Christopher E Wilmer

List of Publications by Year
in descending order

57	9,547	126858	143943
papers	citations	33 h-index	57 g-index

58	58	58	11482
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Metalâ€“Organic Framework Materials with Ultrahigh Surface Areas: Is the Sky the Limit?. Journal of the American Chemical Society, 2012, 134, 15016-15021.	6.6	1,497
2	Nanoscale Forces and Their Uses in Selfâ€Assembly. Small, 2009, 5, 1600-1630.	5.2	1,362
3	Large-scale screening of hypothetical metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 83-89.	6.6	1,098
4	Review and Analysis of Molecular Simulations of Methane, Hydrogen, and Acetylene Storage in Metalâ€“Organic Frameworks. Chemical Reviews, 2012, 112, 703-723.	23.0	1,085
5	Light-Harvesting and Ultrafast Energy Migration in Porphyrin-Based Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 862-869.	6.6	510
6	Self-assembly: from crystals to cells. Soft Matter, 2009, 5, 1110.	1.2	385
7	Structureâ€“property relationships of porous materials for carbon dioxide separation and capture. Energy and Environmental Science, 2012, 5, 9849.	15.6	334
8	Nanoporous Carbohydrate Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 406-417.	6.6	271
9	An Extended Charge Equilibration Method. Journal of Physical Chemistry Letters, 2012, 3, 2506-2511.	2.1	253
10	Thermodynamic analysis of Xe/Kr selectivity in over 137â€‰000 hypothetical metalâ€“organic frameworks. Chemical Science, 2012, 3, 2217.	3.7	248
11	Gram-scale, high-yield synthesis of a robust metalâ€“organic framework for storing methane and other gases. Energy and Environmental Science, 2013, 6, 1158.	15.6	219
12	Designing Higher Surface Area Metalâ€“Organic Frameworks: Are Triple Bonds Better Than Phenyls?. Journal of the American Chemical Society, 2012, 134, 9860-9863.	6.6	198
13	Large-Scale Quantitative Structureâ€“Property Relationship (QSPR) Analysis of Methane Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	1.5	174
14	Towards rapid computational screening of metal-organic frameworks for carbon dioxide capture: Calculation of framework charges via charge equilibration. Chemical Engineering Journal, 2011, 171, 775-781.	6.6	141
15	Simultaneously high gravimetric and volumetric methane uptake characteristics of the metalâ€“organic framework NU-111. Chemical Communications, 2013, 49, 2992.	2.2	137
16	The 'wired' universe of organic chemistry. Nature Chemistry, 2009, 1, 31-36.	6.6	130
17	Effect of pore size and shape on the thermal conductivity of metal-organic frameworks. Chemical Science, 2017, 8, 583-589.	3.7	120
18	Carborane-Based Metalâ€“Organic Framework with High Methane and Hydrogen Storage Capacities. Chemistry of Materials, 2013, 25, 3539-3543.	3.2	115

#	Article	IF	Citations
19	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. Journal of Physical Chemistry C, 2014, 118, 6941-6951.	1.5	108
20	Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates. Nature Communications, 2020, 11, 4010.	5.8	97
21	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
22	Heat Flux for Many-Body Interactions: Corrections to LAMMPS. Journal of Chemical Theory and Computation, 2019, 15, 5579-5587.	2.3	80
23	The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation. Molecular Simulation, 2019, 45, 1082-1121.	0.9	74
24	Mechanisms of Heat Transfer in Porous Crystals Containing Adsorbed Gases: Applications to Metal-Organic Frameworks. Physical Review Letters, 2016, 116, 025902.	2.9	64
25	High-throughput computational prediction of the cost of carbon capture using mixed matrix membranes. Energy and Environmental Science, 2019, 12, 1255-1264.	15.6	62
26	The effect of pyridine modification of Niâ€“DOBDC on CO₂ capture under humid conditions. Chemical Communications, 2014, 50, 3296-3298.	2.2	52
27	Computational Design of Metalâ€“Organic Framework Arrays for Gas Sensing: Influence of Array Size and Composition on Sensor Performance. Journal of Physical Chemistry C, 2017, 121, 6033-6038.	1.5	50
28	Precision Assembly of Oppositely and Like-Charged Nanoobjects Mediated by Charge-Induced Dipole Interactions. Nano Letters, 2010, 10, 2275-2280.	4.5	49
29	Polyporous Metal-Coordination Frameworks. Organic Letters, 2012, 14, 1460-1463.	2.4	47
30	Transient Mass and Thermal Transport during Methane Adsorption into the Metalâ€“Organic Framework HKUST-1. ACS Applied Materials & Interfaces, 2018, 10, 2400-2406.	4.0	46
31	Layer-by-Layer Assembled Films of Perylene Diimide- and Squaraine-Containing Metalâ€“Organic Framework-like Materials: Solar Energy Capture and Directional Energy Transfer. ACS Applied Materials & Interfaces, 2016, 8, 24983-24988.	4.0	44
32	Intelligent Selection of Metalâ€“Organic Framework Arrays for Methane Sensing via Genetic Algorithms. ACS Sensors, 2019, 4, 1586-1593.	4.0	44
33	Thermal Transport in Interpenetrated Metalâ€“Organic Frameworks. Chemistry of Materials, 2018, 30, 2281-2286.	3.2	40
34	Optimizing information content in MOF sensor arrays for analyzing methane-air mixtures. Sensors and Actuators B: Chemical, 2018, 267, 483-493.	4.0	36
35	VOC Mixture Sensing with a MOF Film Sensor Array: Detection and Discrimination of Xylene Isomers and Their Ternary Blends. ACS Sensors, 2022, 7, 1666-1675.	4.0	36
36	Metallacarborane-Based Metalâ€“Organic Framework with a Complex Topology. Crystal Growth and Design, 2014, 14, 1324-1330.	1.4	28

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37	Influence of Missing Linker Defects on the Thermal Conductivity of Metalâ€“Organic Framework HKUST-1. ACS Applied Materials & Interfaces, 2020, 12, 56172-56177.	4.0	25
38	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
39	Modeling of Diffusion of Acetone in UiO-66. Journal of Physical Chemistry C, 2020, 124, 28469-28478.	1.5	23
40	Hybridization from Guestâ€“Host Interactions Reduces the Thermal Conductivity of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2022, 144, 3603-3613.	6.6	23
41	Size Discrimination of Carbohydrates via Conductive Carbon Nanotube@Metal Organic Framework Composites. Journal of the American Chemical Society, 2021, 143, 8022-8033.	6.6	16
42	Discovery of hypothetical hetero-interpenetrated MOFs with arbitrarily dissimilar topologies and unit cell shapes. CrystEngComm, 2017, 19, 4497-4504.	1.3	14
43	Effect of Flexibility on Thermal Transport in Breathing Porous Crystals. Journal of Physical Chemistry C, 2020, 124, 18604-18608.	1.5	13
44	Computational Design of MOF-Based Electronic Noses for Dilute Gas Species Detection: Application to Kidney Disease Detection. ACS Sensors, 2021, 6, 4425-4434.	4.0	12
45	Enhanced Thermal Conductivity in a Diamine-Appended Metalâ€“Organic Framework as a Result of Cooperative CO₂ Adsorption. ACS Applied Materials & Interfaces, 2020, 12, 44617-44621.	4.0	10
46	Genetic Algorithm Design of MOF-based Gas Sensor Arrays for CO2-in-Air Sensing. Sensors, 2020, 20, 924.	2.1	10
47	In Situ Nuclear Magnetic Resonance Investigation of Molecular Adsorption and Kinetics in Metalâ€“Organic Framework UiO-66. Journal of Physical Chemistry Letters, 2021, 12, 892-899.	2.1	10
48	A framework for modeling fraud in E-waste management. Resources, Conservation and Recycling, 2021, 171, 105613.	5.3	10
49	High-Pressure Methane Adsorption in Porous Lennard-Jones Crystals. Journal of Physical Chemistry Letters, 2018, 9, 4275-4281.	2.1	9
50	Large-Scale Generation and Screening of Hypothetical Metal-Organic Frameworks for Applications in Gas Storage and Separations. Topics in Current Chemistry, 2013, 345, 257-289.	4.0	8
51	Efficiently mapping structureâ€“property relationships of gas adsorption in porous materials: application to Xe adsorption. Faraday Discussions, 2017, 201, 221-232.	1.6	5
52	Modeling diffusion of nanocars on a Cu (110) surface. Molecular Systems Design and Engineering, 2020, 5, 1186-1192.	1.7	5
53	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
54	Silver Nanofilament Formation Dynamics in a Polymerâ€“Ionic Liquid Thin Film by Direct Write. Advanced Functional Materials, 2020, 30, 1907950.	7.8	4

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55	Mechanical and electrical properties of nanostructured â€˜plastic metalsâ€™. Journal of Non-Crystalline Solids, 2009, 355, 1313-1317.	1.5	2
56	Towards Comprehensive Exploration of the Physisorption Space in Porous Pseudomaterials Using an Iterative Mutation Search Algorithm. Journal of Chemical Physics, 2021, 155, 234114.	1.2	1
57	(Invited) Progress Towards the Design of Metal-Organic Frameworks with Targeted Thermal Conductivities. ECS Meeting Abstracts, 2018, , .	0.0	0