

Seda Keskin

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/463323/publications.pdf>

Version: 2024-02-01

156
papers

9,131
citations

38720

50
h-index

46771

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. <i>Journal of Supercritical Fluids</i> , 2007, 43, 150-180.	1.6	648
2	Can Metal-Organic Framework Materials Play a Useful Role in Large-Scale Carbon Dioxide Separations?. <i>ChemSusChem</i> , 2010, 3, 879-891.	3.6	556
3	Biomedical Applications of Metal Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 1799-1812.	1.8	520
4	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal-Organic Framework Materials. <i>Industrial & Engineering Chemistry Research</i> , 2009, 48, 2355-2371.	1.8	283
5	Opportunities and challenges of MOF-based membranes in gas separations. <i>Separation and Purification Technology</i> , 2015, 152, 207-237.	3.9	233
6	Ionic Liquid/Metal-Organic Framework Composites: From Synthesis to Applications. <i>ChemSusChem</i> , 2017, 10, 2842-2863.	3.6	210
7	Screening Metal-Organic Framework Materials for Membrane-based Methane/Carbon Dioxide Separations. <i>Journal of Physical Chemistry C</i> , 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. <i>Energy and Environmental Science</i> , 2010, 3, 343.	15.6	172
9	Effect of Metal-Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7828-7837.	7.2	164
10	Efficient Methods for Screening of Metal Organic Framework Membranes for Gas Separations Using Atomically Detailed Models. <i>Langmuir</i> , 2009, 25, 11786-11795.	1.6	161
11	Assessment of a Metal-Organic Framework Membrane for Gas Separations Using Atomically Detailed Calculations: CO ₂ , CH ₄ , N ₂ , H ₂ Mixtures in MOF-5. <i>Industrial & Engineering Chemistry Research</i> , 2009, 48, 914-922.	1.8	143
12	High-Throughput Screening of MOF Adsorbents and Membranes for H ₂ Purification and CO ₂ Capture. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 33693-33706.	4.0	133
13	[BMIM][PF ₆] Incorporation Doubles CO ₂ Selectivity of ZIF-8: Elucidation of Interactions and Their Consequences on Performance. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 30992-31005.	4.0	131
14	Database for CO ₂ Separation Performances of MOFs Based on Computational Materials Screening. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 17257-17268.	4.0	129
15	Recent advances, opportunities, and challenges in high-throughput computational screening of MOFs for gas separations. <i>Coordination Chemistry Reviews</i> , 2020, 422, 213470.	9.5	124
16	Core-Shell Type Ionic Liquid/Metal Organic Framework Composite: An Exceptionally High CO ₂ /CH ₄ Selectivity. <i>Journal of the American Chemical Society</i> , 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. <i>Progress in Materials Science</i> , 2021, 117, 100743.	16.0	120
18	Tuning the Gas Separation Performance of CuBTC by Ionic Liquid Incorporation. <i>Langmuir</i> , 2016, 32, 1139-1147.	1.6	110

#	ARTICLE	IF	CITATIONS
19	High-Throughput Computational Screening of the Metal Organic Framework Database for CH ₄ /H ₂ Separations. ACS Applied Materials & Interfaces, 2018, 10, 3668-3679.	4.0	108
20	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH ₄ /H ₂ and CO ₂ /CH ₄ 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][BF ₄] 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 Metal-Organic Framework-Based Mixed Matrix Membranes. Chemistry - an Asian Journal, 2013, 8, 1692-1704.	1.7	95
25	Computational Screening of Metal-Organic Frameworks for Membrane-Based CO ₂ /N ₂ /H ₂ O 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 CH ₄ /N ₂ 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 CH ₄ and H ₂ 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: Metal-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 CO ₂ /CH ₄ separations: Cu(hfipbb)(H ₂ hfipbb)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 CO ₂ Capture and H ₂ Purification? Computational Screening of the Updated MOF Database. ACS Applied Materials & Interfaces, 2020, 12, 41567-41579.	4.0	74
35	Adsorption and Transport of CH ₄ , CO ₂ , H ₂ 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

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

#	ARTICLE	IF	CITATIONS
55	Multivariable linear models of structural parameters to predict methane uptake in metal-organic frameworks. <i>Chemical Engineering Science</i> , 2015, 124, 125-134.	1.9	47
56	Molecular simulations of MOF adsorbents and membranes for noble gas separations. <i>Chemical Engineering Science</i> , 2017, 164, 108-121.	1.9	47
57	CO ₂ separation from flue gas mixture using [BMIM][BF ₄]/MOF composites: Linking high-throughput computational screening with experiments. <i>Chemical Engineering Journal</i> , 2020, 394, 124916.	6.6	46
58	Molecular modeling of MOF and ZIF-filled MMMs for CO ₂ /N ₂ separations. <i>Journal of Membrane Science</i> , 2014, 454, 407-417.	4.1	45
59	Computational investigation of metal organic frameworks for storage and delivery of anticancer drugs. <i>Journal of Materials Chemistry B</i> , 2017, 5, 7342-7351.	2.9	44
60	MIL-53(Al) as a Versatile Platform for Ionic-Liquid/MOF Composites to Enhance CO ₂ Selectivity over CH ₄ and N ₂ . <i>Chemistry - an Asian Journal</i> , 2019, 14, 3655-3667.	1.7	44
61	Unlocking CO ₂ separation performance of ionic liquid/CuBTC composites: Combining experiments with molecular simulations. <i>Chemical Engineering Journal</i> , 2019, 373, 1179-1189.	6.6	44
62	Computational screening of metal organic frameworks for mixed matrix membrane applications. <i>Journal of Membrane Science</i> , 2012, 407-408, 221-230.	4.1	43
63	Understanding the Potential of Zeolite Imidazolate Framework Membranes in Gas Separations Using Atomically Detailed Calculations. <i>Journal of Physical Chemistry C</i> , 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. <i>Polyhedron</i> , 2013, 50, 314-320.	1.0	41
65	Exploring the performance limits of MOF/polymer MMMs for O ₂ /N ₂ separation using computational screening. <i>Journal of Membrane Science</i> , 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. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 14124-14138.	1.8	40
67	Recent advances in sustainable syngas production by catalytic CO ₂ reforming of ethanol and glycerol. <i>Sustainable Energy and Fuels</i> , 2020, 4, 1029-1047.	2.5	40
68	MOF Membranes for CO ₂ Capture: Past, Present and Future. <i>Carbon Capture Science & Technology</i> , 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. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 32134-32148.	4.0	39
70	High-Throughput Screening of COF Membranes and COF/Polymer MMMs for Helium Separation and Hydrogen Purification. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 21738-21749.	4.0	38
71	Computational assessment of MOF membranes for CH ₄ /H ₂ separations. <i>Journal of Membrane Science</i> , 2016, 514, 313-321.	4.1	37
72	Molecular Simulation Study of CH ₄ /H ₂ Mixture Separations Using Metal Organic Framework Membranes and Composites. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13047-13054.	1.5	36

#	ARTICLE	IF	CITATIONS
73	An unusual 3D metal-organic framework, $\{[Ag_4(\frac{1}{4}\text{-pzdc})_2(\frac{1}{4}\text{-en})_2]\cdot n\text{H}_2\text{O}\}_n$: Câ€™Hâˆ’Ag, Nâ€™Hâˆ’Ag and (Oâ€™H)âˆ’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 CO ₂ /H ₂ Separation. Journal of Physical Chemistry C, 2020, 124, 22577-22590.	1.5	36
76	Oxalamide-Functionalized Metal Organic Frameworks for CO ₂ 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 CO ₂ 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][PF ₆]-Incorporated UiO-66 and NH ₂ -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 H ₂ /CH ₄ 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 CO ₂ /N ₂ 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 CO ₂ /CH ₄ separation. Molecular Systems Design and Engineering, 2020, 5, 532-543.	1.7	31
84	Computational Modeling of bio-MOFs for CO ₂ /CH ₄ separations. Chemical Engineering Science, 2015, 130, 120-128.	1.9	30
85	Recent advances in materials for high purity H ₂ 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 O ₂ /N ₂ Selectivity in Metal-Organic Frameworks via High-Throughput Computational Screening and Machine Learning. ACS Applied Materials & Interfaces, 2022, 14, 736-749.	4.0	30
89	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.	1.4	29
90	Computational screening of ZIFs for CO ₂ separations. Molecular Simulation, 2015, 41, 713-726.	0.9	28

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

#	ARTICLE	IF	CITATIONS
109	Application of MD Simulations to Predict Membrane Properties of MOFs. <i>Journal of Nanomaterials</i> , 2015, 2015, 1-9.	1.5	21
110	A phytochemical-containing metal-organic framework: Synthesis, characterization and molecular simulations for hydrogen adsorption. <i>Inorganica Chimica Acta</i> , 2015, 427, 138-143.	1.2	21
111	Gas adsorption and diffusion in a highly CO ₂ /N ₂ selective metal-organic framework: molecular simulations. <i>Molecular Simulation</i> , 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. <i>Microporous and Mesoporous Materials</i> , 2020, 306, 110446.	2.2	20
113	Effect of Metal-Organic Framework (MOF) Database Selection on the Assessment of Gas Storage and Separation Potentials of MOFs. <i>Angewandte Chemie</i> , 2021, 133, 7907-7916.	1.6	20
114	Soil remediation via an ionic liquid and supercritical CO ₂ . <i>Chemical Engineering and Processing: Process Intensification</i> , 2008, 47, 1693-1704.	1.8	19
115	A new approach for predicting gas separation performances of MOF membranes. <i>Journal of Membrane Science</i> , 2016, 519, 45-54.	4.1	19
116	High-Throughput Screening of Metal Organic Frameworks as Fillers in Mixed Matrix Membranes for Flue Gas Separation. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900109.	1.3	19
117	Analysis of CH ₄ Uptake over Metal-Organic Frameworks Using Data-Mining Tools. <i>ACS Combinatorial Science</i> , 2019, 21, 257-268.	3.8	19
118	Doubling CO ₂ /N ₂ separation performance of CuBTC by incorporation of 1-n-ethyl-3-methylimidazolium diethyl phosphate. <i>Microporous and Mesoporous Materials</i> , 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. <i>Inorganica Chimica Acta</i> , 2013, 399, 19-35.	1.2	18
120	Gas adsorption/separation properties of metal directed self-assembly of two coordination polymers with 5-nitroisophthalate. <i>Journal of Solid State Chemistry</i> , 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. <i>CrystEngComm</i> , 2013, 15, 1244.	1.3	17
122	Revealing the effect of structure curations on the simulated CO ₂ separation performances of MOFs. <i>Materials Advances</i> , 2020, 1, 341-353.	2.6	17
123	Computational Methods for MOF/Polymer Membranes. <i>Chemical Record</i> , 2016, 16, 703-718.	2.9	16
124	An Integrated Computational-Experimental Hierarchical Approach for the Rational Design of an IL/UiO-66 Composite Offering Infinite CO ₂ Selectivity. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	16
125	Computational Screening of MOF-Based Mixed Matrix Membranes for CO ₂ /N ₂ Separations. <i>Journal of Nanomaterials</i> , 2016, 2016, 1-12.	1.5	15
126	Enhanced Water Purification Performance of Ionic Liquid Impregnated Metal-Organic Framework: Dye Removal by [BMIM][PF ₆]/MIL-53(Al) Composite. <i>Frontiers in Chemistry</i> , 2020, 8, 622567.	1.8	14

#	ARTICLE	IF	CITATIONS
127	Combined GCMC, MD, and DFT Approach for Unlocking the Performances of COFs for Methane Purification. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 12999-13012.	1.8	14
128	[BMIM][OAc] coating layer makes activated carbon almost completely selective for CO ₂ . <i>Chemical Engineering Journal</i> , 2022, 437, 135436.	6.6	14
129	Zr-MOFs for CF ₄ /CH ₄ , CH ₄ /H ₂ , and CH ₄ /N ₂ separation: towards the goal of discovering stable and effective adsorbents. <i>Molecular Systems Design and Engineering</i> , 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. <i>Synthetic Metals</i> , 2011, 161, 2471-2480.	2.1	12
131	Multi-scale computational screening to accelerate discovery of IL/COF composites for CO ₂ /N ₂ separation. <i>Separation and Purification Technology</i> , 2022, 287, 120578.	3.9	12
132	A three-dimensional silver(I) framework assembled from 3,3- α^2 -thiodipropionate: Synthesis, structure and molecular simulations for hydrogen gas adsorption. <i>Polyhedron</i> , 2012, 45, 103-106.	1.0	11
133	Effects of molecular simulation parameters on predicting gas separation performance of ZIFs. <i>Journal of Chemical Technology and Biotechnology</i> , 2015, 90, 1707-1718.	1.6	11
134	The role of ovarian reserve markers in prediction of clinical pregnancy. <i>Journal of Obstetrics and Gynaecology</i> , 2017, 37, 492-497.	0.4	11
135	MOF adsorbents for flue gas separation: Comparison of material ranking approaches. <i>Chemical Engineering Research and Design</i> , 2022, 179, 308-318.	2.7	11
136	Hypothetical yet effective: Computational identification of high-performing MOFs for CO ₂ capture. <i>Computers and Chemical Engineering</i> , 2022, 160, 107705.	2.0	11
137	Different dimensionality in Mn(II), Co(II) and Ni(II) aminoisophthalate metal-organic compounds: Synthesis, characterization and gas adsorption properties. <i>Polyhedron</i> , 2012, 48, 199-211.	1.0	10
138	In Silico Design of Metal Organic Frameworks with Enhanced CO ₂ Separation Performances: Role of Metal Sites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28255-28265.	1.5	10
139	Molecular simulations of porous coordination network-based mixed matrix membranes for CO ₂ /N ₂ separations. <i>Molecular Simulation</i> , 2015, 41, 1396-1408.	0.9	9
140	Selection rules for estimating the solubility of C ₄ -hydrocarbons in imidazolium ionic liquids determined by machine-learning tools. <i>Journal of Molecular Liquids</i> , 2019, 284, 511-521.	2.3	9
141	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. <i>Polyhedron</i> , 2015, 100, 108-113.	1.0	8
142	Screening for selectivity. <i>Nature Energy</i> , 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. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 484001.	0.7	8
144	Molecular Modeling of MOF-based Mixed Matrix Membranes. <i>Current Organic Chemistry</i> , 2014, 18, 2364-2380.	0.9	8

#	ARTICLE	IF	CITATIONS
145	Enhanced water stability and high CO ₂ storage capacity of a Lewis basic sites-containing zirconium metal-organic framework. Dalton Transactions, 2021, 50, 16587-16592.	1.6	8
146	Computational insights into efficient CO ₂ and H ₂ S capture through zirconium MOFs. Journal of CO ₂ Utilization, 2022, 55, 101811.	3.3	8
147	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.	0.8	6
148	Reply to Comment on "Database for CO ₂ Separation Performances of MOFs Based on Computational Materials Screening". ACS Applied Materials & Interfaces, 2019, 11, 16266-16271.	4.0	4
149	Exploring covalent organic frameworks for H ₂ S+CO ₂ separation from natural gas using efficient computational approaches. Journal of CO ₂ Utilization, 2022, 62, 102077.	3.3	4
150	Recent Advances in Molecular Dynamics Simulations of Gas Diffusion in Metal Organic Frameworks. , O, , .		3
151	Metal Exchange Boosts the CO ₂ 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 SO ₂ Capture. Journal of Physical Chemistry C, 2022, 126, 9875-9888.	1.5	2
153	Molecular Simulations for Adsorption-Based CO ₂ 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 CO ₂ Capture. , 2021, , 205-238.		0
156	Molecular Modeling of Metal-Organic Frameworks for Carbon Dioxide Separation Applications. , 2015, , 339-379.		0