

Using molecular simulation to characterise metal-organic applications

Chemical Society Reviews

38, 1237

DOI: [10.1039/b803498m](https://doi.org/10.1039/b803498m)

Citation Report

#	ARTICLE	IF	CITATIONS
5	Preferred Hydrogen Adsorption Sites in Various MOFs—A Comparative Computational Study. <i>ChemPhysChem</i> , 2009, 10, 2647-2657.	1.0	75
6	Mixed-ligand coordination polymers constructed from flexible 2,2'-biphenyldicarboxylate and rigid isomeric bipyridines. <i>Polyhedron</i> , 2009, 28, 2997-3004.	1.0	4
7	Novel 3-dimensional sixfold interpenetrating diamondoid networks of copper(I) coordination polymers of polypyridyl ligands—Syntheses, characterization and crystal structures. <i>Inorganic Chemistry Communication</i> , 2009, 12, 1227-1230.	1.8	14
8	Two-Dimensional Networks of Lanthanide Cubane-Shaped Dumbbells. <i>Inorganic Chemistry</i> , 2009, 48, 11748-11754.	1.9	67
9	An Ab Initio Force Field for Predicting Hydrogen Storage in IRMOF Materials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21815-21824.	1.5	47
10	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. <i>CrystEngComm</i> , 2009, 11, 2272.	1.3	217
11	Heats of Adsorption for Seven Gases in Three Metal-Organic Frameworks: Systematic Comparison of Experiment and Simulation. <i>Langmuir</i> , 2009, 25, 7383-7388.	1.6	212
12	Studies of Capillary Phase Transitions of Methane in Metal-Organic Frameworks by Gauge Cell Monte Carlo Simulation. <i>Langmuir</i> , 2010, 26, 5160-5166.	1.6	8
13	Comment on Comparative Molecular Simulation Study of CO ₂ /N ₂ and CH ₄ /N ₂ Separation in Zeolites and Metal-Organic Frameworks. <i>Langmuir</i> , 2010, 26, 2975-2978.	1.6	39
14	Understanding gas separation in metal-organic frameworks using computer modeling. <i>Journal of Materials Chemistry</i> , 2010, 20, 10308.	6.7	80
15	MOFs, MILs and more: concepts, properties and applications for porous coordination networks (PCNs). <i>New Journal of Chemistry</i> , 2010, 34, 2366.	1.4	1,039
16	Hydrogen physisorption in metal-organic frameworks: concepts and quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 259-270.	0.5	18
17	CO ₂ adsorption, selectivity and water tolerance of pillared-layer metal organic frameworks. <i>Microporous and Mesoporous Materials</i> , 2010, 132, 305-310.	2.2	103
18	Molecular simulations of very high pressure hydrogen storage using metal-organic frameworks. <i>Microporous and Mesoporous Materials</i> , 2010, 135, 178-186.	2.2	21
19	New Microporous Materials for Acetylene Storage and C ₂ H ₂ /CO ₂ Separation: Insights from Molecular Simulations. <i>ChemPhysChem</i> , 2010, 11, 2220-2229.	1.0	118
20	A High Heat of Adsorption for Hydrogen in Magnesium Formate. <i>ChemSusChem</i> , 2010, 3, 758-761.	3.6	27
21	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
22	Three New Polycatenation Networks Based on 4,4'-Oxybis(benzoate) and Bis(imidazole) Ligands: Synthesis, Structure and Photoluminescence. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5478-5483.	1.0	29

#	ARTICLE	IF	CITATIONS
23	Engineering Homochiral Metal-Organic Frameworks for Heterogeneous Asymmetric Catalysis and Enantioselective Separation. <i>Advanced Materials</i> , 2010, 22, 4112-4135.	11.1	800
24	Modellierung von Adsorption, Diffusion und katalysierten Reaktionen in porösen Medien. <i>Chemie-Ingenieur-Technik</i> , 2010, 82, 881-890.	0.4	4
25	Metal-Organic Frameworks with Exceptionally High Methane Uptake: Where and How is Methane Stored?. <i>Chemistry - A European Journal</i> , 2010, 16, 5205-5214.	1.7	227
27	Carbon Dioxide Capture: Prospects for New Materials. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6058-6082.	7.2	3,452
28	In silico screening of zeolite membranes for CO ₂ capture. <i>Journal of Membrane Science</i> , 2010, 360, 323-333.	4.1	280
29	Homoleptic silver-bis(pyridine) coordination polymers: [Ag(L1) ₂](PF ₆), [Ag(L1) ₂](SbF ₆), [Ag(L1) ₂](BF ₄), [Ag(L2)](PF ₆), and [Ag(L3)1.5](CF ₃ SO ₃)(H ₂ O) ₂ {L1=(4-py)-CHN-C ₁₀ H ₆ -NCH(4-py); L2=(2-py)-CHN-C ₁₀ H ₆ -NCH(2-py); L3=(3-py)-CHN-C ₁₄ H ₁₂ -NCH(3-py)}. <i>Polyhedron</i> , 2010, 29, 2731-2738.	1.0	23
30	Atomistic theoretical models for nanoporous hybrid materials. <i>Microporous and Mesoporous Materials</i> , 2010, 129, 304-318.	2.2	46
31	Cobalt coordination polymers of flexible bis(pyridine)-type ligands containing an intervening cyclohexyl group: [Co(L1)1.5(NO ₃) ₂], [Co(L2)1.5(NO ₃) ₂], [Co(L1-H ₂) ₂ (NO ₃)](NO ₃) ₅ (CH ₃ OH), and [Co(L2-H ₂)(NO ₃) ₂ (OCH ₃) ₂] {(n-py)CHNC ₆ H ₁₀ NCH(n-py) [n=3 (L1) or 4 (L2)]; (m-py)CH ₂ NHC ₆ H ₁₀ NHCH ₂ (m-py) [m=3 (L1) or 4 (L2)]}. <i>Journal of Molecular Structure</i> , 2010, 975, 247-255.	1.8	10
32	Molecular simulation of hydrogen adsorption in metal-organic frameworks. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2010, 357, 35-42.	2.3	33
33	De novo synthesis of a metal-organic framework material featuring ultrahigh surface area and gas storage capacities. <i>Nature Chemistry</i> , 2010, 2, 944-948.	6.6	1,535
35	Rational synthesis and characterization of porous Cu(ii) coordination polymers. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2519.	1.3	38
36	Rational Design, Synthesis, Purification, and Activation of Metal-Organic Framework Materials. <i>Accounts of Chemical Research</i> , 2010, 43, 1166-1175.	7.6	1,259
37	Aspects of crystal structure prediction: some successes and some difficulties. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8580.	1.3	21
38	Multiscale simulation and modelling of adsorptive processes for energy gas storage and carbon dioxide capture in porous coordination frameworks. <i>Energy and Environmental Science</i> , 2010, 3, 1469.	15.6	138
39	A General Approach for Estimating Framework Charges in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5035-5042.	1.5	118
40	Molecular Simulations and Experimental Studies of CO ₂ , CO, and N ₂ Adsorption in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15735-15740.	1.5	169
41	The Behavior of Flexible MIL-53(Al) upon CH ₄ and CO ₂ Adsorption. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22237-22244.	1.5	197
42	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3354-3359.	2.1	166

#	ARTICLE	IF	CITATIONS
43	Highlighting a Variety of Unusual Characteristics of Adsorption and Diffusion in Microporous Materials Induced by Clustering of Guest Molecules. <i>Langmuir</i> , 2010, 26, 8450-8463.	1.6	55
44	Novel Functionalized Metal-Organic Framework Based on Unique Hexagonal Prismatic Clusters. <i>Inorganic Chemistry</i> , 2010, 49, 8647-8649.	1.9	31
45	Molecular dynamics simulations of stability of metal-organic frameworks against H ₂ O using the ReaxFF reactive force field. <i>Chemical Communications</i> , 2010, 46, 5713.	2.2	121
46	A Porous Metal-Organic Replica of PbO_2 for Capture of Nerve Agent Surrogate. <i>Journal of the American Chemical Society</i> , 2010, 132, 17996-17999.	6.6	66
47	Computational and Experimental Studies on the Adsorption of CO, N ₂ , and CO ₂ on Mg-MOF-74. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11185-11191.	1.5	307
48	An Adaptable Peptide-Based Porous Material. <i>Science</i> , 2010, 329, 1053-1057.	6.0	356
49	Pore Space Partition and Charge Separation in Cage-within-Cage Indium-Organic Frameworks with High CO ₂ Uptake. <i>Journal of the American Chemical Society</i> , 2010, 132, 17062-17064.	6.6	339
50	First-Principles-Derived Force Field for Copper Paddle-Wheel-Based Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14402-14409.	1.5	85
51	Construction of Three Metal-Organic Frameworks Based on Multifunctional T-Shaped Tripodal Ligands, H ₃ PylmDC. <i>Crystal Growth and Design</i> , 2010, 10, 3489-3495.	1.4	82
52	Sorbents for CO ₂ capture from flue gas— aspects from materials and theoretical chemistry. <i>Nanoscale</i> , 2010, 2, 1819.	2.8	213
53	Direct Observation and Quantification of CO ₂ Binding Within an Amine-Functionalized Nanoporous Solid. <i>Science</i> , 2010, 330, 650-653.	6.0	860
54	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
55	Zeolitic Imidazolate Frameworks as H ₂ Adsorbents: Ab Initio Based Grand Canonical Monte Carlo Simulation. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12039-12047.	1.5	57
56	Accurate Prediction of Hydrogen Adsorption in Metal-Organic Frameworks with Unsaturated Metal Sites via a Combined Density-Functional Theory and Molecular Mechanics Approach. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19116-19126.	1.5	46
57	Molecular Understanding for the Adsorption of Water and Alcohols in Hydrophilic and Hydrophobic Zeolitic Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11542-11550.	1.5	111
58	Unusual Adsorption Behavior on Metal-Organic Frameworks. <i>Langmuir</i> , 2010, 26, 14694-14699.	1.6	52
59	Evaluation of Energy Heterogeneity in Metal-Organic Frameworks: Absence of Henry's Region in MIL-53 and MIL-68 Materials?. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17665-17674.	1.5	17
60	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
61	Metal-Organic Framework MIL-101 for Adsorption and Effect of Terminal Water Molecules: From Quantum Mechanics to Molecular Simulation. <i>Langmuir</i> , 2010, 26, 8743-8750.	1.6	113
62	Functionalization of Coordination Nanochannels for Controlling Tacticity in Radical Vinyl Polymerization. <i>Journal of the American Chemical Society</i> , 2010, 132, 4917-4924.	6.6	108
63	Computational screening of metal-organic frameworks for large-molecule chemical sensing. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12621.	1.3	83
64	4-Carboxylphthalhydrazidate-bridged layered Pb(II) coordination polymers. <i>CrystEngComm</i> , 2010, 12, 1850.	1.3	28
65	A new Cd ₄ -2,4-pyridinedicarboxylate layered coordination polymer consisting of intralayer cavities and reversible network self-adaptation upon dehydration/moisture-absorption. <i>CrystEngComm</i> , 2010, 12, 1779.	1.3	21
66	Two unusual binodal highly-connected 3D networks constructed with multiflexible ligands. <i>CrystEngComm</i> , 2011, 13, 6071.	1.3	25
67	Molecular simulation investigation into the performance of Cu-BTC metal-organic frameworks for carbon dioxide-methane separations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20453.	1.3	25
68	Predicting Neopentane Isosteric Enthalpy of Adsorption at Zero Coverage in MCM-41. <i>Langmuir</i> , 2011, 27, 6738-6743.	1.6	8
69	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
70	Computational Study of Hydrocarbon Adsorption in Metal-Organic Framework Ni ₂ (dhtp). <i>Journal of Physical Chemistry B</i> , 2011, 115, 2842-2849.	1.2	13
71	Accurate Treatment of Electrostatics during Molecular Adsorption in Nanoporous Crystals without Assigning Point Charges to Framework Atoms. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4824-4836.	1.5	106
72	Three New Coordination Polymers Based on One Reduced Symmetry Tripodal Linker. <i>Crystal Growth and Design</i> , 2011, 11, 3115-3121.	1.4	67
73	Biofuel purification by pervaporation and vapor permeation in metal-organic frameworks: a computational study. <i>Energy and Environmental Science</i> , 2011, 4, 2107.	15.6	48
74	Metal Alkoxide Functionalization in Metal-Organic Frameworks for Enhanced Ambient-Temperature Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2066-2075.	1.5	111
75	Fluorinated and Nanoporous Graphene Materials As Sorbents for Gas Separations. <i>ACS Applied Materials & Interfaces</i> , 2011, 3, 4451-4458.	4.0	105
76	Atomistic Simulations for Adsorption, Diffusion, and Separation of Gas Mixtures in Zeolite Imidazolate Frameworks. <i>Journal of Physical Chemistry C</i> , 2011, 115, 800-807.	1.5	85
77	Biomedical Applications of Metal Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 1799-1812.	1.8	520
78	Toward Understanding Reactive Adsorption of Ammonia on Cu-MOF/Graphite Oxide Nanocomposites. <i>Langmuir</i> , 2011, 27, 13043-13051.	1.6	137

#	ARTICLE	IF	CITATIONS
79	Neutron Scattering and Spectroscopic Studies of Hydrogen Adsorption in Cr ₃ (BTC) ₂ A Metal-Organic Framework with Exposed Cr ²⁺ Sites. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8414-8421.	1.5	50
80	A Case Study of Zn ^{II} -bmb Meso-Helical Coordination Polymers upon the Spacer Angles and Lengths of Dicarboxylate Coligands. <i>Crystal Growth and Design</i> , 2011, 11, 1869-1879.	1.4	97
81	Molecular simulations for energy, environmental and pharmaceutical applications of nanoporous materials: from zeolites, metal-organic frameworks to protein crystals. <i>Chemical Society Reviews</i> , 2011, 40, 3599.	18.7	130
82	Homochiral Nickel Coordination Polymers Based on Salen(Ni) Metalloligands: Synthesis, Structure, and Catalytic Alkene Epoxidation. <i>Inorganic Chemistry</i> , 2011, 50, 2191-2198.	1.9	103
83	In silico screening of metal-organic frameworks in separation applications. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10593.	1.3	300
84	Solvent and temperature influence structural variation from nonporous 2D \rightarrow 3D parallel polycatenation to 3D microporous metal-organic framework. <i>CrystEngComm</i> , 2011, 13, 3971.	1.3	39
85	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH ₄ /H ₂ and CO ₂ /CH ₄ Mixtures in ZIFs. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12560-12566.	1.5	101
86	Functionalizing Porous Aromatic Frameworks with Polar Organic Groups for High-Capacity and Selective CO ₂ Separation: A Molecular Simulation Study. <i>Langmuir</i> , 2011, 27, 3451-3460.	1.6	124
87	An Interpenetrated Metal-Organic Framework and Its Gas Storage Behavior: Simulation and Experiment. <i>Inorganic Chemistry</i> , 2011, 50, 11055-11063.	1.9	43
88	Adsorption and Transport of CH ₄ , CO ₂ , H ₂ Mixtures in a Bio-MOF Material from Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 6833-6840.	1.5	72
89	Exploring Network Topologies of Copper Paddle Wheel Based Metal-Organic Frameworks with a First-Principles Derived Force Field. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15133-15139.	1.5	47
90	Accurate Prediction of Methane Adsorption in a Metal-Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23074-23080.	1.5	86
92	Ionic Liquid/Metal-Organic Framework Composite for CO ₂ Capture: A Computational Investigation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 21736-21742.	1.5	114
93	Synthesis, Structure, and Photoluminescent Properties of Metal-Organic Coordination Polymers Assembled with Bithiophenedicarboxylic Acid. <i>Inorganic Chemistry</i> , 2011, 50, 3198-3205.	1.9	67
94	From molecules to materials: Molecular paddle-wheel synthons of macromolecules, cage compounds and metal-organic frameworks. <i>Dalton Transactions</i> , 2011, 40, 6834.	1.6	162
95	Molecular Simulations of PIM-1-like Polymers of Intrinsic Microporosity. <i>Macromolecules</i> , 2011, 44, 6944-6951.	2.2	189
96	A Benchmark Test Set for Alchemical Free Energy Transformations and Its Use to Quantify Error in Common Free Energy Methods. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4115-4134.	2.3	123
97	X-Ray crystal structure of [HSm{VIVO(TPPS)}] _n and encapsulation of nitrogen molecules in 1-D channels. <i>Dalton Transactions</i> , 2011, 40, 12826.	1.6	18

#	ARTICLE	IF	CITATIONS
98	Computational screening of metal-organic frameworks for xenon/krypton separation. <i>AIChE Journal</i> , 2011, 57, 1759-1766.	1.8	147
99	Lanthanide, Y and Sc MOFs: where amazing crystal structures meet outstanding material properties. <i>CrystEngComm</i> , 2011, 13, 5031.	1.3	34
100	Combined volumetric, infrared spectroscopic and theoretical investigation of CO ₂ adsorption on Na-A zeolite. <i>Microporous and Mesoporous Materials</i> , 2011, 146, 97-105.	2.2	75
101	Molecular architecture based on manganese triangles: Monomer, dimer, and one-dimensional polymer. <i>Polyhedron</i> , 2011, 30, 3265-3271.	1.0	12
102	Synthesis, structural properties, and catalytic behavior of Cu-BTC and mixed-linker Cu-BTC-PyDC in the oxidation of benzene derivatives. <i>Journal of Catalysis</i> , 2011, 281, 76-87.	3.1	179
103	New pyridine-monoacylhydrazidate-coordinated transition-metal complexes. <i>Inorganica Chimica Acta</i> , 2011, 378, 72-80.	1.2	20
104	Visualisation and characterisation of voids in crystalline materials. <i>CrystEngComm</i> , 2011, 13, 1804-1813.	1.3	397
105	Reconciling the Discrepancies between Crystallographic Porosity and Guest Access As Exemplified by Zn-HKUST-1. <i>Journal of the American Chemical Society</i> , 2011, 133, 18257-18263.	6.6	195
106	Hydrogen Uptake by {H[Mg(HCOO) ₃] \cdot 2NHMe ₂ } _n and Determination of Its H ₂ Adsorption Sites through Monte Carlo Simulations. <i>Langmuir</i> , 2011, 27, 10124-10131.	1.6	21
107	Methane adsorption in PIM-1. <i>Adsorption</i> , 2011, 17, 21-26.	1.4	30
108	Liquid-phase adsorption on metal-organic frameworks. <i>Adsorption</i> , 2011, 17, 219-226.	1.4	33
109	A series of dn transition metal coordination complexes: Structures and comparative study of surface electron behaviors (n=9, 8, 7, 6, 5). <i>Inorganica Chimica Acta</i> , 2011, 368, 101-110.	1.2	25
110	Molecular simulation studies of separation of CH ₄ /H ₂ mixture in metal-organic frameworks with interpenetration and mixed-ligand. <i>Chemical Engineering Science</i> , 2011, 66, 3012-3019.	1.9	28
111	Synthesis, Structure, and Surface Photoelectric Properties of Two Novel Cobalt(II) Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 2282-2287.	0.6	10
112	Synthesis, Structures, and Adsorption Properties of Two New La ^{III} -Mg ^{II} Heterometallic Polymers. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 5299-5304.	1.0	10
113	Oberflächenchemie Metallorganischer Gerüste an der Flüssig-Grenzfläche. <i>Angewandte Chemie</i> , 2011, 123, 184-208.	1.6	43
116	Surface Chemistry of Metal-Organic Frameworks at the Liquid-Solid Interface. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 176-199.	7.2	292
117	A Metal-Organic Framework with Optimized Open Metal Sites and Pore Spaces for High Methane Storage at Room Temperature. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 3178-3181.	7.2	340

#	ARTICLE	IF	CITATIONS
118	Functional Mixed Metal-Organic Frameworks with Metalloligands. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10510-10520.	7.2	384
119	Spin Canting and Metamagnetism in the First Hybrid Cobalt-Hypoxanthine Open Framework with Topology. <i>Chemistry - A European Journal</i> , 2011, 17, 5588-5594.	1.7	41
120	Selective Palladium-Loaded MIL-101 Catalysts. <i>Chemistry - A European Journal</i> , 2011, 17, 8071-8077.	1.7	122
121	Palladium Nanoparticles Encapsulated in a Metal-Organic Framework as Efficient Heterogeneous Catalysts for Direct C2 Arylation of Indoles. <i>Chemistry - A European Journal</i> , 2011, 17, 12706-12712.	1.7	177
122	Modeling Heterogeneous Catalyzed Reactions in Porous Media. <i>Chemie-Ingenieur-Technik</i> , 2011, 83, 2188-2210.	0.4	5
123	Carbon dioxide capture-related gas adsorption and separation in metal-organic frameworks. <i>Coordination Chemistry Reviews</i> , 2011, 255, 1791-1823.	9.5	1,805
124	Towards rapid computational screening of metal-organic frameworks for carbon dioxide capture: Calculation of framework charges via charge equilibration. <i>Chemical Engineering Journal</i> , 2011, 171, 775-781.	6.6	141
125	Diffusion of CH ₄ and H ₂ in ZIF-8. <i>Journal of Membrane Science</i> , 2011, 377, 36-41.	4.1	136
126	Structural diversity of silver (I) azine complexes - Effect of substituents and counter anions. <i>Journal of Molecular Structure</i> , 2011, 1000, 29-34.	1.8	6
127	New 4,5-dichlorophthalhydrazidate-bridged chained coordination polymers. <i>Journal of Solid State Chemistry</i> , 2011, 184, 667-674.	1.4	30
128	Applications of a general random-walk theory for confined diffusion. <i>Physical Review E</i> , 2011, 83, 011120.	0.8	32
129	Molecular simulation of CO ₂ , N ₂ and CH ₄ adsorption and separation in ZIF-78 and ZIF-79. <i>Molecular Simulation</i> , 2011, 37, 1131-1142.	0.9	26
130	Zeolitic imidazolate framework-7 as an ultra-selective nanofilter for H ₂ purification: atomistic simulation study. <i>Molecular Simulation</i> , 2012, 38, 830-837.	0.9	3
131	Crystal structure of aqua-[(2,2'-bipyridine)]-(2,4-dihydropyrimidine-5-carboxylato)] perchloratocopper(II), Cu(H ₂ O)(C ₁₀ H ₈ N ₂)(C ₅ H ₃ N ₂ O ₄)(ClO ₄), C ₁₅ H ₁₃ ClCuN ₄ O ₉ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2012, 227, 365-366.	0.1	0
132	Synthesis, structures, and luminescent properties of four new 3D lanthanide metal-organic frameworks with fluorescent whitener, 4,4'-biphenyldicarboxylate and 1,10-phenanthroline. <i>Inorganic Chemistry Communication</i> , 2012, 24, 114-117.	1.8	11
133	Influence of sterically non-hindering methyl groups on adsorption properties of two classical zinc and copper MOF types. <i>Comptes Rendus Chimie</i> , 2012, 15, 866-877.	0.2	17
134	Prediction of Structure and Properties of Boron-Based Covalent Organic Frameworks by a First-Principles Derived Force Field. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4921-4929.	1.5	52
135	CO ₂ Adsorption in Mono-, Di- and Trivalent Cation-Exchanged Metal-Organic Frameworks: A Molecular Simulation Study. <i>Langmuir</i> , 2012, 28, 3903-3910.	1.6	39

#	ARTICLE	IF	CITATIONS
136	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
137	Prediction of CO ₂ Adsorption Properties in Zeolites Using Force Fields Derived from Periodic Dispersion-Corrected DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10692-10701.	1.5	123
138	Characterization and Comparison of the Performance of IRMOF-1, IRMOF-8, and IRMOF-10 for CO ₂ Adsorption in the Subcritical and Supercritical Regimes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22938-22946.	1.5	25
139	New monoacylhydrazidate-coordinated Mn ²⁺ and Pb ²⁺ compounds. <i>Dalton Transactions</i> , 2012, 41, 6137.	1.6	25
140	New metal complexes with di(mono)acylhydrazidate molecules. <i>Dalton Transactions</i> , 2012, 41, 10267.	1.6	18
141	Experimental and theoretical investigations on the MMOF selectivity for CO ₂ vs. N ₂ in flue gas mixtures. <i>Dalton Transactions</i> , 2012, 41, 4232.	1.6	31
142	Synthesis, structural characterization and photoluminescence property of four di(mono)acylhydrazidate-coordinated Cd ²⁺ and Zn ²⁺ compounds. <i>CrystEngComm</i> , 2012, 14, 8162.	1.3	20
143	Hydrogen thermal desorption spectra: insights from molecular simulation. <i>Dalton Transactions</i> , 2012, 41, 3974.	1.6	8
144	New photoluminescence acylhydrazidate-coordinated complexes. <i>Dalton Transactions</i> , 2012, 41, 2382-2392.	1.6	37
145	An Extended Charge Equilibration Method. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2506-2511.	2.1	253
146	Synthesis and Crystal Structure of a New Co(II) Complex With Surface Photoelectric Property. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2012, 42, 818-822.	0.6	1
147	Calculation and visualization of free energy barriers for several VOCs and TNT in HKUST-1. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15438.	1.3	13
148	Predicting Large CO ₂ Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture. <i>Journal of the American Chemical Society</i> , 2012, 134, 18940-18943.	6.6	129
149	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metal-Organic Frameworks: The Effect of Lateral Interactions for Methane/CPO-27-Mg. <i>Journal of the American Chemical Society</i> , 2012, 134, 18354-18365.	6.6	90
150	Toward Rational Design of Metal-Organic Frameworks for Sensing Applications: Efficient Calculation of Adsorption Characteristics in Zero Loading Regime. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3025-3033.	1.5	48
151	Single-Walled Polytetrazolate Metal-Organic Channels with High Density of Open Nitrogen-Donor Sites and Gas Uptake. <i>Journal of the American Chemical Society</i> , 2012, 134, 784-787.	6.6	169
152	Grand Canonical Monte Carlo Simulation of Low-Pressure Methane Adsorption in Nanoporous Framework Materials for Sensing Applications. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3492-3502.	1.5	30
153	Novel characterization of the adsorption sites in large pore metal-organic frameworks: combination of X-ray powder diffraction and thermal desorption spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12892.	1.3	12

#	ARTICLE	IF	CITATIONS
154	Improving Predictions of Gas Adsorption in Metal-Organic Frameworks with Coordinatively Unsaturated Metal Sites: Model Potentials, ab initio Parameterization, and GCMC Simulations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18899-18909.	1.5	102
155	Catalysis by a Zinc-Porphyrin-Based Metal-Organic Framework: From Theory to Computational Design. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23494-23502.	1.5	33
156	Accelerating Applications of Metal-Organic Frameworks for Gas Adsorption and Separation by Computational Screening of Materials. <i>Langmuir</i> , 2012, 28, 14114-14128.	1.6	202
157	Computer-Aided Design of Interpenetrated Tetrahydrofuran-Functionalized 3D Covalent Organic Frameworks for CO ₂ Capture. <i>Crystal Growth and Design</i> , 2012, 12, 5349-5356.	1.4	37
158	Insights from theoretical calculations on structure, dynamics, phase behavior and hydrogen sorption in nanoporous metal organic frameworks. <i>Computational and Theoretical Chemistry</i> , 2012, 987, 42-56.	1.1	14
159	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
160	Discovering the Active Sites for C3 Separation in MIL-100(Fe) by Using Operando IR Spectroscopy. <i>Chemistry - A European Journal</i> , 2012, 18, 11959-11967.	1.7	97
161	Syntheses, Crystal Structures, and Properties of Lead(II), Zinc(II), and Manganese(II) Complexes Constructed from 2, 3, 5, 6-Tetraiodo-1, 4-benzenedicarboxylic Acid. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, n/a-n/a.	0.6	1
162	Synthesis and structure of silver coordination polymer with extended ditopic ligand containing terminal amino groups [Ag(C ₂₄ H ₂₈ N ₂) _{1.5}]NO ₃ . <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 953-958.	0.3	6
163	Computational Study of Adsorption and Separation of CO ₂ , CH ₄ , and N ₂ by an <i>ir</i> -Type Metal-Organic Framework. <i>Langmuir</i> , 2012, 28, 12122-12133.	1.6	102
164	Adsorption of Hydrocarbons in Metal-Organic Frameworks: A Force Field Benchmark on the Example of Benzene in Metal-Organic Framework 5. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15369-15377.	1.5	14
165	Metal-organic frameworks in mixed-matrix membranes for gas separation. <i>Dalton Transactions</i> , 2012, 41, 14003.	1.6	442
166	Luminescent Properties of Metal-Organic Framework MOF-5: Relativistic Time-Dependent Density Functional Theory Investigations. <i>Inorganic Chemistry</i> , 2012, 51, 12389-12394.	1.9	106
167	Multicomponent Adsorption of Alcohols onto Silicalite-1 from Aqueous Solution: Isotherms, Structural Analysis, and Assessment of Ideal Adsorbed Solution Theory. <i>Langmuir</i> , 2012, 28, 15566-15576.	1.6	71
168	Ion Exchange in Metal-Organic Framework for Water Purification: Insight from Molecular Simulation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6925-6931.	1.5	77
169	Anion Modulated Structural Diversification in the Assembly of Cd(II) Complexes Based on a Balance-like Dipodal Ligand. <i>Crystal Growth and Design</i> , 2012, 12, 2389-2396.	1.4	25
170	Accurate Computation of Gas Uptake in Microporous Organic Molecular Crystals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8865-8871.	1.5	41
171	Adsorption of selected gases on metal-organic frameworks and covalent organic frameworks: A comparative grand canonical Monte Carlo simulation. <i>Journal of Applied Physics</i> , 2012, 111, 112628.	1.1	20

#	ARTICLE	IF	CITATIONS
172	Atomically Detailed Models for Transport of Gas Mixtures in ZIF Membranes and ZIF/Polymer Composite Membranes. <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 3091-3100.	1.8	36
173	Ab Initio Parametrized Force Field for the Flexible Metal-Organic Framework MIL-53(Al). <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3217-3231.	2.3	69
174	Single-Layer [Cu ₂ Br(IN) ₂] _n Coordination Polymer (CP): Electronic and Magnetic Properties, and Implication for Molecular Sensors. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4119-4125.	1.5	27
175	Understanding nanofluid stability through molecular simulation. <i>Chemical Physics Letters</i> , 2012, 551, 115-120.	1.2	10
176	Recent development of in silico molecular modeling for gas and liquid separations in metal-organic frameworks. <i>Current Opinion in Chemical Engineering</i> , 2012, 1, 138-144.	3.8	19
177	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
178	Review and Analysis of Molecular Simulations of Methane, Hydrogen, and Acetylene Storage in Metal-Organic Frameworks. <i>Chemical Reviews</i> , 2012, 112, 703-723.	23.0	1,085
179	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. II. Adsorption of atomic and molecular fluids in a porous material. <i>Journal of Chemical Physics</i> , 2012, 136, 184108.	1.2	41
180	Metal-Organic Frameworks for Separations. <i>Chemical Reviews</i> , 2012, 112, 869-932.	23.0	5,588
181	Mesoporous metal-organic framework materials. <i>Chemical Society Reviews</i> , 2012, 41, 1677-1695.	18.7	830
182	Two- and Three-Dimensional Divalent Metal Coordination Polymers Constructed from a New Tricarboxylate Linker and Dipyridyl Ligands. <i>Crystal Growth and Design</i> , 2012, 12, 4649-4657.	1.4	34
183	Temperature-Dependent Structures of Lanthanide Metal-Organic Frameworks Based on Furan-2,5-Dicarboxylate and Oxalate. <i>Crystal Growth and Design</i> , 2012, 12, 3263-3270.	1.4	76
184	Coordination-Chemistry Control of Proton Conductivity in the Iconic Metal-Organic Framework Material HKUST-1. <i>Journal of the American Chemical Society</i> , 2012, 134, 51-54.	6.6	382
185	A Porous Metal-Organic Framework Based on Triazoledicarboxylate Ligands - Synthesis, Structure, and Gas-Sorption Studies. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3562-3568.	1.0	18
186	Protein-based carbon capture: progress and potential. , 2012, 2, 223-238.		12
187	Finding MOFs for Highly Selective CO ₂ /N ₂ Adsorption Using Materials Screening Based on Efficient Assignment of Atomic Point Charges. <i>Journal of the American Chemical Society</i> , 2012, 134, 4313-4323.	6.6	187
188	Commensurate Adsorption of Hydrocarbons and Alcohols in Microporous Metal Organic Frameworks. <i>Chemical Reviews</i> , 2012, 112, 836-868.	23.0	985
189	Well-studied Cu-BTC still serves surprises: evidence for facile Cu ²⁺ /Cu ⁺ interchange. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4383.	1.3	91

#	ARTICLE	IF	CITATIONS
190	Large-scale computational screening of metal-organic frameworks for CH ₄ /H ₂ separation. <i>AICHE Journal</i> , 2012, 58, 2078-2084.	1.8	91
192	Homochiral Metal-Organic Frameworks for Asymmetric Heterogeneous Catalysis. <i>Chemical Reviews</i> , 2012, 112, 1196-1231.	23.0	2,699
193	Large-scale screening of hypothetical metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 83-89.	6.6	1,098
194	Zinc and cadmium coordination polymers assembled with 2,2'-bipyridine and bithiophenedicarboxylic acid: Effect of metal ions on the conformation of ligand. <i>Inorganica Chimica Acta</i> , 2012, 383, 185-189.	1.2	18
195	Two new 3-D photoluminescence metal-organic frameworks based on cubane Cu ₄ clusters as tetrahedral nodes. <i>Inorganica Chimica Acta</i> , 2012, 384, 287-292.	1.2	16
196	Prediction of a new leveler (N-butyl-methyl piperidinium bromide) for through-hole electroplating using molecular dynamics simulations. <i>Electrochemistry Communications</i> , 2012, 18, 104-107.	2.3	57
197	Epitaxially grown metal-organic frameworks. <i>Materials Today</i> , 2012, 15, 110-116.	8.3	117
198	Computational screening of homochiral metal-organic frameworks for enantioselective adsorption. <i>Microporous and Mesoporous Materials</i> , 2012, 157, 118-123.	2.2	32
199	Atomistic models for disordered nanoporous carbons using reactive force fields. <i>Microporous and Mesoporous Materials</i> , 2012, 154, 24-37.	2.2	76
200	Borromean-Entanglement-Driven Assembly of Porous Molecular Architectures with Anion-Modified Pore Space. <i>Chemistry - A European Journal</i> , 2012, 18, 1924-1931.	1.7	36
201	Competition and Cooperativity in Carbon Dioxide Sorption by Amine-Functionalized Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1826-1829.	7.2	131
202	CO ₂ Adsorption in Porous Materials. , 2013, , 535-558.		1
203	Lithium-Functionalized Metal-Organic Frameworks that Show >10 wt% H ₂ Uptake at Ambient Temperature. <i>ChemPhysChem</i> , 2013, 14, 2698-2703.	1.0	6
204	Adsorption in Metal-Organic Frameworks. , 2013, , 989-1006.		3
205	Carbon Dioxide Capture and Activation ¹¹ This chapter was prepared using literature published before April, 2011.. , 2013, , 475-504.		1
206	Two new Cu(II) complexes constructed by mixed-organic tectonics: Structures, magnetic properties and photocatalytic degradation of organic dyes. <i>Inorganic Chemistry Communication</i> , 2013, 36, 137-140.	1.8	24
207	Molecular Mechanisms of Water-Mediated Proton Transport in MIL-53 Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19508-19516.	1.5	42
208	Gabapentin Coordination Networks: Mechanochemical Synthesis and Behavior under Shelf Conditions. <i>Crystal Growth and Design</i> , 2013, 13, 5007-5017.	1.4	11

#	ARTICLE	IF	CITATIONS
209	H ₂ , N ₂ , and CH ₄ Gas Adsorption in Zeolitic Imidazolate Framework-95 and -100: Ab Initio Based Grand Canonical Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24407-24416.	1.5	51
210	Grafting of hydrophilic ethylene glycols or ethylenediamine on coordinatively unsaturated metal sites in MIL-100(Cr) for improved water adsorption characteristics. <i>Inorganica Chimica Acta</i> , 2013, 407, 145-152.	1.2	75
211	Adsorption of C ₁ –C ₄ Alcohols in Zeolitic Imidazolate Framework-8: Effects of Force Fields, Atomic Charges, and Framework Flexibility. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25628-25635.	1.5	70
212	A microporous metal–organic open framework containing uncoordinated carbonyl groups as postsynthetic modification sites for cation exchange and Tb ³⁺ sensing. <i>Chemical Communications</i> , 2013, 49, 6897.	2.2	112
213	Computational screening of porous carbons, zeolites, and metal organic frameworks for desulfurization and decarburization of biogas, natural gas, and flue gas. <i>AIChE Journal</i> , 2013, 59, 2928-2942.	1.8	77
214	Effects of nitro-functionalization on the gas adsorption properties of isoreticular metal-organic framework-eight (IRMOF-8). <i>Microporous and Mesoporous Materials</i> , 2013, 177, 82-90.	2.2	18
215	New highly ordered hydrophobic siloxane-based coordination polymers. <i>Polymer</i> , 2013, 54, 6096-6104.	1.8	20
216	First principles derived, transferable force fields for CO ₂ adsorption in Na-exchanged cationic zeolites. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12882.	1.3	79
217	Thermal Conductivity of Zeolitic Imidazolate Framework-8: A Molecular Simulation Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18441-18447.	1.5	117
218	Fast and Accurate Electrostatics in Metal Organic Frameworks with a Robust Charge Equilibration Parameterization for High-Throughput Virtual Screening of Gas Adsorption. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3056-3061.	2.1	90
219	Functionalized metal–organic framework MIL-101 for CO ₂ capture: multi-scale modeling from ab initio calculation and molecular simulation to breakthrough prediction. <i>CrystEngComm</i> , 2013, 15, 10358.	1.3	36
220	Computational studies on the adsorption of CO ₂ in the flexible perfluorinated metal–organic framework zinc 1,2-bis(4-pyridyl)ethane tetrafluoroterephthalate. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 176-182.	1.3	11
221	Coordination polymers via self-assembly of silver(i) and cis-bis-nitrile-oxa-bowl derivatives. <i>CrystEngComm</i> , 2013, 15, 9623.	1.3	9
222	Adsorption and Diffusion of Small Alcohols in Zeolitic Imidazolate Frameworks ZIF-8 and ZIF-90. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3169-3176.	1.5	135
223	Gas adsorption and diffusion in a highly CO ₂ selective metal–organic framework: molecular simulations. <i>Molecular Simulation</i> , 2013, 39, 14-24.	0.9	20
224	A rare alb-4,8-Cmce metal–organic coordination network based on tetrazolate and phosphonate functionalized 1,3,5,7-tetraphenyladamantane. <i>CrystEngComm</i> , 2013, 15, 1235.	1.3	42
225	Molecular simulation studies of reversed-phase liquid chromatography. <i>Journal of Chromatography A</i> , 2013, 1287, 60-82.	1.8	96
226	On the Thermodynamics of Refrigerant + Heterogeneous Solid Surfaces Adsorption. <i>Langmuir</i> , 2013, 29, 14494-14502.	1.6	26

#	ARTICLE	IF	CITATIONS
227	Synthesis, structure and properties of zinc(II) coordination polymers with 9H-carbazole-2,7-dicarboxylic acid. <i>Journal of Solid State Chemistry</i> , 2013, 206, 293-299.	1.4	13
228	Copper(I) and silver(I) coordination assemblies of imino-pyridyl and azino-pyridyl ligands: Syntheses, crystal structures, spectroscopic and photophysical properties. <i>Inorganica Chimica Acta</i> , 2013, 404, 131-143.	1.2	17
229	The hydrogen storage capacity of mono-substituted MOF-5 derivatives: An experimental and computational approach. <i>Microporous and Mesoporous Materials</i> , 2013, 171, 65-71.	2.2	30
230	An Adsorbent Performance Indicator as a First Step Evaluation of Novel Sorbents for Gas Separations: Application to Metal-Organic Frameworks. <i>Langmuir</i> , 2013, 29, 3301-3309.	1.6	131
231	Experimental Screening of Porous Materials for High Pressure Gas Adsorption and Evaluation in Gas Separations: Application to MOFs (MIL-100 and CAU-10). <i>ACS Combinatorial Science</i> , 2013, 15, 111-119.	3.8	48
232	Water Sorption Cycle Measurements on Functionalized MIL-101Cr for Heat Transformation Application. <i>Chemistry of Materials</i> , 2013, 25, 790-798.	3.2	238
233	Porous NbO-type metal-organic framework with inserted acylamide groups exhibiting highly selective CO ₂ capture. <i>CrystEngComm</i> , 2013, 15, 3517.	1.3	99
234	Molecular simulations to understand and to design porous organic molecules. <i>Current Opinion in Solid State and Materials Science</i> , 2013, 17, 19-30.	5.6	42
235	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7613-7622.	1.5	79
236	Metal-organic frameworks as platforms for clean energy. <i>Energy and Environmental Science</i> , 2013, 6, 1656.	15.6	858
237	Large-Scale Quantitative Structure-Property Relationship (QSPR) Analysis of Methane Storage in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7681-7689.	1.5	174
238	Carbon Dioxide Capture by PAFs and an Efficient Strategy To Fast Screen Porous Materials for Gas Separation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8353-8364.	1.5	62
239	Methoxy-Modified MOF-5: A MOF-5 Framework Prepared by a Mixed Ligand Approach. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2336-2341.	1.0	12
240	Screening metal-organic frameworks for selective noble gas adsorption in air: effect of pore size and framework topology. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9093.	1.3	92
241	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
242	Toward Effective CO ₂ /CH ₄ Separations by Sulfur-Containing PIMs via Predictive Molecular Simulations. <i>Macromolecules</i> , 2013, 46, 5371-5380.	2.2	58
243	Gas adsorption by nanoporous materials: Future applications and experimental challenges. <i>MRS Bulletin</i> , 2013, 38, 412-421.	1.7	65
244	Complexities in modeling of heterogeneous catalytic reactions. <i>Computers and Mathematics With Applications</i> , 2013, 65, 1674-1697.	1.4	39

#	ARTICLE	IF	CITATIONS
245	Development of Computational Methodologies for Metal-Organic Frameworks and Their Application in Gas Separations. <i>Chemical Reviews</i> , 2013, 113, 8261-8323.	23.0	448
246	Cooperative Carbon Capture Capabilities in Multivariate MOFs Decorated with Amino Acid Side Chains: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14717-14722.	1.5	13
247	MOF-EFF – A flexible first-principles derived force field for metal-organic frameworks. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 1128-1141.	0.7	162
248	Predicting the impact of functionalized ligands on CO ₂ adsorption in MOFs: A combined DFT and Grand Canonical Monte Carlo study. <i>Microporous and Mesoporous Materials</i> , 2013, 168, 225-238.	2.2	47
249	Effect of Room-Temperature Ionic Liquids on CO ₂ Separation by a Cu-BTC Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20762-20768.	1.5	84
250	Hydrothermal syntheses, crystal structures and luminescence properties of zinc(II) and cadmium(II) coordination polymers based on bifunctional 3,2,6-terpyridine-4-carboxylic acid. <i>Journal of Solid State Chemistry</i> , 2013, 198, 416-423.	1.4	17
251	A novel route for preparing highly proton conductive membrane materials with metal-organic frameworks. <i>Chemical Communications</i> , 2013, 49, 143-145.	2.2	130
252	Correlation of Gas Permeability in a Metal-Organic Framework MIL-101(Cr)-Polysulfone Mixed-Matrix Membrane with Free Volume Measurements by Positron Annihilation Lifetime Spectroscopy (PALS). <i>Membranes</i> , 2013, 3, 331-353.	1.4	62
253	MOFIA: a cheminformatic webserver for the prediction of CO ₂ adsorption in metal organic frameworks (MOF). <i>Materials Research Society Symposia Proceedings</i> , 2013, 1523, 801.	0.1	0
254	3D Organization of Dysprosium Cubanes. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 5879-5885.	1.0	29
255	Four Coordination Polymers Containing 2,6-Naphthalenedicarboxylic Acid and 1,10-Phenanthroline: Synthesis, Structure, and Magnetic Properties. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2013, 639, 626-632.	0.6	12
256	Computational studies of adsorption in metal organic frameworks and interaction of nanoparticles in condensed phases. <i>Molecular Simulation</i> , 2014, 40, 571-584.	0.9	21
257	Exploring the interplay between ligand and topology in zeolitic imidazolate frameworks with computational chemistry. <i>Molecular Simulation</i> , 2014, 40, 25-32.	0.9	7
258	A fluorescent 3-D metal-organic framework with unusual tetranuclear zinc secondary building units. <i>Journal of Coordination Chemistry</i> , 2014, 67, 3484-3491.	0.8	12
259	Adsorption of hydrogen in covalent organic frameworks using expanded Wang-Landau simulations. <i>Molecular Simulation</i> , 2014, 40, 71-79.	0.9	15
261	Atomistic modeling toward high-efficiency carbon capture: A brief survey with a few illustrative examples. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 163-175.	1.0	14
262	Metal-organic frameworks based on terephthalic acid: Sorbents of organic dyes. <i>Russian Journal of Applied Chemistry</i> , 2014, 87, 1065-1069.	0.1	5
263	Synthesis, structures, characterization and antimicrobial activity of two novel coordination complexes derived from 2-naphthoxyacetic acid. <i>Journal of the Iranian Chemical Society</i> , 2014, 11, 1321-1328.	1.2	3

#	ARTICLE	IF	CITATIONS
264	Effects of substituent groups on methane adsorption in covalent organic frameworks. RSC Advances, 2014, 4, 15542.	1.7	13
265	Towards imaging electron density inside metal-organic framework structures. Chemical Communications, 2014, 50, 2271.	2.2	7
266	Adsorption-based characterization of hierarchical metal-organic frameworks. Adsorption, 2014, 20, 349-357.	1.4	7
267	Synthesis, Crystal Structure, and Properties of a 3D Cu(I) Coordination Polymer Based on Cu ₃ (CN) ₂ Clusters and 1,3-Di-(1,2,4-Triazole-4-yl)Benzene. Journal of Cluster Science, 2014, 25, 1137-1145.	1.7	10
268	Quantum chemistry investigation of rigid A-IRMOF-MO series (A=zinc, cadmium, and alkaline-earth) properties. Microporous and Mesoporous Materials, 2014, 183, 218-233.	2.2	18
269	High-throughput computational screening of metal-organic frameworks. Chemical Society Reviews, 2014, 43, 5735-5749.	18.7	336
270	Adsorption and Dynamics in Hierarchical Metal-Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 7423-7433.	1.5	25
271	Noble Gas Adsorption in Metal-Organic Frameworks Containing Open Metal Sites. Journal of Physical Chemistry C, 2014, 118, 11685-11698.	1.5	165
272	Multinuclear-based copper coordination architectures constructed from pyridyl-1H-benzimidazol-derived flexible tripodal connector and the magnetic behaviors. Polyhedron, 2014, 78, 1-9.	1.0	6
273	Metal-Organic Frameworks for Air Purification of Toxic Chemicals. Chemical Reviews, 2014, 114, 5695-5727.	23.0	825
274	Stabilization of Scandium Terephthalate MOFs against Reversible Amorphization and Structural Phase Transition by Guest Uptake at Extreme Pressure. Journal of the American Chemical Society, 2014, 136, 8606-8613.	6.6	63
275	Enhanced noble gas adsorption in Ag@MOF-74Ni. Chemical Communications, 2014, 50, 466-468.	2.2	153
276	Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N ₂ and CH ₄ . Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
277	Porous Inorganic Membranes for CO ₂ Capture: Present and Prospects. Chemical Reviews, 2014, 114, 1413-1492.	23.0	481
278	Recent developments in first-principles force fields for molecules in nanoporous materials. Journal of Materials Chemistry A, 2014, 2, 274-291.	5.2	126
279	A pyridyl-carboxylate type linking ligand containing an intervening amide group and its cadmium and nickel coordination polymers: (3-py)-C(O)NH-C ₆ H ₄ -CH ₂ -COOH (HL), {[CdL ₂](H ₂ O)} _n , and {[NiL ₂ (H ₂ O)](H ₂ O)} _n . Polyhedron, 2014, 69, 197-204.	1.0	5
280	Polyoxometallates trapped in a zeolitic imidazolate framework leading to high uptake and selectivity of bioactive molecules. Journal of Materials Chemistry A, 2014, 2, 2168-2173.	5.2	102
281	Comparison of generic force fields for packing of concave molecules. Molecular Physics, 2014, 112, 2241-2248.	0.8	3

#	ARTICLE	IF	CITATIONS
282	Ferromagnetic interaction and slow magnetic relaxation in a Co ₃ cluster-based three-dimensional framework. Dalton Transactions, 2014, 43, 47-50.	1.6	25
283	Structure–property relationships of water adsorption in metal–organic frameworks. New Journal of Chemistry, 2014, 38, 3102-3111.	1.4	252
284	Force field for ZIF-8 flexible frameworks: atomistic simulation of adsorption, diffusion of pure gases as CH ₄ , H ₂ , CO ₂ and N ₂ . RSC Advances, 2014, 4, 16503-16511.	1.7	64
285	Parallel Monte Carlo simulation in the canonical ensemble on the graphics processing unit. International Journal of Parallel, Emergent and Distributed Systems, 2014, 29, 379-400.	0.7	4
286	Water Stability and Adsorption in Metal–Organic Frameworks. Chemical Reviews, 2014, 114, 10575-10612.	23.0	1,951
287	Monte Carlo Modeling of Carbon Dioxide Adsorption in Porous Aromatic Frameworks. Langmuir, 2014, 30, 4147-4156.	1.6	19
288	Molecular simulations in metal–organic frameworks for diverse potential applications. Molecular Simulation, 2014, 40, 516-536.	0.9	31
289	Tuning CO ₂ Selective Adsorption over N ₂ and CH ₄ in UiO-67 Analogues through Ligand Functionalization. Inorganic Chemistry, 2014, 53, 9254-9259.	1.9	239
290	Construction of Three Novel Coordination Complexes by 3-Nitrophthalic Acid Plus N-Donor Ligands: Synthesis, Structure, and Properties. Molecular Crystals and Liquid Crystals, 2014, 593, 214-231.	0.4	0
291	Investigation of SO ₂ gas adsorption in metal–organic frameworks by molecular simulation. Inorganic Chemistry Communication, 2014, 46, 277-281.	1.8	42
292	Perspective of microporous metal–organic frameworks for CO ₂ capture and separation. Energy and Environmental Science, 2014, 7, 2868.	15.6	693
293	Microstructure-Dependent Gas Adsorption: Accurate Predictions of Methane Uptake in Nanoporous Carbons. Journal of Chemical Theory and Computation, 2014, 10, 1-4.	2.3	22
294	A DIH-based equation for separation of CO ₂ –CH ₄ in metal–organic frameworks and covalent–organic materials. Journal of Materials Chemistry A, 2014, 2, 11341.	5.2	28
295	Ionomers of Intrinsic Microporosity: In Silico Development of Ionic-Functionalized Gas-Separation Membranes. Langmuir, 2014, 30, 12039-12048.	1.6	21
296	Metal–Organic Frameworks for Oxygen Storage. Angewandte Chemie - International Edition, 2014, 53, 14092-14095.	7.2	106
297	Molecular simulations of physical and chemical adsorption under gas and liquid environments using force field- and quantum mechanics-based methods. Molecular Simulation, 2014, 40, 678-689.	0.9	9
298	Transferable Force Field for Metal–Organic Frameworks from First-Principles: BTW-FF. Journal of Chemical Theory and Computation, 2014, 10, 4644-4652.	2.3	93
299	Programming MIL-101Cr for selective and enhanced CO ₂ adsorption at low pressure by postsynthetic amine functionalization. Dalton Transactions, 2014, 43, 1338-1347.	1.6	69

#	ARTICLE	IF	CITATIONS
300	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9643-9655.	1.3	57
301	A three-dimensional porous and magnetic framework constructed from copper salt and 5-Methyltetrazole: [Cu ₈ (Metz) ₉](OH)·xH ₂ O. <i>Journal of the Iranian Chemical Society</i> , 2014, 11, 847-852.	1.2	5
302	Adsorption of metal ions by clays and inorganic solids. <i>RSC Advances</i> , 2014, 4, 28537-28586.	1.7	101
303	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO ₂ Capture. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3056-3060.	2.1	234
304	Complexing agent study via computational chemistry for environmentally friendly silver electrodeposition and the application of a silver deposit. <i>RSC Advances</i> , 2014, 4, 40930-40940.	1.7	43
305	Functional materials derived from open framework templates/precursors: synthesis and applications. <i>Energy and Environmental Science</i> , 2014, 7, 2071.	15.6	619
306	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5383-5389.	1.5	84
307	Coordination polymers with nucleobases: From structural aspects to potential applications. <i>Coordination Chemistry Reviews</i> , 2014, 276, 34-58.	9.5	101
308	Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8. <i>Microporous and Mesoporous Materials</i> , 2014, 194, 190-199.	2.2	75
309	The seventh industrial fluid properties simulation challenge. <i>Fluid Phase Equilibria</i> , 2014, 366, 136-140.	1.4	5
312	Computational Approaches to the Design, Crystal Structure Prediction, and Structure-Property Relationships of Metal-Organic Frameworks. , 2015, , 1-52.		0
313	Structural, energetic and dynamic insights into the abnormal xylene separation behavior of hierarchical porous crystal. <i>Scientific Reports</i> , 2015, 5, 11537.	1.6	29
314	Probing the Structural Stability of and Enhanced CO ₂ Storage in MOF MIL-68(In) under High Pressures by FTIR Spectroscopy. <i>Chemistry - A European Journal</i> , 2015, 21, 18739-18748.	1.7	15
315	Synthesis, Structures, and Luminescent Properties of Two Four-connected Polymers Based on 2,2-Dimethylsuccinic Acid. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015, 641, 1906-1910.	0.6	4
316	Exploiting Large-Pore Metal-Organic Frameworks for Separations through Entropic Molecular Mechanisms. <i>ChemPhysChem</i> , 2015, 16, 2046-2067.	1.0	27
317	Effect of chemical functionalization groups on Zr ₆ -AzoBDC to enhance H ₂ , CH ₄ storage and CO ₂ capture: a theoretical investigation. <i>Advances in Natural Sciences: Nanoscience and Nanotechnology</i> , 2015, 6, 035011.	0.7	0
318	Structural diversity of coordination polymers controlled by the metal ion as the sole reaction variable. <i>CrystEngComm</i> , 2015, 17, 4462-4468.	1.3	13
319	Function-led design of new porous materials. <i>Science</i> , 2015, 348, aaa8075.	6.0	1,272

#	ARTICLE	IF	CITATIONS
320	Using neutron powder diffraction and first-principles calculations to understand the working mechanisms of porous coordination polymer sorbents. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 648-660.	0.5	7
321	Carbon Capture and Storage—, 2015, , 329-366.		5
322	Silver-tetrapyrrolyl coordination polymers: [Ag ₂ (L)](NO ₃) ₂ (H ₂ O) ₂ , [Ag(L)](PF ₆), and [Ag ₂ (L)](CH ₂ Cl) ₂ {L = 1,1,2,2-tetrakis(4-(pyridin-3-yl)phenyl)ethene}. <i>Polyhedron</i> , 2015, 87, 338-348.	1.0	7
323	A New Class of Cuprous Bromide Cluster-Based Hybrid Materials: Direct Observation of the Stepwise Replacement of Hydrogen Bonds by Coordination Bonds. <i>Inorganic Chemistry</i> , 2015, 54, 554-559.	1.9	19
324	Direct Measurement of Adsorbed Gas Redistribution in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2015, 137, 2919-2930.	6.6	40
325	Methane Uptakes in Covalent Organic Frameworks with Double Halogen Substitution. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2010-2014.	1.5	24
326	From Inorganic to Organic Strategy To Design Porous Aromatic Frameworks for High-Capacity Gas Storage. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3260-3267.	1.5	15
327	Gas Adsorption and Separation in Realistic and Idealized Frameworks of Organic Pillared Graphene: A Comparative Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1980-1987.	1.5	29
328	A UiO-66 analogue with uncoordinated carboxylic acids for the broad-spectrum removal of toxic chemicals. <i>New Journal of Chemistry</i> , 2015, 39, 2396-2399.	1.4	133
329	Efficient synthesis of aluminum- and zinc-containing metal-organic frameworks. <i>Inorganic Materials</i> , 2015, 51, 236-240.	0.2	3
330	Adsorption of hexavalent chromium by metal organic frameworks from aqueous solution. <i>Journal of Industrial and Engineering Chemistry</i> , 2015, 28, 211-216.	2.9	199
331	Investigation of bio-removing metal ions from wastewater—a viewpoint of micro forces. <i>Desalination and Water Treatment</i> , 2015, 56, 2118-2130.	1.0	2
332	CO ₂ capture in metal-organic frameworks: multiscale modeling from molecular simulation to breakthrough prediction. <i>Journal of Materials Chemistry A</i> , 2015, 3, 16327-16336.	5.2	20
333	Anion-dependent copper(II) coordination polymers based on 1,3-di-(1,2,4-triazole-4-yl)benzene: Syntheses and crystal structures. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2015, 41, 339-344.	0.3	3
334	Aminopyridine derivatives controlled the assembly and various properties of Cu-BTC metal-organic frameworks. <i>Dalton Transactions</i> , 2015, 44, 14008-14018.	1.6	18
335	Co(II)/Mn(II)/Cu(II) Coordination Polymers Based on Flexible 5,5'-(hexane-1,6-diyl)-bis(oxy)diisophthalic Acid: Crystal Structures, Magnetic Properties, and Catalytic Activity. <i>Crystal Growth and Design</i> , 2015, 15, 2712-2722.	1.4	20
336	Zinc-Formate Metal-Organic Frameworks: Watch Out for Reactive Solvents. <i>Journal of Chemical Crystallography</i> , 2015, 45, 178-188.	0.5	10
337	Insights on the physical adsorption of hydrogen and methane in UiO series of MOFs using molecular simulations. <i>Computational and Theoretical Chemistry</i> , 2015, 1061, 36-45.	1.1	18

#	ARTICLE	IF	CITATIONS
339	Amide-containing zinc(ii) metal-organic layered networks: a structure-CO ₂ capture relationship. <i>Inorganic Chemistry Frontiers</i> , 2015, 2, 477-484.	3.0	15
340	Non-covalent Interactions of CO ₂ with Functional Groups of Metal-Organic Frameworks from a CCSD(T) Scheme Applicable to Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1574-1584.	2.3	32
341	Crystalline Capsules: Metal-Organic Frameworks Locked by Size-Matching Ligand Bolts. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5966-5970.	7.2	135
342	Combined experimental and theoretical insight into the drug delivery of nanoporous metal-organic frameworks. <i>RSC Advances</i> , 2015, 5, 85606-85612.	1.7	21
343	Are Quantum Chemistry Semiempirical Methods Effective to Predict Solid State Structure and Adsorption in Metal Organic Frameworks?. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23398-23406.	1.5	24
344	A Comparison of Barostats for the Mechanical Characterization of Metal-Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5583-5597.	2.3	83
345	Intermolecular interaction energies in transition metal coordination compounds. <i>CrystEngComm</i> , 2015, 17, 9300-9310.	1.3	19
346	Transferable force fields for adsorption of small gases in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24048-24055.	1.3	30
347	DFT-based force field development for noble gas adsorption in metal organic frameworks. <i>Journal of Materials Chemistry A</i> , 2015, 3, 23539-23548.	5.2	33
348	A combined experimental and computational study of novel nanocage-based metal-organic frameworks for drug delivery. <i>Dalton Transactions</i> , 2015, 44, 19370-19382.	1.6	83
349	Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2015, 3, 22432-22440.	5.2	64
350	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
351	Opportunities and challenges of MOF-based membranes in gas separations. <i>Separation and Purification Technology</i> , 2015, 152, 207-237.	3.9	233
352	Modelling Gas Adsorption in Porous Solids: Roles of Surface Chemistry and Pore Architecture. <i>Journal of Chemical Sciences</i> , 2015, 127, 1687-1699.	0.7	7
353	Nitrogen-doped porous aromatic frameworks for enhanced CO ₂ adsorption. <i>Journal of Colloid and Interface Science</i> , 2015, 438, 191-195.	5.0	32
354	A Combined Theoretical and Experimental Study for Silver Electroplating. <i>Scientific Reports</i> , 2014, 4, 3837.	1.6	35
355	Propane simulated in silica pores: Adsorption isotherms, molecular structure, and mobility. <i>Chemical Engineering Science</i> , 2015, 121, 292-299.	1.9	43
356	Atomic charges for modeling metal-organic frameworks: Why and how. <i>Journal of Solid State Chemistry</i> , 2015, 223, 144-151.	1.4	47

#	ARTICLE	IF	CITATIONS
357	Review of Recent Developments in CO ₂ Capture Using Solid Materials: Metal Organic Frameworks (MOFs)., 0, , .		17
358	Grand Canonical Monte Carlo Simulation of Nitrogen Adsorption in a Silica Aerogel Model. Computation, 2016, 4, 18.	1.0	5
359	Bio-Inspired Metal-Organic Frameworks in the Pharmaceutical World: A Brief Review. , 0, , .		5
360	Molecular Simulations for Adsorption-Based CO ₂ Separation Using Metal Organic Frameworks. , 2016, , .		0
361	Study of the Discrepancies between Crystallographic Porosity and Guest Access into Cadmium-Imidazolate Frameworks and Tunable Luminescence Properties by Incorporation of Lanthanides. Chemistry - A European Journal, 2016, 22, 6905-6913.	1.7	26
362	Computational Evaluation of the Impact of Incorporated Nitrogen and Oxygen Heteroatoms on the Affinity of Polyaromatic Ligands for Carbon Dioxide and Methane in Metal-Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 27342-27348.	1.5	9
363	Adsorption Properties of MFM-400 and MFM-401 with CO ₂ and Hydrocarbons: Selectivity Derived from Directed Supramolecular Interactions. Inorganic Chemistry, 2016, 55, 7219-7228.	1.9	41
364	Outlook and challenges for hydrogen storage in nanoporous materials. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	1.1	129
365	The Eighth Industrial Fluids Properties Simulation Challenge. Adsorption Science and Technology, 2016, 34, 3-12.	1.5	3
366	Molecular simulation of CH ₄ , CO ₂ , H ₂ O and N ₂ molecules adsorption on heterogeneous surface models of coal. Applied Surface Science, 2016, 389, 894-905.	3.1	121
367	Olefin/Paraffin Separation Potential of ZIF-9 and ZIF-71: A Combined Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2016, 2016, 4440-4449.	1.0	33
368	Noria: A Highly Xe-Selective Nanoporous Organic Solid. Chemistry - A European Journal, 2016, 22, 12618-12623.	1.7	48
369	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. Langmuir, 2016, 32, 12664-12675.	1.6	33
370	Influence of Pore Dimension on the Host-Guest Interaction in Metal-Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 27319-27327.	1.5	15
371	A Combined Experimental and Theoretical Study on the Extraction of Uranium by Amino-Derived Metal-Organic Frameworks through Post-Synthetic Strategy. ACS Applied Materials & Interfaces, 2016, 8, 31032-31041.	4.0	161
372	Mechanistic insight into the displacement of CH ₄ by CO ₂ in calcite slit nanopores: the effect of competitive adsorption. RSC Advances, 2016, 6, 104456-104462.	1.7	44
373	Multiscale Computational Study on the Adsorption and Separation of CO ₂ /CH ₄ and CO ₂ /H ₂ on Li ⁺ -Doped Mixed-Ligand Metal-Organic Framework Zn ₂ (NDC) ₂ (diPyNI). ChemPhysChem, 2016, 17, 4124-4133.	1.0	20
374	A porous magnesium metal-organic framework showing selective adsorption and separation of nitrile guest molecules. RSC Advances, 2016, 6, 104451-104455.	1.7	7

#	ARTICLE	IF	CITATIONS
375	Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory. Chemistry - A European Journal, 2016, 22, 18045-18050.	1.7	11
376	What can molecular simulation do for global warming?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 173-197.	6.2	32
377	Adsorption Methodology. , 0, , 575-605.		1
378	Conversion of Ni Nd and Ni Tb compartment compounds into one-dimensional coordination polymers or tetranuclear dimers. Polyhedron, 2016, 117, 231-243.	1.0	12
379	Computation of the Heat and Entropy of Adsorption in Proximity of Inflection Points. Journal of Physical Chemistry C, 2016, 120, 1727-1738.	1.5	21
380	Towards accurate porosity descriptors based on guest-host interactions. Journal of Molecular Graphics and Modelling, 2016, 66, 91-98.	1.3	1
381	Highly Dispersed HKUST-1 on Milimeter-Sized Mesoporous Al_2O_3 Beads for Highly Effective Adsorptive Desulfurization. Industrial & Engineering Chemistry Research, 2016, 55, 7249-7258.	1.8	56
382	Tuning the Gas Separation Performance of CuBTC by Ionic Liquid Incorporation. Langmuir, 2016, 32, 1139-1147.	1.6	110
383	Composites of metal-organic frameworks and carbon-based materials: preparations, functionalities and applications. Journal of Materials Chemistry A, 2016, 4, 3584-3616.	5.2	301
384	Adsorption properties of CH_4 and CO_2 in quartz nanopores studied by molecular simulation. RSC Advances, 2016, 6, 32770-32778.	1.7	40
385	Model Study of Thermoresponsive Behavior of Metal-Organic Frameworks Modulated by Linker Functionalization. Journal of Physical Chemistry C, 2016, 120, 6835-6841.	1.5	14
386	The effects of framework dynamics on the behavior of water adsorbed in the [Zn(L)(Cl)] and Co-MOF-74 metal-organic frameworks. Physical Chemistry Chemical Physics, 2016, 18, 8196-8204.	1.3	12
387	Multiscale adsorption and transport in hierarchical porous materials. New Journal of Chemistry, 2016, 40, 4078-4094.	1.4	88
388	Superparamagnetic Luminescent $\text{MOF@Fe}_3\text{O}_4/\text{SiO}_2$ Composite Particles for Signal Augmentation by Magnetic Harvesting as Potential Water Detectors. ACS Applied Materials & Interfaces, 2016, 8, 5445-5452.	4.0	70
389	Experimental and simulation study on structural characterization and hydrogen storage of metal organic structured compounds. International Journal of Hydrogen Energy, 2016, 41, 8256-8263.	3.8	13
390	Coarse graining of force fields for metal-organic frameworks. Dalton Transactions, 2016, 45, 4370-4379.	1.6	32
391	Systematic evaluation of materials for post-combustion CO_2 capture in a Temperature Swing Adsorption process. Chemical Engineering Journal, 2016, 284, 438-447.	6.6	118
392	Computational screening of MOFs for $\text{C}_2\text{H}_6/\text{C}_2\text{H}_4$ and $\text{C}_2\text{H}_6/\text{CH}_4$ separations. Chemical Engineering Science, 2016, 139, 49-60.	1.9	64

#	ARTICLE	IF	CITATIONS
393	Effects of ionic liquid dispersion in metal-organic frameworks and covalent organic frameworks on CO ₂ capture: A computational study. <i>Chemical Engineering Science</i> , 2016, 140, 1-9.	1.9	53
394	Computational characterization and prediction of metal-organic framework properties. <i>Coordination Chemistry Reviews</i> , 2016, 307, 211-236.	9.5	206
395	Effect of temperature on hydrogen and carbon dioxide adsorption hysteresis in an ultramicroporous MOF. <i>Microporous and Mesoporous Materials</i> , 2016, 219, 186-189.	2.2	35
396	Adsorption Kinetics Emulation With Lattice Gas Cellular Automata. <i>Heat Transfer Engineering</i> , 2017, 38, 409-416.	1.2	3
397	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4462-4470.	1.5	17
398	Adsorption of propylene, propane, ethylene and ethane in an isorecticular series of MOF-74 structures. <i>Adsorption</i> , 2017, 23, 507-514.	1.4	6
399	Nanoporous Materials for the Onboard Storage of Natural Gas. <i>Chemical Reviews</i> , 2017, 117, 1796-1825.	23.0	241
400	Synthesis and Structures of 1D and 2D Zn ₂ Gd Coordination Polymers: [ZnGd(L)(NO ₃) ₃] ₂ (4-ppa)(EtOH)] and [ZnGd(L)(NO ₃) ₃] ₂ (4-pca) (H ₂ L = Tj ₄ Qq1 1 6.784314 4- <i>pyridinecarboxylic acid</i>). <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 177-182.		
401	Accurate Evaluation of the Dispersion Energy in the Simulation of Gas Adsorption into Porous Zeolites. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1756-1768.	2.3	12
402	Metal-organic frameworks for H ₂ and CH ₄ storage: insights on the pore geometry-adsorption energetics relationship. <i>IUCr</i> , 2017, 4, 131-135.	1.0	33
403	CO ₂ Capture and Separations Using MOFs: Computational and Experimental Studies. <i>Chemical Reviews</i> , 2017, 117, 9674-9754.	23.0	837
404	An atomistic model of a disordered nanoporous solid: Interplay between Monte Carlo simulations and gas adsorption experiments. <i>AIP Advances</i> , 2017, 7, 045013.	0.6	3
405	A New Split Charge Equilibration Model and REPEAT Electrostatic Potential Fitted Charges for Periodic Frameworks with a Net Charge. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2858-2869.	2.3	12
406	Application of computational methods to the design and characterisation of porous molecular materials. <i>Chemical Society Reviews</i> , 2017, 46, 3286-3301.	18.7	68
407	Hybrid computational approaches for deriving quantum mechanical insights into metal-organic frameworks. <i>Tetrahedron Letters</i> , 2017, 58, 2309-2317.	0.7	15
408	Molecular simulations of adsorption and separation of acetylene and methane and their binary mixture on MOF-5, HKUST-1 and MOF-505 metal-organic frameworks. <i>Molecular Simulation</i> , 2017, 43, 260-266.	0.9	12
409	Molecular simulation of CO ₂ /CH ₄ adsorption in brown coal: Effect of oxygen-, nitrogen-, and sulfur-containing functional groups. <i>Applied Surface Science</i> , 2017, 423, 33-42.	3.1	99
410	Ab Initio Prediction of Adsorption Isotherms for Gas Mixtures by Grand Canonical Monte Carlo Simulations on a Lattice of Sites. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2713-2718.	2.1	21

#	ARTICLE	IF	CITATIONS
411	Molecular insight into the micro-behaviors of CH ₄ and CO ₂ in montmorillonite slit-nanopores. <i>Molecular Simulation</i> , 2017, 43, 1004-1011.	0.9	38
412	Establishing upper bounds on CO ₂ swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2017, 5, 12258-12265.	5.2	44
413	Metal-organic and covalent organic frameworks as single-site catalysts. <i>Chemical Society Reviews</i> , 2017, 46, 3134-3184.	18.7	861
414	Metal-organic frameworks for the removal of toxic industrial chemicals and chemical warfare agents. <i>Chemical Society Reviews</i> , 2017, 46, 3357-3385.	18.7	707
415	The right isotherms for the right reasons? Validation of generic force fields for prediction of methane adsorption in metal-organic frameworks. <i>Molecular Simulation</i> , 2017, 43, 828-837.	0.9	18
416	A Transferable Model for Adsorption in MOFs with Unsaturated Metal Sites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 441-458.	1.5	28
417	Split-Charge Equilibration Parameters for Generating Rapid Partial Atomic Charges in Metal-Organic Frameworks and Porous Polymer Networks for High-Throughput Screening. <i>Journal of Physical Chemistry C</i> , 2017, 121, 903-910.	1.5	12
418	Siloxane-based metal-organic frameworks with remarkable catalytic activity in mild environmental photodegradation of azo dyes. <i>Applied Catalysis B: Environmental</i> , 2017, 205, 78-92.	10.8	62
419	Balancing gravimetric and volumetric hydrogen density in MOFs. <i>Energy and Environmental Science</i> , 2017, 10, 2459-2471.	15.6	127
420	The coordination chemistry of N-heterocyclic carboxylic acid: A comparison of the coordination polymers constructed by 4,5-imidazoledicarboxylic acid and 1H-1,2,3-triazole-4,5-dicarboxylic acid. <i>Coordination Chemistry Reviews</i> , 2017, 352, 108-150.	9.5	104
421	Probing adsorption sites of carbon dioxide in metal organic framework of [Zn(bdc)(dpds)] _n : A molecular simulation study. <i>Chemical Physics</i> , 2017, 497, 1-9.	0.9	4
422	CO ₂ adsorption and separation in covalent organic frameworks with interlayer slipping. <i>CrystEngComm</i> , 2017, 19, 6950-6963.	1.3	51
423	New lanthanide(III) coordination polymers: synthesis, structural features, and catalytic activity in CO ₂ fixation. <i>Dalton Transactions</i> , 2017, 46, 16426-16431.	1.6	28
424	Statistical Mechanical Model for Adsorption Coupled with SAFT-VR Mie Equation of State. <i>Langmuir</i> , 2017, 33, 11291-11298.	1.6	29
425	Theoretical Simulation of CH ₄ Separation from H ₂ in CAU-17 Materials. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20197-20204.	1.5	6
426	Porous Carbon Materials Based on Graphdiyne Basis Units by the Incorporation of the Functional Groups and Li Atoms for Superior CO ₂ Capture and Sequestration. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 30002-30013.	4.0	37
427	Machine Learning Using Combined Structural and Chemical Descriptors for Prediction of Methane Adsorption Performance of Metal Organic Frameworks (MOFs). <i>ACS Combinatorial Science</i> , 2017, 19, 640-645.	3.8	158
428	Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25309-25322.	1.5	34

#	ARTICLE	IF	CITATIONS
429	Modelling adsorption in fluorinated TKL MOFs. <i>Molecular Simulation</i> , 2017, 43, 213-221.	0.9	1
430	Structures and properties of coordination polymers with a rigid zwitterionic pyridinium-based tricarboxylate ligand. <i>Inorganica Chimica Acta</i> , 2017, 456, 207-215.	1.2	0
431	Evaluation of CH ₄ and CO ₂ adsorption on HKUST-1 and MIL-101(Cr) MOFs employing Monte Carlo simulation and comparison with experimental data. <i>Applied Thermal Engineering</i> , 2017, 110, 891-900.	3.0	66
432	Exploring mechanochemistry to turn organic bio-relevant molecules into metal-organic frameworks: a short review. <i>Beilstein Journal of Organic Chemistry</i> , 2017, 13, 2416-2427.	1.3	27
433	Porous Organic Cages. , 2017, , 139-197.		7
434	Mechanochemical Assembly of Nalidixic Acid Bioinspired Metal-Organic Compounds and Complexes toward Improved Solubility. <i>Crystal Growth and Design</i> , 2018, 18, 2067-2081.	1.4	25
435	Metal-organic framework-based materials: superior adsorbents for the capture of toxic and radioactive metal ions. <i>Chemical Society Reviews</i> , 2018, 47, 2322-2356.	18.7	1,438
436	Towards a better understanding of adsorption of indoor air pollutants in porous media—From mechanistic model to molecular simulation. <i>Building Simulation</i> , 2018, 11, 997-1010.	3.0	11
437	Computational evaluation of the impact of metal substitution on the 14CH ₄ storage in PCN-14 metal-organic frameworks. <i>Catalysis Today</i> , 2018, 312, 168-173.	2.2	4
438	Pd- and Pt- Ln complexes of a bi-compartmental ligand: [MLn(L)(NO ₃) ₃] (M = Pd, Pt; Ln = Eu, Tb); <i>Tj ETQq1 1 0.784314</i>	1.2	6
439	Rapid and selective adsorption of cationic dyes by a unique metal-organic framework with decorated pore surface. <i>Applied Surface Science</i> , 2018, 440, 1219-1226.	3.1	137
440	Syntheses, structures and photoluminescence properties of three M(II)-coordination polymers (M) <i>Tj ETQq1 1 0.784314 rgBT /Overlo</i> 145-151.	1.8	8
441	Structure and adsorptive desulfurization performance of the composite material MOF-5@AC. <i>New Journal of Chemistry</i> , 2018, 42, 3840-3850.	1.4	53
442	New functionalized IRMOF-10 with strong affinity for methanol: A simulation study. <i>Applied Surface Science</i> , 2018, 440, 351-358.	3.1	20
443	Adsorptive desulfurization of thiophene from the model fuels onto graphite oxide/metal-organic framework composites. <i>Petroleum Science and Technology</i> , 2018, 36, 141-147.	0.7	29
444	Molecular Mechanism of Loading Sulfur Hexafluoride in β -Cyclodextrin Metal-Organic Framework. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5225-5233.	1.2	24
445	Extra low friction coefficient caused by the formation of a solid-like layer: A new lubrication mechanism found through molecular simulation of the lubrication of MoS ₂ nanoslits. <i>Chinese Journal of Chemical Engineering</i> , 2018, 26, 2412-2419.	1.7	10
446	Ionic-Functionalized Polymers of Intrinsic Microporosity for Gas Separation Applications. <i>Langmuir</i> , 2018, 34, 3949-3960.	1.6	22

#	ARTICLE	IF	CITATIONS
447	Molecular simulations of adsorption and separation of ethylene/ethane and propylene/propane mixtures on Ni ₂ (dobdc) and Ni ₂ (m-dobdc) metal-organic frameworks. <i>Molecular Simulation</i> , 2018, 44, 389-395.	0.9	10
448	Gas adsorption and dynamics in Pillared Graphene Frameworks. <i>Microporous and Mesoporous Materials</i> , 2018, 257, 222-231.	2.2	31
449	Enhancing Van der Waals Interactions of Functionalized UiO-66 with Non-polar Adsorbates: The Unique Effect of para Hydroxyl Groups. <i>Chemistry - A European Journal</i> , 2018, 24, 1931-1937.	1.7	7
450	Synthesis, Structure, and Magnetic Properties of a Copper(II) Metal-Organic Framework with Biphenyl-2,2',4,4'-tetracarboxylic Acid. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 109-113.	0.6	1
452	A charge-separated diamondoid metal-organic framework. <i>Chemical Communications</i> , 2018, 54, 12654-12657.	2.2	11
453	CO ₂ capture and separation over N ₂ and CH ₄ in nanoporous MFM-300(In, Al, Ga, and In-3N): Insight from GCMC simulations. <i>Journal of CO₂ Utilization</i> , 2018, 28, 145-151.	3.3	16
454	Reviewing Rare Earth Succinate Frameworks from the Reticular Chemistry Point of View: Structures, Nets, Catalytic and Photoluminescence Applications. <i>Israel Journal of Chemistry</i> , 2018, 58, 1044-1061.	1.0	17
455	Adsorption Thicknesses of Confined Pure and Mixing Fluids in Nanopores. <i>Langmuir</i> , 2018, 34, 12815-12826.	1.6	29
456	Molecular Modeling of Carbon Dioxide Adsorption in Metal-Organic Frameworks. , 2018, , 99-149.		6
457	Modeling Amorphous Microporous Polymers for CO ₂ Capture and Separations. <i>Chemical Reviews</i> , 2018, 118, 5488-5538.	23.0	208
458	Monte Carlo Simulations to Examine the Role of Pore Structure on Ambient Air Separation in Metal-Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 9240-9253.	1.8	14
459	Capture of CO ₂ in carbon nanotube bundles supported with room-temperature ionic liquids: A molecular simulation study. <i>Chemical Engineering Science</i> , 2018, 192, 94-102.	1.9	29
461	The First C-Cl Activation in Ullmann C-O Coupling by MOFs. <i>ChemCatChem</i> , 2018, 10, 4636-4651.	1.8	8
462	Coordination polymers and metal-organic frameworks built up with poly(tetrazolate) ligands. <i>Coordination Chemistry Reviews</i> , 2018, 372, 1-30.	9.5	74
463	On the structure of superbasic (MgO) _n sites solvated in a faujasite zeolite. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18503-18514.	1.3	7
464	Ln-MOFs using a compartmental ligand with a unique combination of hard-soft terminals and their magnetic, gas adsorption and luminescence properties. <i>CrystEngComm</i> , 2019, 21, 5665-5672.	1.3	11
465	Theoretical prediction of thermal and electronic properties of metal-organic frameworks. <i>Journal of Industrial and Engineering Chemistry</i> , 2019, 80, 136-151.	2.9	10
466	Large-scale Screening and Design of Metal-Organic Frameworks for CH ₄ /N ₂ Separation. <i>Chemistry - an Asian Journal</i> , 2019, 14, 3688-3693.	1.7	24

#	ARTICLE	IF	CITATIONS
467	Trends in Solid Adsorbent Materials Development for CO ₂ Capture. ACS Applied Materials & Interfaces, 2019, 11, 34533-34559.	4.0	215
468	Insight into Fluorocarbon Adsorption in Metal-Organic Frameworks via Experiments and Molecular Simulations. Scientific Reports, 2019, 9, 10289.	1.6	34
469	Elucidating the Interaction of CO ₂ in the Giant Metal-Organic Framework MIL-100 through Large-Scale Periodic Ab Initio Modeling. Journal of Physical Chemistry C, 2019, 123, 28677-28687.	1.5	15
470	Adsorption of Methane, Nitrogen, and Carbon Dioxide in Atomic-Scale Fractal Nanopores by Monte Carlo Simulation I: Single-Component Adsorption. Energy & Fuels, 2019, 33, 10457-10475.	2.5	14
471	Molecular simulation of flue gas and CH ₄ competitive adsorption in dry and wet coal. Journal of Natural Gas Science and Engineering, 2019, 71, 102980.	2.1	34
472	Early stages of phase selection in MOF formation observed in molecular Monte Carlo simulations. RSC Advances, 2019, 9, 14382-14390.	1.7	8
473	Electrochemical Studies and Molecular Dynamics Simulation of the Interaction between Accelerators and Cu Surface During the Electroplating Process. International Journal of Electrochemical Science, 2019, , 4705-4717.	0.5	14
474	Metal-organic frameworks (MOFs) and their composites as electrodes for lithium battery applications: Novel means for alternative energy storage. Coordination Chemistry Reviews, 2019, 393, 48-78.	9.5	198
475	Surfactants as promising media in the field of metal-organic frameworks. Coordination Chemistry Reviews, 2019, 391, 30-43.	9.5	296
476	Theoretical study of heterofullerene-linked metal-organic framework with lithium doping for CO ₂ capture and separation from CO ₂ /CH ₄ and CO ₂ /H ₂ mixtures. Microporous and Mesoporous Materials, 2019, 284, 385-392.	2.2	16
477	Schiff-base reaction induced selective sensing of trace dopamine based on a Pt ₄₁ Rh ₅₉ alloy/ZIF-90 nanocomposite. Nanotechnology, 2019, 30, 335708.	1.3	9
478	H ₂ S separation from biogas by adsorption on functionalized MIL-47-X (X = OH and OCH ₃): A simulation study. Applied Surface Science, 2019, 479, 1006-1013.	3.1	16
479	Deep neural network learning of complex binary sorption equilibria from molecular simulation data. Chemical Science, 2019, 10, 4377-4388.	3.7	38
480	Flexible and Transferable ab Initio Force Field for Zeolitic Imidazolate Frameworks: ZIF-FF. Journal of Physical Chemistry A, 2019, 123, 3000-3012.	1.1	34
481	Understanding the effect of host flexibility on the adsorption of CH ₄ , CO ₂ and SF ₆ in porous organic cages. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 547-555.	0.4	3
482	A generalized van der Waals model for light gas adsorption prediction in IRMOFs. Physical Chemistry Chemical Physics, 2019, 21, 8906-8914.	1.3	1
483	Utilization of zeolite as a potential multi-functional proppant for CO ₂ enhanced shale gas recovery and CO ₂ sequestration: A molecular simulation study on the competitive adsorption of CH ₄ and CO ₂ in zeolite and organic matter. Fuel, 2019, 249, 119-129.	3.4	17
484	In Silico Design and Characterization of Graphene Oxide Membranes with Variable Water Content and Flake Oxygen Content. ACS Nano, 2019, 13, 2995-3004.	7.3	32

#	ARTICLE	IF	CITATIONS
486	On the structure of a confined ideal gas: A statistical mechanical description with an external field. <i>Fluid Phase Equilibria</i> , 2019, 489, 99-103.	1.4	8
487	Characterization of the adsorption site energies and heterogeneous surfaces of porous materials. <i>Journal of Materials Chemistry A</i> , 2019, 7, 10104-10137.	5.2	187
488	Integration of Metal Nanoparticles into Metal-Organic Frameworks for Composite Catalysts: Design and Synthetic Strategy. <i>Small</i> , 2019, 15, e1804849.	5.2	67
489	Modeling and simulation of adsorption of methane, ethane, hydrogen sulfide and water from natural gas in (FP)YEu Metal-Organic Framework. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 579, 012020.	0.3	3
490	Integrating multiple adsorption sites and tortuous diffusion paths into a metal-organic framework for C ₃ H ₄ /C ₃ H ₆ separation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 25254-25257.	5.2	26
491	Molecular simulation of coal-fired plant flue gas competitive adsorption and diffusion on coal. <i>Fuel</i> , 2019, 239, 87-96.	3.4	64
492	Indium-Organic Frameworks Based on Dual Secondary Building Units Featuring Halogen-Decorated Channels for Highly Effective CO ₂ Fixation. <i>Chemistry of Materials</i> , 2019, 31, 1084-1091.	3.2	142
493	Pt/ZSM-22 with Partially Filled Micropore Channels as Excellent Shape-Selective Hydroisomerization Catalyst. <i>ChemCatChem</i> , 2019, 11, 1431-1436.	1.8	26
494	Anion Pillared Metal-Organic Framework Embedded with Molecular Rotors for Size-Selective Capture of CO ₂ from CH ₄ and N ₂ . <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 3138-3144.	3.2	47
495	Improving SAPO-34 performance for CO ₂ /CH ₄ separation and optimization of adsorption conditions using central composite design. <i>Separation Science and Technology</i> , 2020, 55, 1260-1276.	1.3	3
496	The effect of atomic point charges on adsorption isotherms of CO ₂ and water in metal organic frameworks. <i>Adsorption</i> , 2020, 26, 663-685.	1.4	36
497	Application of computational chemistry for adsorption studies on metal-organic frameworks used for carbon capture. <i>Physical Sciences Reviews</i> , 2020, 5, .	0.8	0
498	Recent developments in luminescent coordination polymers: Designing strategies, sensing application and theoretical evidences. <i>Coordination Chemistry Reviews</i> , 2020, 406, 213145.	9.5	366
500	Atomistic Insight Into the Host-Guest Interaction of a Photoresponsive Metal-Organic Framework. <i>Chemistry - A European Journal</i> , 2020, 26, 1263-1268.	1.7	17
501	Computational study of the effect of functionalization on natural gas components separation and adsorption in NUM-3a MOF. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107731.	1.3	8
502	Progress and potential of metal-organic frameworks (MOFs) as novel desiccants for built environment control: A review. <i>Renewable and Sustainable Energy Reviews</i> , 2020, 133, 110246.	8.2	58
503	One-pot synthesis and characterization of a dual-function hierarchical multiporous composite H ₃ PW ₁₂ O ₄₀ @HKUST-1/Al ₂ O ₃ with enhanced performance in adsorptive desulfurization and acid catalysis. <i>Journal of Coordination Chemistry</i> , 2020, 73, 2479-2498.	0.8	5
504	Effective strategy to fabricate ZIF-8@ZIF-8/polyacrylonitrile nanofibers with high loading efficiency and improved removing of Cr(VI). <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125292.	2.3	41

#	ARTICLE	IF	CITATIONS
505	A fast procedure for the estimation of the hydrogen storage capacity by cryoadsorption of metal-organic framework materials from their available porous properties. <i>International Journal of Hydrogen Energy</i> , 2020, , .	3.8	4
506	Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database. <i>Chemistry of Materials</i> , 2020, 32, 9849-9867.	3.2	132
507	Design of Zeolite-Covalent Organic Frameworks for Methane Storage. <i>Materials</i> , 2020, 13, 3322.	1.3	6
508	Screening of electroplating additive for improving throwing power of copper pyrophosphate bath via molecular dynamics simulation. <i>Chemical Physics Letters</i> , 2020, 757, 137848.	1.2	13
509	A historical overview of the activation and porosity of metal-organic frameworks. <i>Chemical Society Reviews</i> , 2020, 49, 7406-7427.	18.7	367
510	Computational Material Screening Using Artificial Neural Networks for Adsorption Gas Separation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21446-21460.	1.5	16
511	High-Performing Deep Learning Regression Models for Predicting Low-Pressure CO ₂ Adsorption Properties of Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27996-28005.	1.5	39
512	On the capture of polar indoor air pollutants at sub-ppm level—A molecular simulation study. <i>Building Simulation</i> , 2020, 13, 989-997.	3.0	9
513	Topological Descriptors Help Predict Guest Adsorption in Nanoporous Materials. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9360-9368.	1.5	33
514	Metal-Organic Frameworks against Toxic Chemicals. <i>Chemical Reviews</i> , 2020, 120, 8130-8160.	23.0	406
515	A Robotics-Inspired Screening Algorithm for Molecular Caging Prediction. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1302-1316.	2.5	6
516	Remarkable adsorption performance of MOF-199 derived porous carbons for benzene vapor. <i>Environmental Research</i> , 2020, 184, 109323.	3.7	42
517	Transfer Learning Study of Gas Adsorption in Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 34041-34048.	4.0	58
518	Standard Practices of Reticular Chemistry. <i>ACS Central Science</i> , 2020, 6, 1255-1273.	5.3	142
519	Charge-Separated and Lewis Paired Metal-Organic Framework for Anion Exchange and CO ₂ Chemical Fixation. <i>Chemistry - A European Journal</i> , 2020, 26, 13788-13791.	1.7	7
520	Impact of intrinsic framework flexibility for selective adsorption of sarin in non-aqueous solvents using metal-organic frameworks. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6441-6448.	1.3	22
521	The Chemistry of Reticular Framework Nanoparticles: MOF, ZIF, and COF Materials. <i>Advanced Functional Materials</i> , 2020, 30, 1909062.	7.8	174
523	Genetic Algorithm Design of MOF-based Gas Sensor Arrays for CO ₂ -in-Air Sensing. <i>Sensors</i> , 2020, 20, 924.	2.1	10

#	ARTICLE	IF	CITATIONS
524	Charge-Separated Metal-Organic Frameworks Derived from Boron-Centered Tetrapods. <i>Crystal Growth and Design</i> , 2020, 20, 1598-1608.	1.4	5
525	On the Universality of Capillary Condensation and Adsorption Hysteresis Phenomena in Ordered and Crystalline Mesoporous Materials. <i>Advanced Materials Interfaces</i> , 2020, 7, 2000184.	1.9	23
526	The role of flexibility in MOFs. , 2020, , 93-110.		4
527	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
528	Molecular simulation of hydrogen storage and transport in cellulose. <i>Molecular Simulation</i> , 2021, 47, 170-179.	0.9	3
529	Molecular simulation of adsorption and diffusion of CH ₄ and H ₂ O in flexible metal-organic framework ZIF-8. <i>Fuel</i> , 2021, 286, 119342.	3.4	20
530	Evaluating the purification and activation of metal-organic frameworks from a technical and circular economy perspective. <i>Coordination Chemistry Reviews</i> , 2021, 428, 213578.	9.5	28
531	Novel Systems and Membrane Technologies for Carbon Capture. <i>International Journal of Chemical Engineering</i> , 2021, 2021, 1-23.	1.4	10
532	Concluding remarks: current and next generation MOFs. <i>Faraday Discussions</i> , 2021, 231, 397-417.	1.6	17
533	Backbonding contributions to small molecule chemisorption in a metal-organic framework with open copper(<i>scp</i>) centers. <i>Chemical Science</i> , 2021, 12, 2156-2164.	3.7	21
534	Advancing Computational Analysis of Porous Materials—Modeling Three-Dimensional Gas Adsorption in Organic Gels. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1960-1969.	1.2	3
535	Molecular simulations of the adsorption and separation of hydrogen sulfide, carbon dioxide, methane, and nitrogen and their binary mixtures (H ₂ S/CH ₄), (CO ₂ /CH ₄) on NUM-3a metal-organic frameworks. <i>Journal of Molecular Modeling</i> , 2021, 27, 133.	0.8	5
536	Molecular Insight into the Swelling of a MOF: A Force-Field Investigation of Methanol Uptake in MIL-88B(Fe)-Cl. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12837-12847.	1.5	13
537	Impact of binding positions of 1,3-alternate calix[4]arene tetrabenzoic acids on geometry of coordination polymers. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 0, , 1.	0.9	0
538	25 Jahre retikuläre Chemie. <i>Angewandte Chemie</i> , 2021, 133, 24142.	1.6	6
539	Predicting hydrogen storage in MOFs via machine learning. <i>Patterns</i> , 2021, 2, 100291.	3.1	51
540	The synergistic effects of surface functional groups and pore sizes on CO ₂ adsorption by GCMC and DFT simulations. <i>Chemical Engineering Journal</i> , 2021, 415, 128824.	6.6	51
541	25 Years of Reticular Chemistry. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 23946-23974.	7.2	204

#	ARTICLE	IF	CITATIONS
542	Impact of Structural Functionalization, Pore Size, and Presence of Extra-Framework Ions on the Capture of Gaseous I ₂ by MOF Materials. <i>Nanomaterials</i> , 2021, 11, 2245.	1.9	7
543	Hydrogen Adsorption in Metal-Organic Framework MIL-101(Cr) Adsorbate Densities and Enthalpies from Sorption, Neutron Scattering, In Situ X-ray Diffraction, Calorimetry, and Molecular Simulations. <i>ACS Applied Energy Materials</i> , 2021, 4, 7839-7847.	2.5	2
544	Understanding the adsorption and separation of sulfur dioxide in flue gas by Zeolitic imidazolate frameworks via molecular simulation. <i>Chemical Physics Letters</i> , 2021, 778, 138788.	1.2	3
545	Potential application of metal-organic frameworks (MOFs) for hydrogen storage: Simulation by artificial intelligent techniques. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 36336-36347.	3.8	20
546	Analysis of energetics and economics of sub-ambient hybrid combustion carbon dioxide capture. <i>AIChE Journal</i> , 2021, 67, e17403.	1.8	7
547	Functionalized Zr-Uio-67 metal-organic frameworks: Structural landscape and application. <i>Coordination Chemistry Reviews</i> , 2021, 445, 214050.	9.5	57
548	Synthesis, identification and application of metal organic framework for removal of industrial cationic dyes. <i>Journal of Molecular Liquids</i> , 2021, 342, 117435.	2.3	56
549	ZIF-67 derived magnetic nanoporous carbon coated by poly(m-phenylenediamine) for hexavalent chromium removal. <i>Separation and Purification Technology</i> , 2021, 277, 119436.	3.9	21
550	Accurate ab initio Description of Adsorption on Coordinatively Unsaturated Sites in Metal-Organic Frameworks. , 2015, , 175-206.		3
551	Predicting Hydrogen Storage in Mofs & via Machine Learning. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
552	Modified Dual-Site Langmuir Adsorption Equilibrium Models from A GCMC Molecular Simulation. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 1311.	1.3	13
553	Novel Lanthanide Coordination Polymers Prepared by Microwave Heating: [Ln(L) ₃ (H ₂ O) ₂](H ₂ O) ₃ (Ln = Tj ETQq1 1,0,784314 rgBT /Ove	1.0	5
554	A Series of Transition-metal Coordination Complexes Assembled from 3-Nitrophthalic Acid and Thiabendazole: Synthesis, Structure and Properties. <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 218-224.	1.0	3
555	A Two-Dimensional Zinc Coordination Polymer Based on a Pyridyl-Carboxylate Linking Ligand Containing an Intervening Amide Group: [ZnCl(L)] ⁿ (HL = 6-(nicotinamido)-2-naphthoic acid). <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 2179-2182.	1.0	1
556	Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. <i>ACS Omega</i> , 2021, 6, 27898-27904.	1.6	2
557	Microwave-assisted Preparation, Structures, and Photoluminescent Properties of [Ln(NO ₃) ₃ (H ₂ O) ₂](NO ₃) ₃ (L ₂)(NO ₃) ₃ (H ₂ O) ₂ (Ln = Tb, Eu; L ₂ = 2-(4-pyridyl)ethanesulfonate, (4-pyH) ⁺ -CH ₂ -CH ₂ -SO ₃ ⁻). <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 1858-1864.	1.0	1
558	Structural Isomers of a Potential Linking Ligand Containing a Pyridyl and a Carboxylate Terminals: (n-py)-CH=N-C ₆ H ₄ -CH ₂ -COOH (n = 3, 4). <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 647-650.	1.0	1
559	Molecular Modeling of Metal-Organic Frameworks for Carbon Dioxide Separation Applications. , 2015, , 339-379.		0

#	ARTICLE	IF	CITATIONS
560	Synthesis, structure and hydrogen sorption properties of a pyrazine-bridged copper(I) nitrate metal-organic framework. <i>European Journal of Chemistry</i> , 2019, 10, 195-200.	0.3	2
561	Smart Metal-Organic Frameworks for Biotechnological Applications: A Mini-Review. <i>ACS Applied Bio Materials</i> , 2021, 4, 8159-8171.	2.3	26
562	Molecular simulation for physisorption characteristics of O ₂ in low-rank coals. <i>Energy</i> , 2022, 242, 122538.	4.5	26
563	Two-Dimensional Polymers and Polymerizations. <i>Chemical Reviews</i> , 2022, 122, 442-564.	23.0	128
564	Computational Design of MOF-Based Electronic Noses for Dilute Gas Species Detection: Application to Kidney Disease Detection. <i>ACS Sensors</i> , 2021, 6, 4425-4434.	4.0	12
565	Valorisation of glycerol through catalytic hydrogenolysis routes for sustainable production of value-added C ₃ chemicals: current and future trends. <i>Sustainable Energy and Fuels</i> , 2022, 6, 596-639.	2.5	18
566	Development of PPTA/cellulose three-layer composite insulating paper with low dielectric constant and good mechanical strength based on molecular dynamics simulation. <i>Polymer Composites</i> , 2022, 43, 1698-1710.	2.3	10
567	Are you using the right probe molecules for assessing the textural properties of metal-organic frameworks?. <i>Journal of Materials Chemistry A</i> , 2021, 10, 157-173.	5.2	33
568	Preferential adsorption sites for propane/propylene separation on ZIF-8 as revealed by solid-state NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6535-6543.	1.3	4
569	Insights into desiccant-based internally-cooled dehumidification using porous sorbents: From a modeling viewpoint. <i>Applied Energy</i> , 2022, 311, 118732.	5.1	12
570	Fabrication of metal-organic framework-mixed matrix membranes with abundant open metal sites through dual-induction mechanism. <i>Separation and Purification Technology</i> , 2022, 290, 120850.	3.9	12
571	Grand canonical Monte Carlo (GCMC) study on adsorption performance of metal organic frameworks (MOFs) for carbon capture. <i>Sustainable Materials and Technologies</i> , 2022, 32, e00383.	1.7	10
572	Polarity, thermal stability, and hydrophilicity of three-layer crosslinked PPTA/cellulose composite insulation system: Molecular dynamics simulations. <i>Materials Today Communications</i> , 2022, 31, 103533.	0.9	9
573	Discrepancy Quantification between Experimental and Simulated Data of CO ₂ Adsorption Isotherm Using Hierarchical Bayesian Estimation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
574	Stable Bimetallic Metal-Organic Framework with Dual-Functional Pyrazolate-Carboxylate Ligand: Rational Construction and C ₂ H ₂ /CO ₂ Separation. , 2022, 4, 1032-1036.		15
575	Particle size effect on the catalytic properties of zeolitic imidazolate frameworks. <i>Russian Chemical Bulletin</i> , 2022, 71, 599-612.	0.4	8
576	Deep-Learning-Based End-to-End Predictions of CO ₂ Capture in Metal-Organic Frameworks. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3281-3290.	2.5	9
577	Benchmarking various types of partial atomic charges for classical all-atom simulations of metal-organic frameworks. <i>Nanoscale</i> , 2022, 14, 9466-9473.	2.8	5

#	ARTICLE	IF	CITATIONS
578	Discrepancy quantification between experimental and simulated data of CO ₂ adsorption isotherm using hierarchical Bayesian estimation. Separation and Purification Technology, 2022, 296, 121371.	3.9	6
579	Lead(II)-Azido Metal-Organic Coordination Polymers: Synthesis, Structure and Application in PbO Nanomaterials Preparation. Nanomaterials, 2022, 12, 2257.	1.9	4
580	Ti(IV)-MOF with Specific Facet-Ag Nanoparticle Composites for Enhancing the Photocatalytic Activity and Selectivity of CO ₂ Reduction. ACS Applied Materials & Interfaces, 2022, 14, 32350-32359.	4.0	26
582	System of sequences in multivariate reticular structures. Nature Reviews Materials, 2023, 8, 331-340.	23.3	28
583	Structural study of water/alcohol mixtures adsorbed in MFI and MEL porosils. Journal of Molecular Liquids, 2022, , 120527.	2.3	0
584	Porous Materials for Water Purification. Angewandte Chemie - International Edition, 2023, 62, .	7.2	38
585	Porous Materials for Water Purification. Angewandte Chemie, 2023, 135, .	1.6	0
586	ARC-MOF: A Diverse Database of Metal-Organic Frameworks with DFT-Derived Partial Atomic Charges and Descriptors for Machine Learning. Chemistry of Materials, 2023, 35, 900-916.	3.2	20
587	Chemical transformations of highly toxic H ₂ S to promising clean energy in MOFs. Coordination Chemistry Reviews, 2023, 485, 215135.	9.5	11
588	Development of Integrated Blog-Based Teaching Materials of Dyestuffs Adsorption to Improve Students' Literacy in Chemistry. , 2023, , 157-165.		0
589	Porous Organic Cages. Chemical Reviews, 2023, 123, 4602-4634.	23.0	60
590	Green Route Synthesis and Adsorption Studies of Copper-Benzimidazole Coordination Polymer for Removal of Methyl Orange from Water. Chemistry Africa, 0, , .	1.2	1
603	Efficient SF ₆ capture and separation in robust gallium- and vanadium-based metal-organic frameworks. Journal of Materials Chemistry A, 2023, 11, 26435-26441.	5.2	0