Seda KeskIn

List of Publications by Citations

149 papers	6,503 citations	41 h-index	76 g-index
160 ext. papers	7,703 ext. citations	6.7 avg, IF	6.87 L-index

#	Paper	IF	Citations
149	A review of ionic liquids towards supercritical fluid applications. *Journal of Supercritical Fluids*, **2007**, 43, 150-180	4.2	591
148	Can metal-organic framework materials play a useful role in large-scale carbon dioxide separations?. *ChemSusChem*, **2010**, 3, 879-91	8.3	518
147	Biomedical Applications of Metal Organic Frameworks. *Industrial & Engineering Chemistry Research*, **2011**, 50, 1799-1812	3.9	420
146	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal□Organic Framework Materials. *Industrial & Engineering Chemistry Research*, **2009**, 48, 2355-2371	3.9	270
145	Opportunities and challenges of MOF-based membranes in gas separations. *Separation and Purification Technology*, **2015**, 152, 207-237	8.3	182
144	Screening Metal□Organic Framework Materials for Membrane-based Methane/Carbon Dioxide Separations. *Journal of Physical Chemistry C*, **2007**, 111, 14055-14059	3.8	173
143	Selecting metal organic frameworks as enabling materials in mixed matrix membranes for high efficiency natural gas purification. *Energy and Environmental Science*, **2010**, 3, 343	35.4	159
142	Efficient methods for screening of metal organic framework membranes for gas separations using atomically detailed models. *Langmuir*, **2009**, 25, 11786-95	4	149
141	Ionic Liquid/Metal-Organic Framework Composites: From Synthesis to Applications. *ChemSusChem*, **2017**, 10, 2842-2863	8.3	138
140	Assessment of a Metal□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	3.9	129
139	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	3.8	95
138	Database for CO Separation Performances of MOFs Based on Computational Materials Screening. *ACS Applied Materials & Interfaces*, **2018**, 10, 17257-17268	9.5	90
137	[BMIM][PF] Incorporation Doubles CO Selectivity of ZIF-8: Elucidation of Interactions and Their Consequences on Performance. *ACS Applied Materials & Interfaces*, **2016**, 8, 30992-31005	9.5	89
136	Atomically detailed models of gas mixture diffusion through CuBTC membranes. *Microporous and Mesoporous Materials*, **2009**, 125, 101-106	5.3	86
135	Tuning the Gas Separation Performance of CuBTC by Ionic Liquid Incorporation. *Langmuir*, **2016**, 32, 1139-47	4	85
134	Recent advances in metal-organic framework-based mixed matrix membranes. *Chemistry - an Asian Journal*, **2013**, 8, 1692-704	4.5	83
133	High-Throughput Screening of MOF Adsorbents and Membranes for H Purification and CO Capture. *ACS Applied Materials & Interfaces*, **2018**, 10, 33693-33706	9.5	79

132	Simulation and modelling of MOFs for hydrogen storage. *CrystEngComm*, **2015**, 17, 261-275	3.3	77
131	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, 11389-94	3.6	77
130	Atomistic Simulations for Adsorption, Diffusion, and Separation of Gas Mixtures in Zeolite Imidazolate Frameworks. *Journal of Physical Chemistry C*, **2011**, 115, 800-807	3.8	76
129	Core-Shell Type Ionic Liquid/Metal Organic Framework Composite: An Exceptionally High CO/CH Selectivity. *Journal of the American Chemical Society*, **2018**, 140, 10113-10116	16.4	73
128	Site characteristics in metal organic frameworks for gas adsorption. *Progress in Surface Science*, **2014**, 89, 56-79	6.6	71
127	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	3.8	70
126	High-Throughput Computational Screening of the Metal Organic Framework Database for CH/H Separations. *ACS Applied Materials & Interfaces*, **2018**, 10, 3668-3679	9.5	70
125	Computational Screening of Metal-Organic Frameworks for Membrane-Based CO/N/HO Separations: Best Materials for Flue Gas Separation. *Journal of Physical Chemistry C*, **2018**, 122, 17347-17357	3.8	66
124	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	3.8	64
123	Testing the accuracy of correlations for multicomponent mass transport of adsorbed gases in metal-organic frameworks: diffusion of H2/CH4 mixtures in CuBTC. *Langmuir*, **2008**, 24, 8254-61	4	64
122	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	13	60
121	Screening Metal□Organic Framework-Based Mixed-Matrix Membranes for CO2/CH4Separations. *Industrial & Engineering Chemistry Research*, **2011**, 50, 12606-12616	3.9	59
120	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	3.9	58
119	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	3.8	57
118	Recent advances, opportunities, and challenges in high-throughput computational screening of MOFs for gas separations. *Coordination Chemistry Reviews*, **2020**, 422, 213470	23.2	56
117	Efficient Storage of Drug and Cosmetic Molecules in Biocompatible Metal Organic Frameworks: A Molecular Simulation Study. *Industrial & Engineering Chemistry Research*, **2016**, 55, 1929-1939	3.9	53
116	Molecular Simulations of MOF Membranes and Performance Predictions of MOF/Polymer Mixed Matrix Membranes for CO/CH Separations. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 2739-2750	8.3	48
115	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	4.4	47

114	An Emerging Family of Hybrid Nanomaterials: Metal–Organic Framework/Aerogel Composites. *ACS Applied Nano Materials*, **2018**, 1, 5959-5980	5.6	47
113	Novel nanostructured composites of silica aerogels with a metal organic framework. *Microporous and Mesoporous Materials*, **2013**, 170, 352-358	5.3	46
112	Atomically Detailed Modeling of Metal Organic Frameworks for Adsorption, Diffusion, and Separation of Noble Gas Mixtures. *Industrial & Engineering Chemistry Research*, **2012**, 51, 7373-7382	3.9	45
111	Ranking of MOF Adsorbents for CO2 Separations: A Molecular Simulation Study. *Industrial & Engineering Chemistry Research*, **2016**, 55, 10404-10419	3.9	43
110	Effect of Metal-Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. *Angewandte Chemie - International Edition*, **2021**, 60, 7828-7837	16.4	42
109	Identifying Highly Selective Metal Organic Frameworks for CH4/H2 Separations Using Computational Tools. *Industrial & Engineering Chemistry Research*, **2015**, 54, 8479-8491	3.9	41
108	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	3.9	41
107	Computational screening of metal organic frameworks for mixed matrix membrane applications. *Journal of Membrane Science*, **2012**, 407-408, 221-230	9.6	40
106	Large-Scale Computational Screening of Metal Organic Framework (MOF) Membranes and MOF-Based Polymer Membranes for H/N Separations. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 9525-9536	8.3	38
105	Computer simulations of 4240 MOF membranes for H/CH separations: insights into structure-performance relations. *Journal of Materials Chemistry A*, **2018**, 6, 5836-5847	13	37
104	Computational investigation of metal organic frameworks for storage and delivery of anticancer drugs. *Journal of Materials Chemistry B*, **2017**, 5, 7342-7351	7.3	37
103	Understanding the Potential of Zeolite Imidazolate Framework Membranes in Gas Separations Using Atomically Detailed Calculations. *Journal of Physical Chemistry C*, **2012**, 116, 15525-15537	3.8	37
102	Multivariable linear models of structural parameters to predict methane uptake in metal–organic frameworks. *Chemical Engineering Science*, **2015**, 124, 125-134	4.4	36
101	Molecular modeling of MOF and ZIF-filled MMMs for CO2/N2 separations. *Journal of Membrane Science*, **2014**, 454, 407-417	9.6	36
100	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	2.7	35
99	An unusual 3D metal–organic framework, {[Ag4(μ4-pzdc)2(μ-en)2]·H2O}n: C–H···Ag, N–H···Ag and (O–H)···Ag interactions and an unprecedented coordination mode for pyrazine-2,3-dicarboxylate. *CrystEngComm*, **2012**, 14, 2817	3.3	34
98	Atomically Detailed Models for Transport of Gas Mixtures in ZIF Membranes and ZIF/Polymer Composite Membranes. *Industrial & Engineering Chemistry Research*, **2012**, 51, 3091-3100	3.9	34
97	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. *Journal of Chemical Theory and Computation*, **2019**, 15, 382-401	6.4	33

96	Molecular Simulation Study of CH4/H2 Mixture Separations Using Metal Organic Framework Membranes and Composites. *Journal of Physical Chemistry C*, **2010**, 114, 13047-13054	3.8	32
95	Unlocking CO2 separation performance of ionic liquid/CuBTC composites: Combining experiments with molecular simulations. *Chemical Engineering Journal*, **2019**, 373, 1179-1189	14.7	30
94	Efficient separation of helium from methane using MOF membranes. *Separation and Purification Technology*, **2018**, 191, 192-199	8.3	30
93	Computational assessment of MOF membranes for CH4/H2 separations. *Journal of Membrane Science*, **2016**, 514, 313-321	9.6	29
92	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	42.2	29
91	Enhancing CO2/CH4 and CO2/N2 separation performances of ZIF-8 by post-synthesis modification with [BMIM][SCN]. *Polyhedron*, **2018**, 155, 485-492	2.7	29
90	CO2 separation from flue gas mixture using [BMIM][BF4]/MOF composites: Linking high-throughput computational screening with experiments. *Chemical Engineering Journal*, **2020**, 394, 124916	14.7	28
89	Predicting Noble Gas Separation Performance of Metal Organic Frameworks Using Theoretical Correlations. *Journal of Physical Chemistry C*, **2013**, 117, 5229-5241	3.8	28
88	Parametric study of methane steam reforming to syngas in a catalytic microchannel reactor. *Applied Catalysis A: General*, **2012**, 411-412, 114-122	5.1	28
87	Molecular simulations of MOF adsorbents and membranes for noble gas separations. *Chemical Engineering Science*, **2017**, 164, 108-121	4.4	27
86	2D-3D polycatenated and 3D-3D interpenetrated metal-organic frameworks constructed from thiophene-2,5-dicarboxylate and rigid bis(imidazole) ligands. *Journal of Solid State Chemistry*, **2014**, 210, 261-266	3.3	27
85	Do New MOFs Perform Better for CO Capture and H Purification? Computational Screening of the Updated MOF Database. *ACS Applied Materials & Interfaces*, **2020**, 12, 41567-41579	9.5	27
84	Adsorption- and Membrane-Based CH4/N2 Separation Performances of MOFs. *Industrial & Engineering Chemistry Research*, **2017**, 56, 8713-8722	3.9	26
83	Effects of Force Field Selection on the Computational Ranking of MOFs for CO Separations. *Industrial & Engineering Chemistry Research*, **2018**, 57, 2298-2309	3.9	25
82	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	13	25
81	Machine Learning Meets with Metal Organic Frameworks for Gas Storage and Separation. *Journal of Chemical Information and Modeling*, **2021**, 61, 2131-2146	6.1	25
80	Computational Screening of Porous Coordination Networks for Adsorption and Membrane-Based Gas Separations. *Journal of Physical Chemistry C*, **2014**, 118, 13988-13997	3.8	24
79	High CO2Selectivity of A Microporous Metal-Imidazolate Framework: A Molecular Simulation Study. *Industrial & Engineering Chemistry Research*, **2011**, 50, 8230-8236	3.9	24

78	Simulation of H/CH mixture permeation through MOF membranes using non-equilibrium molecular dynamics. *Journal of Materials Chemistry A*, **2019**, 7, 2301-2314	13	22
77	Computational Modeling of bio-MOFs for CO2/CH4 separations. *Chemical Engineering Science*, **2015**, 130, 120-128	4.4	22
76	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	4.6	22
75	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	3.8	22
74	Toward Rational Design of Ionic Liquid/Metal-Organic Framework Composites: Effects of Interionic Interaction Energy. *ACS Omega*, **2017**, 2, 6613-6618	3.9	21
73	High-Throughput Molecular Simulations of Metal Organic Frameworks for CO2 Separation: Opportunities and Challenges. *Frontiers in Materials*, **2018**, 5,	4	21
72	Computational screening of ZIFs for CO2 separations. *Molecular Simulation*, **2015**, 41, 713-726	2	20
71	Modeling and simulation of water-gas shift in a heat exchange integrated microchannel converter. *International Journal of Hydrogen Energy*, **2018**, 43, 1094-1104	6.7	20
70	Comparing Performance of CPO and IRMOF Membranes for Gas Separations Using Atomistic Models. *Industrial & Engineering Chemistry Research*, **2010**, 49, 11689-11696	3.9	20
69	MIL-53(Al) as a Versatile Platform for Ionic-Liquid/MOF Composites to Enhance CO Selectivity over CH and N. *Chemistry - an Asian Journal*, **2019**, 14, 3655-3667	4.5	19
68	Predicting Gas Separation Performances of Porous Coordination Networks Using Atomistic Simulations. *Industrial & Engineering Chemistry Research*, **2013**, 52, 17627-17639	3.9	19
67	Application of MD Simulations to Predict Membrane Properties of MOFs. *Journal of Nanomaterials*, **2015**, 2015, 1-9	3.2	19
66	A phytochemical-containing metal-organic framework: Synthesis, characterization and molecular simulations for hydrogen adsorption. *Inorganica Chimica Acta*, **2015**, 427, 138-143	2.7	19
65	Effects of electrostatic interactions on gas adsorption and permeability of MOF membranes. *Molecular Simulation*, **2014**, 40, 557-570	2	18
64	Soil remediation via an ionic liquid and supercritical CO2. *Chemical Engineering and Processing: Process Intensification*, **2008**, 47, 1693-1704	3.7	18
63	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	3.3	17
62	Computational Selection of High-Performing Covalent Organic Frameworks for Adsorption and Membrane-Based CO/H Separation. *Journal of Physical Chemistry C*, **2020**, 124, 22577-22590	3.8	17
61	Improving CO Separation Performance of MIL-53(Al) by Incorporating 1--Butyl-3-Methylimidazolium Methyl Sulfate. *Energy Technology*, **2019**, 7, 1900157	3.5	16

60	Computational Screening of MOFs for Acetylene Separation. *Frontiers in Chemistry*, **2018**, 6, 36	5	16
59	Gas adsorption and diffusion in a highly CO2 selective metal-organic framework: molecular simulations. *Molecular Simulation*, **2013**, 39, 14-24	2	16
58	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	3.3	16
57	Exploring the performance limits of MOF/polymer MMMs for O2/N2 separation using computational screening. *Journal of Membrane Science*, **2021**, 618, 118555	9.6	16
56	Effect of methylation of ionic liquids on the gas separation performance of ionic liquid/metal-organic framework composites. *CrystEngComm*, **2018**, 20, 7137-7143	3.3	16
55	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	3.9	15
54	Molecular simulations of MOF membranes for separation of ethane/ethene and ethane/methane mixtures. *RSC Advances*, **2017**, 7, 52283-52295	3.7	15
53	Recent advances in sustainable syngas production by catalytic CO2 reforming of ethanol and glycerol. *Sustainable Energy and Fuels*, **2020**, 4, 1029-1047	5.8	15
52	Computational Screening of MOF-Based Mixed Matrix Membranes for CO2/N2Separations. *Journal of Nanomaterials*, **2016**, 2016, 1-12	3.2	15
51	A new approach for predicting gas separation performances of MOF membranes. *Journal of Membrane Science*, **2016**, 519, 45-54	9.6	14
50	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	2.7	14
49	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	3.5	13
48	Computational Methods for MOF/Polymer Membranes. *Chemical Record*, **2016**, 16, 703-18	6.6	13
47	Recent advances in materials for high purity H2 production by ethanol and glycerol steam reforming. *International Journal of Hydrogen Energy*, **2020**, 45, 34888-34917	6.7	13
46	A new class of porous materials for efficient CO2 separation: Ionic liquid/graphene aerogel composites. *Carbon*, **2021**, 171, 79-87	10.4	13
45	Unlocking the Effect of HO on CO Separation Performance of Promising MOFs Using Atomically Detailed Simulations. *Industrial & Engineering Chemistry Research*, **2020**, 59, 3141-3152	3.9	12
44	Assessing CH4/N2 separation potential of MOFs, COFs, IL/MOF, MOF/Polymer, and COF/Polymer composites. *Chemical Engineering Journal*, **2022**, 428, 131239	14.7	12
43	How Reproducible are Surface Areas Calculated from the BET Equation?. *Advanced Materials*,2201502	24	12

42	Analysis of CH Uptake over Metal-Organic Frameworks Using Data-Mining Tools. *ACS Combinatorial Science*, **2019**, 21, 257-268	3.9	11
41	A three-dimensional silver(I) framework assembled from 3,3?-thiodipropionate: Synthesis, structure and molecular simulations for hydrogen gas adsorption. *Polyhedron*, **2012**, 45, 103-106	2.7	11
40	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	3.6	11
39	Revealing the effect of structure curations on the simulated CO2 separation performances of MOFs. *Materials Advances*, **2020**, 1, 341-353	3.3	11
38	Effect of Metal Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. *Angewandte Chemie*, **2021**, 133, 7907-7916	3.6	11
37	High-Throughput Screening of Metal Organic Frameworks as Fillers in Mixed Matrix Membranes for Flue Gas Separation. *Advanced Theory and Simulations*, **2019**, 2, 1900109	3.5	10
36	Molecular simulations of porous coordination network-based mixed matrix membranes for CO2/N2 separations. *Molecular Simulation*, **2015**, 41, 1396-1408	2	9
35	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	5.3	9
34	Different dimensionality in Mn(II), Co(II) and Ni(II) aminoisophthalate metal organic compounds: Synthesis, characterization and gas adsorption properties. *Polyhedron*, **2012**, 48, 199-211	2.7	9
33	Effects of molecular simulation parameters on predicting gas separation performance of ZIFs. *Journal of Chemical Technology and Biotechnology*, **2015**, 90, 1707-1718	3.5	8
32	A Review on Computational Modeling Tools for MOF-Based Mixed Matrix Membranes. *Computation* , **2019**, 7, 36	2.2	8
31	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	6	7
30	A zinc(II) metal organic framework based on flexible o-phenylenediacetate and rigid 4,4?-azobis(pyridine) ligands: Synthesis, crystal structure and hydrogen gas adsorption property. *Polyhedron*, **2015**, 100, 108-113	2.7	7
29	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	3.8	7
28	Molecular Modeling of MOF-based Mixed Matrix Membranes. *Current Organic Chemistry*, **2014**, 18, 2364-2380	2.7	7
27	Doubling CO2/N2 separation performance of CuBTC by incorporation of 1-n-ethyl-3-methylimidazolium diethyl phosphate. *Microporous and Mesoporous Materials*, **2021**, 316, 110947	5.3	7
26	The role of ovarian reserve markers in prediction of clinical pregnancy. *Journal of Obstetrics and Gynaecology*, **2017**, 37, 492-497	1.3	6
25	The synthesis, characterization, and theoretical hydrogen gas adsorption properties of copper(II)-3,3?-thiodipropionate complexes with imidazole derivatives. *Journal of Coordination Chemistry*, **2013**, 66, 4093-4106	1.6	6

24	MOF Membranes for CO2 Capture: Past, Present and Future. *Carbon Capture Science & Technology*, **2022**, 2, 100026		6
23	Accelerating discovery of COFs for CO2 capture and H2 purification using structurally guided computational screening. *Chemical Engineering Journal*, **2022**, 427, 131574	14.7	6
22	Oxalamide-Functionalized Metal Organic Frameworks for CO Adsorption. *ACS Applied Materials & Interfaces*, **2021**, 13, 33188-33198	9.5	5
21	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**,	1.8	4
20	Composites of porous materials with ionic liquids: Synthesis, characterization, applications, and beyond. *Microporous and Mesoporous Materials*, **2022**, 332, 111703	5.3	4
19	Reply to Comment on "Database for CO Separation Performances of MOFs Based on Computational Materials Screening". *ACS Applied Materials & Interfaces*, **2019**, 11, 16266-16271	9.5	3
18	Recent advances in simulating gas permeation through MOF membranes. *Materials Advances*, **2021**, 2, 5300-5317	3.3	3
17	MOF-based MMMs Breaking the Upper Bounds of Polymers for a Large Variety of Gas Separations. *Separation and Purification Technology*, **2021**, 119811	8.3	3
16	[BMIM][OAc] coating layer makes activated carbon almost completely selective for CO2. *Chemical Engineering Journal*, **2022**, 437, 135436	14.7	3
15	Recent Advances in Molecular Dynamics Simulations of Gas Diffusion in Metal Organic Frameworks **2012**,		2
14	Enhanced Water Purification Performance of Ionic Liquid Impregnated Metal-Organic Framework: Dye Removal by [BMIM][PF]/MIL-53(Al) Composite. *Frontiers in Chemistry*, **2020**, 8, 622567	5	2
13	Zr-MOFs for CF/CH, CH/H, and CH/N separation: towards the goal of discovering stable and effective adsorbents. *Molecular Systems Design and Engineering*, **2021**, 6, 627-642	4.6	2
12	Combined GCMC, MD, and DFT Approach for Unlocking the Performances of COFs for Methane Purification. *Industrial & Engineering Chemistry Research*, **2021**, 60, 12999-13012	3.9	2
11	MOF adsorbents for flue gas separation: Comparison of material ranking approaches. *Chemical Engineering Research and Design*, **2022**, 179, 308-318	5.5	1
10	Hypothetical yet effective: Computational identification of high-performing MOFs for CO2 capture. *Computers and Chemical Engineering*, **2022**, 160, 107705	4	1
9	Enhanced water stability and high CO storage capacity of a Lewis basic sites-containing zirconium metal-organic framework. *Dalton Transactions*, **2021**, 50, 16587-16592	4.3	1
8	Multi-scale computational screening to accelerate discovery of IL/COF composites for CO2/N2 separation. *Separation and Purification Technology*, **2022**, 287, 120578	8.3	0
7	Computational insights into efficient CO2 and H2S capture through zirconium MOFs. *Journal of CO2 Utilization*, **2021**, 55, 101811	7.6	0

6 Molecular Modeling of MOF Membranes for Gas Separations **2017**, 97-143

5 Numerical solution techniques **2016**, 253-268

4 Molecular Modeling of Metal Organic Frameworks for Carbon Dioxide Separation Applications **2015**, 339-379

3 Metal Exchange Boosts the CO Selectivity of Metal Organic Frameworks Having Zn-Oxide Nodes. *Journal of Physical Chemistry C*, **2021**, 125, 17311-17322 3.8

2 Computational Screening of MOFs for CO2 Capture **2021**, 205-238

1 Metal-Organic Frameworks for Hydrogen Storage **2022**, 1-35