Seda KeskÄ°n

List of Publications by Year
in descending order

156 papers	9,131 citations	38660 50 h-index	46693 89 g-index
160 all docs	160 docs citations	160 times ranked	7374 citing authors

#	Article	IF	Citations
1	A review of ionic liquids towards supercritical fluid applications. Journal of Supercritical Fluids, 2007, 43, 150-180.	1.6	648
2	Can Metalâ€"Organic Framework Materials Play a Useful Role in Largeâ€Scale Carbon Dioxide Separations?. ChemSusChem, 2010, 3, 879-891.	3.6	556
3	Biomedical Applications of Metal Organic Frameworks. Industrial & Engineering Chemistry Research, 2011, 50, 1799-1812.	1.8	520
4	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metalâ^'Organic Framework Materials. Industrial & Engineering Chemistry Research, 2009, 48, 2355-2371.	1.8	283
5	Opportunities and challenges of MOF-based membranes in gas separations. Separation and Purification Technology, 2015, 152, 207-237.	3.9	233
6	Ionic Liquid/Metalâ€"Organic Framework Composites: From Synthesis to Applications. ChemSusChem, 2017, 10, 2842-2863.	3.6	210
7	Screening Metalâ^'Organic Framework Materials for Membrane-based Methane/Carbon Dioxide Separations. Journal of Physical Chemistry C, 2007, 111, 14055-14059.	1.5	186
8	Selecting metal organic frameworks as enabling materials in mixed matrix membranes for high efficiency natural gas purification. Energy and Environmental Science, 2010, 3, 343.	15.6	172
9	Effect of Metalâ€"Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. Angewandte Chemie - International Edition, 2021, 60, 7828-7837.	7.2	164
10	Efficient Methods for Screening of Metal Organic Framework Membranes for Gas Separations Using Atomically Detailed Models. Langmuir, 2009, 25, 11786-11795.	1.6	161
11	Assessment of a Metalâ^'Organic Framework Membrane for Gas Separations Using Atomically Detailed Calculations: CO₂, CH₄, N₂, H₂ Mixtures in MOF-5. Industrial & Engineering Chemistry Research, 2009, 48, 914-922.	1.8	143
12	High-Throughput Screening of MOF Adsorbents and Membranes for H₂ Purification and CO₂ Capture. ACS Applied Materials & Interfaces, 2018, 10, 33693-33706.	4.0	133
13	[BMIM][PF₆] Incorporation Doubles CO₂ Selectivity of ZIF-8: Elucidation of Interactions and Their Consequences on Performance. ACS Applied Materials & Interfaces, 2016, 8, 30992-31005.	4.0	131
14	Database for CO₂ Separation Performances of MOFs Based on Computational Materials Screening. ACS Applied Materials & Interfaces, 2018, 10, 17257-17268.	4.0	129
15	Recent advances, opportunities, and challenges in high-throughput computational screening of MOFs for gas separations. Coordination Chemistry Reviews, 2020, 422, 213470.	9.5	124
16	Coreâ€"Shell Type Ionic Liquid/Metal Organic Framework Composite: An Exceptionally High CO₂/CH₄ Selectivity. Journal of the American Chemical Society, 2018, 140, 10113-10116.	6.6	120
17	MOF materials as therapeutic agents, drug carriers, imaging agents and biosensors in cancer biomedicine: Recent advances and perspectives. Progress in Materials Science, 2021, 117, 100743.	16.0	120
18	Tuning the Gas Separation Performance of CuBTC by Ionic Liquid Incorporation. Langmuir, 2016, 32, 1139-1147.	1.6	110

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19	High-Throughput Computational Screening of the Metal Organic Framework Database for CH₄/H₂ Separations. ACS Applied Materials & Interfaces, 2018, 10, 3668-3679.	4.0	108
20	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH₄/H₂ and CO₂/CH₄ Mixtures in ZIFs. Journal of Physical Chemistry C, 2011, 115, 12560-12566.	1.5	101
21	Improving Gas Separation Performance of ZIF-8 by [BMIM][BF₄] Incorporation: Interactions and Their Consequences on Performance. Journal of Physical Chemistry C, 2017, 121, 10370-10381.	1.5	101
22	Machine Learning Meets with Metal Organic Frameworks for Gas Storage and Separation. Journal of Chemical Information and Modeling, 2021, 61, 2131-2146.	2.5	97
23	Simulation and modelling of MOFs for hydrogen storage. CrystEngComm, 2015, 17, 261-275.	1.3	96
24	Recent Advances in Metalâ€“Organic Frameworkâ€Based Mixed Matrix Membranes. Chemistry - an Asian Journal, 2013, 8, 1692-1704.	1.7	95
25	Computational Screening of Metalâ€“Organic Frameworks for Membrane-Based CO₂/N₂/H₂O Separations: Best Materials for Flue Gas Separation. Journal of Physical Chemistry C, 2018, 122, 17347-17357.	1.5	92
26	Atomically detailed models of gas mixture diffusion through CuBTC membranes. Microporous and Mesoporous Materials, 2009, 125, 101-106.	2.2	90
27	Assessing CH4/N2 separation potential of MOFs, COFs, IL/MOF, MOF/Polymer, and COF/Polymer composites. Chemical Engineering Journal, 2022, 428, 131239.	6.6	89
28	An extensive comparative analysis of two MOF databases: high-throughput screening of computation-ready MOFs for CH₄ and H₂ adsorption. Journal of Materials Chemistry A, 2019, 7, 9593-9608.	5.2	87
29	Site characteristics in metal organic frameworks for gas adsorption. Progress in Surface Science, 2014, 89, 56-79.	3.8	86
30	Atomistic Simulations for Adsorption, Diffusion, and Separation of Gas Mixtures in Zeolite Imidazolate Frameworks. Journal of Physical Chemistry C, 2011, 115, 800-807.	1.5	85
31	An Emerging Family of Hybrid Nanomaterials: Metalâ€“Organic Framework/Aerogel Composites. ACS Applied Nano Materials, 2018, 1, 5959-5980.	2.4	84
32	Computational identification of a metal organic framework for high selectivity membrane-based CO2/CH4 separations: Cu(hfipbb)(H2hfipbb)0.5. Physical Chemistry Chemical Physics, 2009, 11, 11389.	1.3	83
33	How Reproducible are Surface Areas Calculated from the BET Equation?. Advanced Materials, 2022, 34, .	11.1	82
34	Do New MOFs Perform Better for CO₂ Capture and H₂ Purification? Computational Screening of the Updated MOF Database. ACS Applied Materials & Interfaces, 2020, 12, 41567-41579.	4.0	74
35	Adsorption and Transport of CH₄, CO₂, H₂ Mixtures in a Bio-MOF Material from Molecular Simulations. Journal of Physical Chemistry C, 2011, 115, 6833-6840.	1.5	72
36	Efficient Storage of Drug and Cosmetic Molecules in Biocompatible Metal Organic Frameworks: A Molecular Simulation Study. Industrial & Engineering Chemistry Research, 2016, 55, 1929-1939.	1.8	71

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37	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. Journal of Chemical Theory and Computation, 2019, 15, 382-401.	2.3	70
38	Molecular Simulations of MOF Membranes and Performance Predictions of MOF/Polymer Mixed Matrix Membranes for CO₂/CH₄ Separations. ACS Sustainable Chemistry and Engineering, 2019, 7, 2739-2750.	3.2	69
39	Can COFs replace MOFs in flue gas separation? high-throughput computational screening of COFs for CO₂/N₂ separation. Journal of Materials Chemistry A, 2020, 8, 14609-14623.	5.2	69
40	Predicting the Performance of Zeolite Imidazolate Framework/Polymer Mixed Matrix Membranes for CO₂, CH₄, and H₂ Separations Using Molecular Simulations. Industrial & Engineering Chemistry Research, 2012, 51, 14218-14228.	1.8	68
41	Testing the Accuracy of Correlations for Multicomponent Mass Transport of Adsorbed Gases in Metalâ^'Organic Frameworks: Diffusion of H₂/CH₄ Mixtures in CuBTC. Langmuir, 2008, 24, 8254-8261.	1.6	67
42	Adsorption, Diffusion, and Separation of CH₄/H₂ Mixtures in Covalent Organic Frameworks: Molecular Simulations and Theoretical Predictions. Journal of Physical Chemistry C, 2012, 116, 1772-1779.	1.5	67
43	Large-Scale Computational Screening of Metal Organic Framework (MOF) Membranes and MOF-Based Polymer Membranes for H₂/N₂ Separations. ACS Sustainable Chemistry and Engineering, 2019, 7, 9525-9536.	3.2	65
44	Computational screening of MOFs for C 2 H 6 /C 2 H 4 and C 2 H 6 /CH 4 separations. Chemical Engineering Science, 2016, 139, 49-60.	1.9	64
45	Screening Metalâ€"Organic Framework-Based Mixed-Matrix Membranes for CO₂/CH₄ Separations. Industrial & Engineering Chemistry Research, 2011, 50, 12606-12616.	1.8	62
46	Ranking of MOF Adsorbents for CO₂ Separations: A Molecular Simulation Study. Industrial & Engineering Chemistry Research, 2016, 55, 10404-10419.	1.8	56
47	Computer simulations of 4240 MOF membranes for H₂/CH₄ separations: insights into structureâ€"performance relations. Journal of Materials Chemistry A, 2018, 6, 5836-5847.	5.2	56
48	Novel nanostructured composites of silica aerogels with a metal organic framework. Microporous and Mesoporous Materials, 2013, 170, 352-358.	2.2	55
49	Atomically Detailed Modeling of Metal Organic Frameworks for Adsorption, Diffusion, and Separation of Noble Gas Mixtures. Industrial & Engineering Chemistry Research, 2012, 51, 7373-7382.	1.8	53
50	Adsorption- and Membrane-Based CH₄/N₂ Separation Performances of MOFs. Industrial & Engineering Chemistry Research, 2017, 56, 8713-8722.	1.8	53
51	Identifying Highly Selective Metal Organic Frameworks for CH₄/H₂ Separations Using Computational Tools. Industrial & Engineering Chemistry Research, 2015, 54, 8479-8491.	1.8	51
52	Enhancing CO2/CH4 and CO2/N2 separation performances of ZIF-8 by post-synthesis modification with [BMIM][SCN]. Polyhedron, 2018, 155, 485-492.	1.0	50
53	Efficient separation of helium from methane using MOF membranes. Separation and Purification Technology, 2018, 191, 192-199.	3.9	49
54	High CO₂ Selectivity of an Amine-Functionalized Metal Organic Framework in Adsorption-Based and Membrane-Based Gas Separations. Industrial & Engineering Chemistry Research, 2013, 52, 3462-3472.	1.8	47

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55	Multivariable linear models of structural parameters to predict methane uptake in metalâ€“organic frameworks. Chemical Engineering Science, 2015, 124, 125-134.	1.9	47
56	Molecular simulations of MOF adsorbents and membranes for noble gas separations. Chemical Engineering Science, 2017, 164, 108-121.	1.9	47
57	CO2 separation from flue gas mixture using [BMIM][BF4]/MOF composites: Linking high-throughput computational screening with experiments. Chemical Engineering Journal, 2020, 394, 124916.	6.6	46
58	Molecular modeling of MOF and ZIF-filled MMMs for CO2/N2 separations. Journal of Membrane Science, 2014, 454, 407-417.	4.1	45
59	Computational investigation of metal organic frameworks for storage and delivery of anticancer drugs. Journal of Materials Chemistry B, 2017, 5, 7342-7351.	2.9	44
60	MILâ€53(Al) as a Versatile Platform for Ionicâ€Liquid/MOF Composites to Enhance CO₂ Selectivity over CH₄ and N₂. Chemistry - an Asian Journal, 2019, 14, 3655-3667.	1.7	44
61	Unlocking CO2 separation performance of ionic liquid/CuBTC composites: Combining experiments with molecular simulations. Chemical Engineering Journal, 2019, 373, 1179-1189.	6.6	44
62	Computational screening of metal organic frameworks for mixed matrix membrane applications. Journal of Membrane Science, 2012, 407-408, 221-230.	4.1	43
63	Understanding the Potential of Zeolite Imidazolate Framework Membranes in Gas Separations Using Atomically Detailed Calculations. Journal of Physical Chemistry C, 2012, 116, 15525-15537.	1.5	42
64	A two-dimensional photoluminescent cadmium(II) coordination polymer containing a new coordination mode of pyridine-2,3-dicarboxylate: Synthesis, structure and molecular simulations for gas storage and separation applications. Polyhedron, 2013, 50, 314-320.	1.0	41
65	Exploring the performance limits of MOF/polymer MMMs for O2/N2 separation using computational screening. Journal of Membrane Science, 2021, 618, 118555.	4.1	41
66	Structural Factors Determining Thermal Stability Limits of Ionic Liquid/MOF Composites: Imidazolium Ionic Liquids Combined with CuBTC and ZIF-8. Industrial & Engineering Chemistry Research, 2019, 58, 14124-14138.	1.8	40
67	Recent advances in sustainable syngas production by catalytic CO₂ reforming of ethanol and glycerol. Sustainable Energy and Fuels, 2020, 4, 1029-1047.	2.5	40
68	MOF Membranes for CO2 Capture: Past, Present and Future. Carbon Capture Science & Technology, 2022, 2, 100026.	4.9	39
69	Combining Machine Learning and Molecular Simulations to Unlock Gas Separation Potentials of MOF Membranes and MOF/Polymer MMMs. ACS Applied Materials & Interfaces, 2022, 14, 32134-32148.	4.0	39
70	High-Throughput Screening of COF Membranes and COF/Polymer MMMs for Helium Separation and Hydrogen Purification. ACS Applied Materials & Interfaces, 2022, 14, 21738-21749.	4.0	38
71	Computational assessment of MOF membranes for CH4/H2 separations. Journal of Membrane Science, 2016, 514, 313-321.	4.1	37
72	Molecular Simulation Study of CH₄/H₂ Mixture Separations Using Metal Organic Framework Membranes and Composites. Journal of Physical Chemistry C, 2010, 114, 13047-13054.	1.5	36

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73	An unusual 3D metalâ€“organic framework, {[Ag4(Î¼4-pzdc)2(Î¼4-en)2]Â·H2O}n: Câ€“Hâ‹¯Ag, Nâ€“Hâ‹¯Ag and (Oâ€“H)â‹¯Ag interactions and an unprecedented coordination mode for pyrazine-2,3-dicarboxylate. CrystEngComm, 2012, 14, 2817.	1.3	36
74	Atomically Detailed Models for Transport of Gas Mixtures in ZIF Membranes and ZIF/Polymer Composite Membranes. Industrial & Engineering Chemistry Research, 2012, 51, 3091-3100.	1.8	36
75	Computational Selection of High-Performing Covalent Organic Frameworks for Adsorption and Membrane-Based CO₂/H₂ Separation. Journal of Physical Chemistry C, 2020, 124, 22577-22590.	1.5	36
76	Oxalamide-Functionalized Metal Organic Frameworks for CO₂ Adsorption. ACS Applied Materials & Interfaces, 2021, 13, 33188-33198.	4.0	35
77	Predicting Noble Gas Separation Performance of Metal Organic Frameworks Using Theoretical Correlations. Journal of Physical Chemistry C, 2013, 117, 5229-5241.	1.5	34
78	A new class of porous materials for efficient CO2 separation: Ionic liquid/graphene aerogel composites. Carbon, 2021, 171, 79-87.	5.4	34
79	Fast and Selective Adsorption of Methylene Blue from Water Using [BMIM][PF₆]-Incorporated UiO-66 and NH₂-UiO-66. Crystal Growth and Design, 2020, 20, 3590-3595.	1.4	33
80	Parametric study of methane steam reforming to syngas in a catalytic microchannel reactor. Applied Catalysis A: General, 2012, 411-412, 114-122.	2.2	32
81	Simulation of H₂/CH₄ mixture permeation through MOF membranes using non-equilibrium molecular dynamics. Journal of Materials Chemistry A, 2019, 7, 2301-2314.	5.2	32
82	A novel IL/MOF/polymer mixed matrix membrane having superior CO2/N2 selectivity. Journal of Membrane Science, 2022, 658, 120712.	4.1	32
83	Role of partial charge assignment methods in high-throughput screening of MOF adsorbents and membranes for CO₂/CH₄ separation. Molecular Systems Design and Engineering, 2020, 5, 532-543.	1.7	31
84	Computational Modeling of bio-MOFs for CO2/CH4 separations. Chemical Engineering Science, 2015, 130, 120-128.	1.9	30
85	Recent advances in materials for high purity H2 production by ethanol and glycerol steam reforming. International Journal of Hydrogen Energy, 2020, 45, 34888-34917.	3.8	30
86	MOF-based MMMs breaking the upper bounds of polymers for a large variety of gas separations. Separation and Purification Technology, 2022, 281, 119811.	3.9	30
87	Composites of porous materials with ionic liquids: Synthesis, characterization, applications, and beyond. Microporous and Mesoporous Materials, 2022, 332, 111703.	2.2	30
88	Prediction of O₂/N₂ Selectivity in Metalâ€“Organic Frameworks via High-Throughput Computational Screening and Machine Learning. ACS Applied Materials & Interfaces, 2022, 14, 736-749.	4.0	30
89	2Dâ†’3D polycatenated and 3Dâ†’3D interpenetrated metalâ€“organic frameworks constructed from thiophene-2,5-dicarboxylate and rigid bis(imidazole) ligands. Journal of Solid State Chemistry, 2014, 210, 261-266.	1.4	29
90	Computational screening of ZIFs for CO₂separations. Molecular Simulation, 2015, 41, 713-726.	0.9	28

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91	Effects of Force Field Selection on the Computational Ranking of MOFs for CO₂ Separations. Industrial & Engineering Chemistry Research, 2018, 57, 2298-2309.	1.8	28
92	Computational Screening of Porous Coordination Networks for Adsorption and Membrane-Based Gas Separations. Journal of Physical Chemistry C, 2014, 118, 13988-13997.	1.5	27
93	High CO₂ Selectivity of A Microporous Metalâ€“Imidazolate Framework: A Molecular Simulation Study. Industrial & Engineering Chemistry Research, 2011, 50, 8230-8236.	1.8	26
94	High-Throughput Molecular Simulations of Metal Organic Frameworks for CO2 Separation: Opportunities and Challenges. Frontiers in Materials, 2018, 5, .	1.2	26
95	Improving CO₂ Separation Performance of MILâ€53(Al) by Incorporating 1â€<i>n</i>â€Butylâ€3â€Methylimidazolium Methyl Sulfate. Energy Technology, 2019, 7, 1900157.	1.8	26
96	Unlocking the Effect of H₂O on CO₂ Separation Performance of Promising MOFs Using Atomically Detailed Simulations. Industrial & Engineering Chemistry Research, 2020, 59, 3141-3152.	1.8	26
97	Accelerating discovery of COFs for CO2 capture and H2 purification using structurally guided computational screening. Chemical Engineering Journal, 2022, 427, 131574.	6.6	26
98	Toward Rational Design of Ionic Liquid/Metalâ€“Organic Framework Composites: Effects of Interionic Interaction Energy. ACS Omega, 2017, 2, 6613-6618.	1.6	25
99	Molecular simulations of MOF membranes for separation of ethane/ethene and ethane/methane mixtures. RSC Advances, 2017, 7, 52283-52295.	1.7	25
100	Effect of methylation of ionic liquids on the gas separation performance of ionic liquid/metalâ€“organic framework composites. CrystEngComm, 2018, 20, 7137-7143.	1.3	25
101	Separation of CO₂ Mixtures Using Zn(bdc)(ted)_{0.5} Membranes and Composites: A Molecular Simulation Study. Journal of Physical Chemistry C, 2011, 115, 13637-13644.	1.5	23
102	A Review on Computational Modeling Tools for MOF-Based Mixed Matrix Membranes. Computation, 2019, 7, 36.	1.0	23
103	Comparing Performance of CPO and IRMOF Membranes for Gas Separations Using Atomistic Models. Industrial & Engineering Chemistry Research, 2010, 49, 11689-11696.	1.8	22
104	Effects of electrostatic interactions on gas adsorption and permeability of MOF membranes. Molecular Simulation, 2014, 40, 557-570.	0.9	22
105	Modeling and simulation of water-gas shift in a heat exchange integrated microchannel converter. International Journal of Hydrogen Energy, 2018, 43, 1094-1104.	3.8	22
106	Computational Screening of MOFs for Acetylene Separation. Frontiers in Chemistry, 2018, 6, 36.	1.8	22
107	Recent advances in simulating gas permeation through MOF membranes. Materials Advances, 2021, 2, 5300-5317.	2.6	22
108	Predicting Gas Separation Performances of Porous Coordination Networks Using Atomistic Simulations. Industrial & Engineering Chemistry Research, 2013, 52, 17627-17639.	1.8	21

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109	Application of MD Simulations to Predict Membrane Properties of MOFs. Journal of Nanomaterials, 2015, 2015, 1-9.	1.5	21
110	A phytochemical-containing metalâ€“organic framework: Synthesis, characterization and molecular simulations for hydrogen adsorption. Inorganica Chimica Acta, 2015, 427, 138-143.	1.2	21
111	Gas adsorption and diffusion in a highly CO₂selective metalâ€“organic framework: molecular simulations. Molecular Simulation, 2013, 39, 14-24.	0.9	20
112	Influence of anion size and electronic structure on the gas separation performance of ionic liquid/ZIF-8 composites. Microporous and Mesoporous Materials, 2020, 306, 110446.	2.2	20
113	Effect of Metalâ€“Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. Angewandte Chemie, 2021, 133, 7907-7916.	1.6	20
114	Soil remediation via an ionic liquid and supercritical CO2. Chemical Engineering and Processing: Process Intensification, 2008, 47, 1693-1704.	1.8	19
115	A new approach for predicting gas separation performances of MOF membranes. Journal of Membrane Science, 2016, 519, 45-54.	4.1	19
116	Highâ€Throughput Screening of Metal Organic Frameworks as Fillers in Mixed Matrix Membranes for Flue Gas Separation. Advanced Theory and Simulations, 2019, 2, 1900109.	1.3	19
117	Analysis of CH₄Uptake over Metalâ€“Organic Frameworks Using Data-Mining Tools. ACS Combinatorial Science, 2019, 21, 257-268.	3.8	19
118	Doubling CO2/N2 separation performance of CuBTC by incorporation of 1-n-ethyl-3-methylimidazolium diethyl phosphate. Microporous and Mesoporous Materials, 2021, 316, 110947.	2.2	19
119	Synthesis, crystal structures, molecular simulations for hydrogen gas adsorption, fluorescent and antimicrobial properties of pyrazine-2,3-dicarboxylate complexes. Inorganica Chimica Acta, 2013, 399, 19-35.	1.2	18
120	Gas adsorption/separation properties of metal directed self-assembly of two coordination polymers with 5-nitroisophthalate. Journal of Solid State Chemistry, 2014, 210, 280-286.	1.4	18
121	Construction of homo- and heterometallic-pyridine-2,3-dicarboxylate metallosupramolecular networks with structural diversity: 1D T5(2) water tape and unexpected coordination mode of pyridine-2,3-dicarboxylate. CrystEngComm, 2013, 15, 1244.	1.3	17
122	Revealing the effect of structure curations on the simulated CO₂ separation performances of MOFs. Materials Advances, 2020, 1, 341-353.	2.6	17
123	Computational Methods for MOF/Polymer Membranes. Chemical Record, 2016, 16, 703-718.	2.9	16
124	An Integrated Computationalâ€“Experimental Hierarchical Approach for the Rational Design of an IL/UiOâ€66 Composite Offering Infinite CO₂ Selectivity. Advanced Functional Materials, 2022, 32, .	7.8	16
125	Computational Screening of MOF-Based Mixed Matrix Membranes for CO₂/N₂Separations. Journal of Nanomaterials, 2016, 2016, 1-12.	1.5	15
126	Enhanced Water Purification Performance of Ionic Liquid Impregnated Metalâ€“Organic Framework: Dye Removal by [BMIM][PF6]/MIL-53(Al) Composite. Frontiers in Chemistry, 2020, 8, 622567.	1.8	14

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127	Combined GCMC, MD, and DFT Approach for Unlocking the Performances of COFs for Methane Purification. Industrial & Engineering Chemistry Research, 2021, 60, 12999-13012.	1.8	14
128	[BMIM][OAc] coating layer makes activated carbon almost completely selective for CO2. Chemical Engineering Journal, 2022, 437, 135436.	6.6	14
129	Zr-MOFs for CF₄/CH₄, CH₄/H₂, and CH₄/N₂ separation: towards the goal of discovering stable and effective adsorbents. Molecular Systems Design and Engineering, 2021, 6, 627-642.	1.7	13
130	Two novel 2D and 3D coordination polymers constructed from pyrazine-2,3-dicarboxylic acid and chloride bridged secondary building units. Synthetic Metals, 2011, 161, 2471-2480.	2.1	12
131	Multi-scale computational screening to accelerate discovery of IL/COF composites for CO2/N2 separation. Separation and Purification Technology, 2022, 287, 120578.	3.9	12
132	A three-dimensional silver(I) framework assembled from 3,3â€²-thiodipropionate: Synthesis, structure and molecular simulations for hydrogen gas adsorption. Polyhedron, 2012, 45, 103-106.	1.0	11
133	Effects of molecular simulation parameters on predicting gas separation performance of ZIFs. Journal of Chemical Technology and Biotechnology, 2015, 90, 1707-1718.	1.6	11
134	The role of ovarian reserve markers in prediction of clinical pregnancy. Journal of Obstetrics and Gynaecology, 2017, 37, 492-497.	0.4	11
135	MOF adsorbents for flue gas separation: Comparison of material ranking approaches. Chemical Engineering Research and Design, 2022, 179, 308-318.	2.7	11
136	Hypothetical yet effective: Computational identification of high-performing MOFs for CO2 capture. Computers and Chemical Engineering, 2022, 160, 107705.	2.0	11
137	Different dimensionality in Mn(II), Co(II) and Ni(II) aminoisophthalate metalâ€“organic compounds: Synthesis, characterization and gas adsorption properties. Polyhedron, 2012, 48, 199-211.	1.0	10
138	In Silico Design of Metal Organic Frameworks with Enhanced CO2 Separation Performances: Role of Metal Sites. Journal of Physical Chemistry C, 2019, 123, 28255-28265.	1.5	10
139	Molecular simulations of porous coordination network-based mixed matrix membranes for CO₂/N₂separations. Molecular Simulation, 2015, 41, 1396-1408.	0.9	9
140	Selection rules for estimating the solubility of C4-hydrocarbons in imidazolium ionic liquids determined by machine-learning tools. Journal of Molecular Liquids, 2019, 284, 511-521.	2.3	9
141	A zinc(II) metal organic framework based on flexible o-phenylenediacetate and rigid 4,4â€²-azobis(pyridine) ligands: Synthesis, crystal structure and hydrogen gas adsorption property. Polyhedron, 2015, 100, 108-113.	1.0	8
142	Screening for selectivity. Nature Energy, 2020, 5, 8-9.	19.8	8
143	Towards complete elucidation of structural factors controlling thermal stability of IL/MOF composites: effects of ligand functionalization on MOFs. Journal of Physics Condensed Matter, 2020, 32, 484001.	0.7	8
144	Molecular Modeling of MOF-based Mixed Matrix Membranes. Current Organic Chemistry, 2014, 18, 2364-2380.	0.9	8

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145	Enhanced water stability and high CO₂ storage capacity of a Lewis basic sites-containing zirconium metalâ€"organic framework. Dalton Transactions, 2021, 50, 16587-16592.	1.6	8
146	Computational insights into efficient CO2 and H2S capture through zirconium MOFs. Journal of CO2 Utilization, 2022, 55, 101811.	3.3	8
147	The synthesis, characterization, and theoretical hydrogen gas adsorption properties of copper(II)-3,3â€²-thiodipropionate complexes with imidazole derivatives. Journal of Coordination Chemistry, 2013, 66, 4093-4106.	0.8	6
148	Reply to Comment on â€œDatabase for CO₂ Separation Performances of MOFs Based on Computational Materials Screeningâ€. ACS Applied Materials & Interfaces, 2019, 11, 16266-16271.	4.0	4
149	Exploring covalent organic frameworks for H2S+CO2 separation from natural gas using efficient computational approaches. Journal of CO2 Utilization, 2022, 62, 102077.	3.3	4
150	Recent Advances in Molecular Dynamics Simulations of Gas Diffusion in Metal Organic Frameworks. , 0, , .		3
151	Metal Exchange Boosts the CO2 Selectivity of Metal Organic Frameworks Having Zn-Oxide Nodes. Journal of Physical Chemistry C, 2021, 125, 17311-17322.	1.5	3
152	Multi-Level Computational Screening of <i>in Silico</i> Designed MOFs for Efficient SO₂ Capture. Journal of Physical Chemistry C, 2022, 126, 9875-9888.	1.5	2
153	Molecular Simulations for Adsorption-Based CO2 Separation Using Metal Organic Frameworks. , 2016, , .		0
154	Molecular Modeling of MOF Membranes for Gas Separations. , 2017, , 97-143.		0
155	Computational Screening of MOFs for CO2 Capture. , 2021, , 205-238.		0
156	Molecular Modeling of Metalâ€"Organic Frameworks for Carbon Dioxide Separation Applications. , 2015, , 339-379.		0