, 8425-8429.	2.0	38
51	Hybrid Ultra-Microporous Materials for Selective Xenon Adsorption and Separation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8285-8289.	13.8	137
52	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. <i>Chemical Science</i> , 2016, 7, 5470-5476.	7.4	66
53	Dynamics of H <sub>2</sub> adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17141-17158.	2.8	23
54	Accurate H <sub>2</sub> Sorption Modeling in the rht-MOF NOTT-112 Using Explicit Polarization. <i>Crystal Growth and Design</i> , 2016, 16, 6024-6032.	3.0	17

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55	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO <sub>2</sub> . <i>Angewandte Chemie</i> , 2016, 128, 10424-10428.	2.0	43
56	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10268-10272.	13.8	237
57	Theoretical Investigations of CO <sub>2</sub> and H <sub>2</sub> Sorption in Robust Molecular Porous Materials. <i>Langmuir</i> , 2016, 32, 11492-11505.	3.5	17
58	Dramatic Effect of the Electrostatic Parameters on H <sub>2</sub> Sorption in an M-MOF-74 Analogue. <i>Crystal Growth and Design</i> , 2016, 16, 867-874.	3.0	23
59	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in <i>&lt; i&gt;rht&lt;/i&gt;</i> -Metalâ€Organic Frameworks. <i>ChemPhysChem</i> , 2015, 16, 3170-3179.	2.1	14
60	Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metalâ€Organic Frameworks. <i>Chemistry of Materials</i> , 2015, 27, 2144-2151.	6.7	72
61	Investigating H <sub>2</sub> Sorption in a Fluorinated Metalâ€Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. <i>Langmuir</i> , 2015, 31, 7328-7336.	3.5	26
62	Modeling PCN-61 and PCN-66: Isostructural <i>&lt; i&gt;rht&lt;/i&gt;</i> -Metalâ€Organic Frameworks with Distinct CO <sub>2</sub> Sorption Mechanisms. <i>Crystal Growth and Design</i> , 2014, 14, 5599-5607.	3.0	23
63	Simulations of hydrogen sorption in rht-MOF-1: identifying the binding sites through explicit polarization and quantum rotation calculations. <i>Journal of Materials Chemistry A</i> , 2014, 2, 2088-2100.	10.3	55
64	Capturing the H <sub>2</sub> â€Metal Interaction in Mg-MOF-74 Using Classical Polarization. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22683-22690.	3.1	40
65	Insights into an intriguing gas sorption mechanism in a polar metalâ€organic framework with open-metal sites and narrow channels. <i>Chemical Communications</i> , 2014, 50, 7283-7286.	4.1	16
66	Porous materials with optimal adsorption thermodynamics and kinetics for CO <sub>2</sub> separation. <i>Nature</i> , 2013, 495, 80-84.	27.8	2,005
67	A Polarizable and Transferable PHAST CO <sub>2</sub> Potential for Materials Simulation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5421-5429.	5.3	39
68	Simulation of the Mechanism of Gas Sorption in a Metalâ€Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15538-15549.	3.1	76
69	Highly Selective CO <sub>2</sub> Uptake in Uninodal 6-Connected â€œmmoâ€Nets Based upon MO <sub>4</sub> <sup>2-</sup> (M = Cr, Mo) Pillars. <i>Journal of the American Chemical Society</i> , 2012, 134, 19556-19559.	13.7	110