

Christopher E Wilmer

List of Publications by Year in descending order

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57
papers

9,547
citations

126907
33
h-index

144013
57
g-index

58
all docs

58
docs citations

58
times ranked

11482
citing authors

#	ARTICLE	IF	CITATIONS
1	Hybridization from Guest-Host Interactions Reduces the Thermal Conductivity of Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2022, 144, 3603-3613.	13.7	23
2	VOC Mixture Sensing with a MOF Film Sensor Array: Detection and Discrimination of Xylene Isomers and Their Ternary Blends. <i>ACS Sensors</i> , 2022, 7, 1666-1675.	7.8	36
3	In Situ Nuclear Magnetic Resonance Investigation of Molecular Adsorption and Kinetics in Metal-Organic Framework UiO-66. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 892-899.	4.6	10
4	Size Discrimination of Carbohydrates via Conductive Carbon Nanotube@Metal Organic Framework Composites. <i>Journal of the American Chemical Society</i> , 2021, 143, 8022-8033.	13.7	16
5	A framework for modeling fraud in E-waste management. <i>Resources, Conservation and Recycling</i> , 2021, 171, 105613.	10.8	10
6	Towards Comprehensive Exploration of the Physisorption Space in Porous Pseudomaterials Using an Iterative Mutation Search Algorithm. <i>Journal of Chemical Physics</i> , 2021, 155, 234114.	3.0	1
7	Computational Design of MOF-Based Electronic Noses for Dilute Gas Species Detection: Application to Kidney Disease Detection. <i>ACS Sensors</i> , 2021, 6, 4425-4434.	7.8	12
8	Silver Nanofilament Formation Dynamics in a Polymer-Ionic Liquid Thin Film by Direct Write. <i>Advanced Functional Materials</i> , 2020, 30, 1907950.	14.9	4
9	Influence of Missing Linker Defects on the Thermal Conductivity of Metal-Organic Framework HKUST-1. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 56172-56177.	8.0	25
10	Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates. <i>Nature Communications</i> , 2020, 11, 4010.	12.8	97
11	Effect of Flexibility on Thermal Transport in Breathing Porous Crystals. <i>Journal of Physical Chemistry C</i> , 2020, 124, 18604-18608.	3.1	13
12	Enhanced Thermal Conductivity in a Diamine-Appended Metal-Organic Framework as a Result of Cooperative CO ₂ Adsorption. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 44617-44621.	8.0	10
13	Modeling of Diffusion of Acetone in UiO-66. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28469-28478.	3.1	23
14	Modeling diffusion of nanocars on a Cu (110) surface. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1186-1192.	3.4	5
15	Genetic Algorithm Design of MOF-based Gas Sensor Arrays for CO ₂ -in-Air Sensing. <i>Sensors</i> , 2020, 20, 924.	3.8	10
16	Heat Flux for Many-Body Interactions: Corrections to LAMMPS. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5579-5587.	5.3	80
17	The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation. <i>Molecular Simulation</i> , 2019, 45, 1082-1121.	2.0	74
18	High-throughput computational prediction of the cost of carbon capture using mixed matrix membranes. <i>Energy and Environmental Science</i> , 2019, 12, 1255-1264.	30.8	62

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19	Intelligent Selection of Metal-Organic Framework Arrays for Methane Sensing via Genetic Algorithms. ACS Sensors, 2019, 4, 1586-1593.	7.8	44
20	Optimizing information content in MOF sensor arrays for analyzing methane-air mixtures. Sensors and Actuators B: Chemical, 2018, 267, 483-493.	7.8	36
21	Thermal Transport in Interpenetrated Metal-Organic Frameworks. Chemistry of Materials, 2018, 30, 2281-2286.	6.7	40
22	Transient Mass and Thermal Transport during Methane Adsorption into the Metal-Organic Framework HKUST-1. ACS Applied Materials & Interfaces, 2018, 10, 2400-2406.	8.0	46
23	High-Pressure Methane Adsorption in Porous Lennard-Jones Crystals. Journal of Physical Chemistry Letters, 2018, 9, 4275-4281.	4.6	9
24	(Invited) Progress Towards the Design of Metal-Organic Frameworks with Targeted Thermal Conductivities. ECS Meeting Abstracts, 2018, , .	0.0	0
25	Computational Design of Metal-Organic Framework Arrays for Gas Sensing: Influence of Array Size and Composition on Sensor Performance. Journal of Physical Chemistry C, 2017, 121, 6033-6038.	3.1	50
26	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	3.2	4
27	Efficiently mapping structure-property relationships of gas adsorption in porous materials: application to Xe adsorption. Faraday Discussions, 2017, 201, 221-232.	3.2	5
28	Discovery of hypothetical hetero-interpenetrated MOFs with arbitrarily dissimilar topologies and unit cell shapes. CrystEngComm, 2017, 19, 4497-4504.	2.6	14
29	Effect of pore size and shape on the thermal conductivity of metal-organic frameworks. Chemical Science, 2017, 8, 583-589.	7.4	120
30	Layer-by-Layer Assembled Films of Perylene Diimide- and Squaraine-Containing Metal-Organic Framework-like Materials: Solar Energy Capture and Directional Energy Transfer. ACS Applied Materials & Interfaces, 2016, 8, 24983-24988.	8.0	44
31	Mechanisms of Heat Transfer in Porous Crystals Containing Adsorbed Gases: Applications to Metal-Organic Frameworks. Physical Review Letters, 2016, 116, 025902.	7.8	64
32	The effect of pyridine modification of Ni-DOBDC on CO ₂ capture under humid conditions. Chemical Communications, 2014, 50, 3296-3298.	4.1	52
33	Metallacarborane-Based Metal-Organic Framework with a Complex Topology. Crystal Growth and Design, 2014, 14, 1324-1330.	3.0	28
34	Exploring the Limits of Methane Storage and Delivery in Nanoporous Materials. Journal of Physical Chemistry C, 2014, 118, 6941-6951.	3.1	108
35	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, 10432-10436.	4.0	24
36	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. Journal of Physical Chemistry C, 2014, 118, 5383-5389.	3.1	84

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37	Carborane-Based Metal-Organic Framework with High Methane and Hydrogen Storage Capacities. Chemistry of Materials, 2013, 25, 3539-3543.	6.7	115
38	Light-Harvesting and Ultrafast Energy Migration in Porphyrin-Based Metal-Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 862-869.	13.7	510
39	Gram-scale, high-yield synthesis of a robust metal-organic framework for storing methane and other gases. Energy and Environmental Science, 2013, 6, 1158.	30.8	219
40	Simultaneously high gravimetric and volumetric methane uptake characteristics of the metal-organic framework NU-111. Chemical Communications, 2013, 49, 2992.	4.1	137
41	Large-Scale Quantitative Structure-Property Relationship (QSPR) Analysis of Methane Storage in Metal-Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	3.1	174
42	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
43	Structure-property relationships of porous materials for carbon dioxide separation and capture. Energy and Environmental Science, 2012, 5, 9849.	30.8	334
44	Polyporous Metal-Coordination Frameworks. Organic Letters, 2012, 14, 1460-1463.	4.6	47
45	An Extended Charge Equilibration Method. Journal of Physical Chemistry Letters, 2012, 3, 2506-2511.	4.6	253
46	Metal-Organic Framework Materials with Ultrahigh Surface Areas: Is the Sky the Limit?. Journal of the American Chemical Society, 2012, 134, 15016-15021.	13.7	1,497
47	Designing Higher Surface Area Metal-Organic Frameworks: Are Triple Bonds Better Than Phenyls?. Journal of the American Chemical Society, 2012, 134, 9860-9863.	13.7	198
48	Nanoporous Carbohydrate Metal-Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 406-417.	13.7	271
49	Review and Analysis of Molecular Simulations of Methane, Hydrogen, and Acetylene Storage in Metal-Organic Frameworks. Chemical Reviews, 2012, 112, 703-723.	47.7	1,085
50	Thermodynamic analysis of Xe/Kr selectivity in over 137,000 hypothetical metal-organic frameworks. Chemical Science, 2012, 3, 2217.	7.4	248
51	Large-scale screening of hypothetical metal-organic frameworks. Nature Chemistry, 2012, 4, 83-89.	13.6	1,098
52	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.	12.7	141
53	Precision Assembly of Oppositely and Like-Charged Nanoobjects Mediated by Charge-Induced Dipole Interactions. Nano Letters, 2010, 10, 2275-2280.	9.1	49
54	Nanoscale Forces and Their Uses in Self-Assembly. Small, 2009, 5, 1600-1630.	10.0	1,362

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55	The 'wired' universe of organic chemistry. Nature Chemistry, 2009, 1, 31-36.	13.6	130
56	Mechanical and electrical properties of nanostructured "plastic metals". Journal of Non-Crystalline Solids, 2009, 355, 1313-1317.	3.1	2
57	Self-assembly: from crystals to cells. Soft Matter, 2009, 5, 1110.	2.7	385