List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	<i>In situ</i> fabricated MOF–cellulose composite as an advanced ROS deactivator-convertor: fluoroswitchable bi-phasic tweezers for free chlorine detoxification and size-exclusive catalytic insertion of aqueous H <sub>2</sub> O <sub>2</sub> . Journal of Materials Chemistry A, 2022, 10, 4316-4332.	5.2	19
2	Evaluating the performance of Cr-Soc-MOF Super-Adsorbents for CO2 capture from flue gas under humid condition through molecular simulation. Separation and Purification Technology, 2022, 295, 121298.	3.9	14
3	Molecular level investigation on the impact of geometric isomers as fluorinated ligands in SIFSIX MOF for natural gas sweetening. Separation Science and Technology, 2022, 57, 2554-2565.	1.3	1
4	Significance of extra-framework monovalent and divalent cation motion upon CO2 and N2 sorption in zeolite X. Materials Today: Proceedings, 2022, 68, 85-92.	0.9	2
5	Nanoencapsulation of Ru( <i>p</i> -cymene) Complex Bearing Ginger-based Natural Product into Liposomal Nanoformulation to Improve Its Cellular Uptake and Antiproliferative Activity. ACS Applied Bio Materials, 2022, 5, 3241-3256.	2.3	8
6	Tunable Capacitive Behavior in Metallopolymer-based Electrochromic Thin Film Supercapacitors. ACS Applied Materials & Interfaces, 2022, 14, 31900-31910.	4.0	10
7	Fluorinated metal organic frameworks, MFFIVE-Ni-L (M = Fe/Al, L = pyr), with coordinatively unsaturated metal site for CO <sub>2</sub> separation from flue gas in the presence of humidity by computational methods. Dalton Transactions, 2021, 50, 466-471.	1.6	13
8	An ultralight charged MOF as fluoro-switchable monitor for assorted organo-toxins: size-exclusive dye scrubbing and anticounterfeiting applications <i>via</i> Tb <sup>3+</sup> sensitization. Inorganic Chemistry Frontiers, 2021, 8, 296-310.	3.0	41
9	Efficient chemical fixation of CO <sub>2</sub> from direct air under environment-friendly co-catalyst and solvent-free ambient conditions. Journal of Materials Chemistry A, 2021, 9, 23127-23139.	5.2	51
10	Highly selective detection of TNP over other nitro compounds in water: the role of selective host–guest interactions in Zr-NDI MOF. New Journal of Chemistry, 2021, 45, 12931-12937.	1.4	24
11	N-Functionality actuated improved CO <sub>2</sub> adsorption and turn-on detection of organo-toxins with guest-induced fluorescence modulation in isostructural diamondoid MOFs. Journal of Materials Chemistry C, 2021, 9, 7142-7153.	2.7	32
12	Chemically Robust and Bifunctional Co(II)-Framework for Trace Detection of Assorted Organo-toxins and Highly Cooperative Deacetalization–Knoevenagel Condensation with Pore-Fitting-Induced Size-Selectivity. ACS Applied Materials & Interfaces, 2021, 13, 28378-28389.	4.0	40
13	Structural engineering in pre-functionalized, imine-based covalent organic framework via anchoring active Ru(II)-complex for visible-light triggered and aerobic cross-coupling of α-amino esters with indoles. Applied Catalysis B: Environmental, 2021, 292, 120149.	10.8	30
14	Chemical Fixation of CO <sub>2</sub> Under Solvent and Co-Catalyst-free Conditions Using a Highly Porous Two-fold Interpenetrated Cu(II)-Metal–Organic Framework. Crystal Growth and Design, 2021, 21, 1233-1241.	1.4	27
15	A disappearing metastable hydrate form of L-citrulline: Variable conformations in polymorphs and hydrates. Journal of Molecular Structure, 2020, 1201, 127179.	1.8	2
16	Supramolecular Surface Charge Regulation in Ionic Covalent Organic Nanosheets: Reversible Exfoliation and Controlled Bacterial Growth. Angewandte Chemie, 2020, 132, 8791-8797.	1.6	40
17	Supramolecular Surface Charge Regulation in Ionic Covalent Organic Nanosheets: Reversible Exfoliation and Controlled Bacterial Growth. Angewandte Chemie - International Edition, 2020, 59, 8713-8719.	7.2	59
18	CO2 fixation by cycloaddition of mono/disubstituted epoxides using acyl amide decorated Co(II) MOF as a synergistic beterogeneous catalyst. Applied Catalysis A: General, 2020, 590, 117375	2.2	42

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19	Tuning the Ultra-Micropore Size of Fluorinated MOFs (M′F6-Ni-L) for CO2 Capture from Flue Gases by Advanced Computational Methods. Journal of Physical Chemistry C, 2020, 124, 16975-16989.	1.5	23
20	Rational Design of a Zn <sup>II</sup> MOF with Multiple Functional Sites for Highly Efficient Fixation of CO <sub>2</sub> under Mild Conditions: Combined Experimental and Theoretical Investigation. Chemistry - A European Journal, 2020, 26, 17445-17454.	1.7	42
21	Oneâ€pot synthesis of [2+2]â€helicateâ€like macrocycle and 2+4â€î¼ <sub>4</sub> â€oxo tetranuclear open fra complexes: Chiroptical properties and asymmetric oxidative coupling of 2â€naphthols. Applied Organometallic Chemistry, 2020, 34, e5666.	me 1.7	8
22	EVALUATION OF TETRA-n-BUTYLAMMONIUM BROMIDE AS CORROSION INHIBITOR FOR MILD STEEL IN 1N HCl MEDIUM: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS. Rasayan Journal of Chemistry, 2020, 13, 499-513.	0.2	1
23	A DFT study on the interaction of small molecules with alkali metal ion-exchanged ETS-10. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 483-493.	0.4	1
24	Cycloaddition of CO <sub>2</sub> with an Epoxide-Bearing Oxindole Scaffold by a Metal–Organic Framework-Based Heterogeneous Catalyst under Ambient Conditions. Inorganic Chemistry, 2019, 58, 10084-10096.	1.9	65
25	Water-Tolerant DUT-Series Metal–Organic Frameworks: A Theoretical–Experimental Study for the Chemical Fixation of CO <sub>2</sub> and Catalytic Transfer Hydrogenation of Ethyl Levulinate to γ-Valerolactone. ACS Applied Materials & Interfaces, 2019, 11, 41458-41471.	4.0	55
26	Efficient catalytic conversion of terminal/internal epoxides to cyclic carbonates by porous Co( <scp>ii</scp> ) MOF under ambient conditions: structure–property correlation and computational studies. Journal of Materials Chemistry A, 2019, 7, 2884-2894.	5.2	96
27	Computational prediction of promising pyrazine and bipyridine analogues of a fluorinated MOF platform, MFN-Ni-L (M = SI/AL; N = SIX/FIVE; L = pyr/bipyr), for CO2 capture under pre-humidified conditions. Physical Chemistry Chemical Physics, 2019, 21, 16127-16136.	1.3	13
28	lonicâ€Liquidâ€Functionalized UiOâ€66 Framework: An Experimental and Theoretical Study on the Cycloaddition of CO <sub>2</sub> and Epoxides. ChemSusChem, 2019, 12, 1033-1042.	3.6	61
29	The effect of crystallite size on pressure amplification in switchable porous solids. Nature Communications, 2018, 9, 1573.	5.8	92
30	Metal-Organic Frameworks for Cultural Heritage Preservation: The Case of Acetic Acid Removal. ACS Applied Materials & Interfaces, 2018, 10, 13886-13894.	4.0	32
31	A promising metal–organic framework (MOF), MIL-96(Al), for CO <sub>2</sub> separation under humid conditions. Journal of Materials Chemistry A, 2018, 6, 2081-2090.	5.2	78
32	Natural gas upgrading using a fluorinated MOF with tuned H2S and CO2 adsorption selectivity. Nature Energy, 2018, 3, 1059-1066.	19.8	214
33	Porous zinc and cobalt 2-nitroimidazolate frameworks with six-membered ring windows and a layered cobalt 2-nitroimidazolate polymorph. CrystEngComm, 2017, 19, 1377-1388.	1.3	6
34	Metal–organic frameworks to satisfy gas upgrading demands: fine-tuning the <b>soc</b> -MOF platform for the operative removal of H <sub>2</sub> S. Journal of Materials Chemistry A, 2017, 5, 3293-3303.	5.2	94
35	Hydrolytically stable fluorinated metal-organic frameworks for energy-efficient dehydration. Science, 2017, 356, 731-735.	6.0	275
36	Gas/vapour separation using ultra-microporous metal–organic frameworks: insights into the structure/separation relationship. Chemical Society Reviews, 2017, 46, 3402-3430.	18.7	1,033

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37	Selective nitrogen capture by porous hybrid materials containing accessible transition metal ion sites. Nature Materials, 2017, 16, 526-531.	13.3	201
38	A Fine-Tuned MOF for Gas and Vapor Separation: A Multipurpose Adsorbent for Acid Gas Removal, Dehydration, and BTX Sieving. CheM, 2017, 3, 822-833.	5.8	83
39	N <sub>2</sub> Capture Performances of the Hybrid Porous MIL-101(Cr): From Prediction toward Experimental Testing. Journal of Physical Chemistry C, 2017, 121, 22130-22138.	1.5	21
40	Diffusion of Carbon Dioxide and Nitrogen in the Smallâ€Pore Titanium Bis(phosphonate) Metal–Organic Framework MILâ€91 (Ti): A Combination of Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. ChemPhysChem, 2017, 18, 2739-2746.	1.0	11
41	Revisiting the Aluminum Trimesate-Based MOF (MIL-96): From Structure Determination to the Processing of Mixed Matrix Membranes for CO <sub>2</sub> Capture. Chemistry of Materials, 2017, 29, 10326-10338.	3.2	78
42	Computational exploration of interesting gas adsorption/separation in MOFs. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C548-C548.	0.0	0
43	Current Trend in the Application of Nanoparticles for Waste Water Treatment and Purification: A Review. Current Organic Synthesis, 2017, 14, 206-226.	0.7	37
44	A pressure-amplifying framework material with negative gas adsorption transitions. Nature, 2016, 532, 348-352.	13.7	490
45	MIL-91(Ti), a small pore metal–organic framework which fulfils several criteria: an upscaled green synthesis, excellent water stability, high CO <sub>2</sub> selectivity and fast CO <sub>2</sub> transport. Journal of Materials Chemistry A, 2016, 4, 1383-1389.	5.2	82
46	Structure and properties of Al-MIL-53-ADP, a breathing MOF based on the aliphatic linker molecule adipic acid. Dalton Transactions, 2016, 45, 4179-4186.	1.6	54
47	The flexibility of modified-linker MIL-53 materials. Dalton Transactions, 2016, 45, 4162-4168.	1.6	37
48	C2-Hydrocarbon Adsorption in Nano-porous Faujasite: A DFT Study. Materials Today: Proceedings, 2015, 2, 436-445.	0.9	4
49	CO2 and N2 Adsorption in Nano-porous BEA Type Zeolite with Different Cations. Materials Today: Proceedings, 2015, 2, 446-455.	0.9	7
50	A density functional theory study on the interaction of paraffins, olefins, and acetylenes with Na-ETS-10. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
51	Highly Selective CO <sub>2</sub> Capture by Small Pore Scandium-Based Metal–Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 23592-23598.	1.5	38
52	Understanding Gas Adsorption Selectivity in IRMOF-8 Using Molecular Simulation. ACS Applied Materials & Interfaces, 2015, 7, 624-637.	4.0	73
53	Molecular Simulation of the Adsorption of Methane in Engelhard Titanosilicate Frameworks. Langmuir, 2014, 30, 7435-7446.	1.6	8
54	Interaction of atmospheric gases with ETS-10: A DFT study. Microporous and Mesoporous Materials, 2014, 190, 38-45.	2.2	10

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55	Grand canonical Monte Carlo simulation and volumetric equilibrium studies for adsorption of nitrogen, oxygen, and argon in cadmium (II) exchanged zeolite A. Journal of Porous Materials, 2012, 19, 683-693.	1.3	9
56	CO2 and N2 adsorption in alkali metal ion exchanged X-Faujasite: Grand canonical Monte Carlo simulation and equilibrium adsorption studies. Microporous and Mesoporous Materials, 2012, 162, 143-151.	2.2	31
57	Sorption of nitrogen, oxygen, and argon in Cd (II) exchanged zeolite X: volumetric equilibrium adsorption and grand canonical Monte Carlo study. Journal of Porous Materials, 2011, 18, 113-124.	1.3	8
58	Computational Study for Water Sorption in AlPO <sub>4</sub> -5 and AlPO <sub>4</sub> -11 Molecular Sieves. Langmuir, 2010, 26, 1755-1764.	1.6	26
59	Ionic liquid as catalytic and reusable media for cyanoethoxycarbonylation of aldehydes. Catalysis Communications, 2010, 11, 907-912.	1.6	12
60	Sorption of CO, CH <sub>4</sub> , and N <sub>2</sub> in Alkali Metal Ion Exchanged Zeolite-X: Grand Canonical Monte Carlo Simulation and Volumetric Measurements. Industrial & Engineering Chemistry Research, 2010, 49, 5816-5825.	1.8	46
61	Sorption of Methane, Nitrogen, Oxygen, and Argon in ZSM-5 with different SiO2/Al2O3 Ratios: Grand Canonical Monte Carlo Simulation and Volumetric Measurements. Industrial & Engineering Chemistry Research, 2010, 49, 2353-2362.	1.8	45
62	A density functional theory study on the interaction of hydrogen molecule with MOF-177. Molecular Simulation, 2010, 36, 373-381.	0.9	9
63	Adsorption of hydrogen in nickel and rhodium exchanged zeolite X. International Journal of Hydrogen Energy, 2008, 33, 735-745.	3.8	70
64	Adsorption of carbon dioxide, methane, nitrogen, oxygen and argon in NaETS-4. Microporous and Mesoporous Materials, 2008, 113, 268-276.	2.2	87
65	Hydrogen uptake in palladium and ruthenium exchanged zeolite X. Journal of Alloys and Compounds, 2008, 466, 439-446.	2.8	22
66	Sorption of N2, O2, and Ar in Mn(II)-Exchanged Zeolites A and X Using Volumetric Measurements and Grand Canonical Monte Carlo Simulation. Industrial & Engineering Chemistry Research, 2007, 46, 6293-6302.	1.8	22
67	Correlation of Sorption Behavior of Nitrogen, Oxygen, and Argon with Ca <sup>2+</sup> Locations in Zeolite A:  A Grand Canonical Monte Carlo Simulation Study. Langmuir, 2007, 23, 8899-8908. 	1.6	19
68	Assembly of Discrete and Oligomeric Structures of Organotin Double-decker Silsesquioxanes: Inherent Stability Studies. New Journal of Chemistry, 0, , .	1.4	8