Qingyuan Yang

List of Publications by Year
in descending order

146 papers	11,410 citations	22132 59 h-index	30058 103 g-index
147 all docs	147 docs citations	147 times ranked	10083 citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Simulation of Carbon Dioxide/Methane/Hydrogen Mixture Adsorption in Metal–Organic Frameworks. Journal of Physical Chemistry B, 2006, 110, 17776-17783.	1.2	503
2	Development of Computational Methodologies for Metal–Organic Frameworks and Their Application in Gas Separations. Chemical Reviews, 2013, 113, 8261-8323.	23.0	448
3	A Series of Isoreticular, Highly Stable, Porous Zirconium Oxide Based Metal–Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 9267-9271.	7.2	407
4	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration. Chemical Communications, 2011, 47, 9603.	2.2	345
5	An in situ self-assembly template strategy for the preparation of hierarchical-pore metal-organic frameworks. Nature Communications, 2015, 6, 8847.	5.8	309
6	A Water Stable Metal–Organic Framework with Optimal Features for CO_2 Capture. Angewandte Chemie - International Edition, 2013, 52, 10316-10320.	7.2	303
7	Confinement of Ionic Liquids in Nanocages: Tailoring the Molecular Sieving Properties of ZIF-8 for Membrane-Based CO_2 Capture. Angewandte Chemie - International Edition, 2015, 54, 15483-15487.	7.2	303
8	Influence of framework metal ions on the dye capture behavior of MIL-100 (Fe, Cr) MOF type solids. Journal of Materials Chemistry A, 2013, 1, 8534.	5.2	291
9	Molecular Simulation of Adsorption and Diffusion of Hydrogen in Metal–Organic Frameworks. Journal of Physical Chemistry B, 2005, 109, 11862-11864.	1.2	276
10	Computational Study of CO_2 Storage in Metal–Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 1562-1569.	1.5	240
11	Molecular simulation of separation of CO_2 from flue gases in CU-BTC metal–organic framework. AICHE Journal, 2007, 53, 2832-2840.	1.8	235
12	Rational construction of defects in a metal–organic framework for highly efficient adsorption and separation of dyes. Chemical Engineering Journal, 2016, 289, 486-493.	6.6	205
13	Understanding Hydrogen Adsorption in Metal–Organic Frameworks with Open Metal Sites: A Computational Study. Journal of Physical Chemistry B, 2006, 110, 655-658.	1.2	204
14	An Evaluation of UiO-66 for Gas-Based Applications. Chemistry - an Asian Journal, 2011, 6, 3270-3280.	1.7	192
15	Materials genomics methods for high-throughput construction of COFs and targeted synthesis. Nature Communications, 2018, 9, 5274.	5.8	182
16	CH4 storage and CO2 capture in highly porous zirconium oxide based metal–organic frameworks. Chemical Communications, 2012, 48, 9831.	2.2	180
17	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimental–modelling exploration. Chemical Science, 2012, 3, 1100.	3.7	176
18	Acid-functionalized UiO-66(Zr) MOFs and their evolution after intra-framework cross-linking: structural features and sorption properties. Journal of Materials Chemistry A, 2015, 3, 3294-3309.	5.2	174

#	Article	IF	Citations
19	Efficient capture of nitrobenzene from waste water using metal–organic frameworks. Chemical Engineering Journal, 2014, 246, 142-149.	6.6	168
20	Understanding the Thermodynamic and Kinetic Behavior of the CO_2/CH_4 Gas Mixture within the Porous Zirconium Terephthalate UiO-66(Zr): A Joint Experimental and Modeling Approach. Journal of Physical Chemistry C, 2011, 115, 13768-13774.	1.5	166
21	The stability and defluoridation performance of MOFs in fluoride solutions. Microporous and Mesoporous Materials, 2014, 185, 72-78.	2.2	165
22	Protic ionic liquid [Bim][NTf$_2$] with strong hydrogen bond donating ability for highly efficient ammonia absorption. Green Chemistry, 2017, 19, 937-945.	4.6	156
23	A GO-assisted method for the preparation of ultrathin covalent organic framework membranes for gas separation. Journal of Materials Chemistry A, 2016, 4, 13444-13449.	5.2	143
24	Electrostatic-Field-Induced Enhancement of Gas Mixture Separation in Metal-Organic Frameworks: A Computational Study. ChemPhysChem, 2006, 7, 1417-1421.	1.0	140
25	Mixed matrix membranes incorporated with amine-functionalized titanium-based metal-organic framework for CO2/CH4 separation. Journal of Membrane Science, 2015, 478, 130-139.	4.1	140
26	Probing the Dynamics of CO_2 and CH_4 within the Porous Zirconium Terephthalate UiO–66(Zr): A Synergic Combination of Neutron Scattering Measurements and Molecular Simulations. Chemistry - A European Journal, 2011, 17, 8882-8889.	1.7	137
27	Adsorption and separation of binary mixtures in a metal-organic framework Cu-BTC: A computational study. Separation and Purification Technology, 2008, 60, 30-35.	3.9	136
28	A robust amino-functionalized titanium(iv) based MOF for improved separation of acid gases. Chemical Communications, 2013, 49, 10082.	2.2	135
29	Novel Biological Functions of ZIF–NP as a Delivery Vehicle: High Pulmonary Accumulation, Favorable Biocompatibility, and Improved Therapeutic Outcome. Advanced Functional Materials, 2016, 26, 2715-2727.	7.8	128
30	Probing the adsorption performance of the hybrid porous MIL-68(Al): a synergic combination of experimental and modelling tools. Journal of Materials Chemistry, 2012, 22, 10210.	6.7	124
31	Two-Dimensional Covalent Triazine Framework Membrane for Helium Separation and Hydrogen Purification. ACS Applied Materials & Interfaces, 2016, 8, 8694-8701.	4.0	121
32	Enhanced Adsorption Selectivity of Hydrogen/Methane Mixtures in Metal˜Organic Frameworks with Interpenetration: A Molecular Simulation Study. Journal of Physical Chemistry C, 2008, 112, 9854-9860.	1.5	120
33	Understanding the Adsorption and Diffusion of Carbon Dioxide in Zeolitic Imidazolate Frameworks: A Molecular Simulation Study. Journal of Physical Chemistry C, 2009, 113, 5004-5009.	1.5	120
34	Li-modified metal–organic frameworks for CO_2/CH_4 separation: a route to achieving high adsorption selectivity. Journal of Materials Chemistry, 2010, 20, 706-714.	6.7	115
35	Preparation of thin film nanocomposite membranes with surface modified MOF for high flux organic solvent nanofiltration. AICHE Journal, 2017, 63, 1303-1312.	1.8	113
36	PEG-stabilized coaxial stacking of two-dimensional covalent organic frameworks for enhanced photocatalytic hydrogen evolution. Nature Communications, 2021, 12, 3934.	5.8	111

#	Article	IF	Citations
37	Revealing the Structure–Property Relationships of Metal–Organic Frameworks for CO_2 Capture from Flue Gas. Langmuir, 2012, 28, 12094-12099.	1.6	110
38	Exploring the structure-property relationships of covalent organic frameworks for noble gas separations. Chemical Engineering Science, 2017, 168, 456-464.	1.9	102
39	Pebax-based composite membranes with high gas transport properties enhanced by ionic liquids for CO_2 separation. RSC Advances, 2017, 7, 6422-6431.	1.7	100
40	High-Flux Graphene Oxide Membranes Intercalated by Metal–Organic Framework with Highly Selective Separation of Aqueous Organic Solution. ACS Applied Materials & Interfaces, 2017, 9, 1710-1718.	4.0	96
41	Crystal–State Photochromism and Dual–Mode Mechanochromism of an Organic Molecule with Fluorescence, Room–Temperature Phosphorescence, and Delayed Fluorescence. Angewandte Chemie - International Edition, 2019, 58, 16445-16450.	7.2	96
42	Large–scale computational screening of metal–organic frameworks for CH_4/H_2 separation. AICHE Journal, 2012, 58, 2078-2084.	1.8	91
43	Comparative Study of Separation Performance of COFs and MOFs for $CH_4/CO_2/H_2$ Mixtures. Industrial & Engineering Chemistry Research, 2010, 49, 2902-2906.	1.8	88
44	Ionic Liquid/Metal–Organic Framework Composites for H_2S Removal from Natural Gas: A Computational Exploration. Journal of Physical Chemistry C, 2015, 119, 3674-3683.	1.5	86
45	Adsorption and Diffusion of Light Hydrocarbons in UiO-66(Zr): A Combination of Experimental and Modeling Tools. Journal of Physical Chemistry C, 2014, 118, 27470-27482.	1.5	84
46	A hybrid zeolitic imidazolate framework membrane by mixed-linker synthesis for efficient CO_2 capture. Chemical Communications, 2013, 49, 600-602.	2.2	83
47	Few-layered ultrathin covalent organic framework membranes for gas separation: a computational study. Journal of Materials Chemistry A, 2016, 4, 124-131.	5.2	83
48	Theoretical investigation of gas separation in functionalized nanoporous graphene membranes. Applied Surface Science, 2017, 407, 532-539.	3.1	80
49	Computational Study on the Influences of Framework Charges on CO_2 Uptake in Metal–Organic Frameworks. Industrial & Engineering Chemistry Research, 2009, 48, 10479-10484.	1.8	76
50	Adsorption Behavior of Metal–Organic Frameworks for Thiophenic Sulfur from Diesel Oil. Industrial & Engineering Chemistry Research, 2012, 51, 12449-12455.	1.8	73
51	Mixed-matrix membranes containing functionalized porous metal–organic polyhedrons for the effective separation of CO_2–CH_4 mixture. Chemical Communications, 2015, 51, 4249-4251.	2.2	72
52	Enhancing CO 2 adsorption and separation ability of Zr(IV)-based metal–organic frameworks through ligand functionalization under the guidance of the quantitative structure–property relationship model. Chemical Engineering Journal, 2016, 289, 247-253.	6.6	72
53	A robust calcium-based microporous metal-organic framework for efficient CH4/N2 separation. Chemical Engineering Journal, 2021, 408, 127294.	6.6	72
54	Revealing the structure–property relationship of covalent organic frameworks for CO_2 capture from postcombustion gas: a multi-scale computational study. Physical Chemistry Chemical Physics, 2014, 16, 15189-15198.	1.3	69

#	ARTICLE	IF	CITATIONS
55	A new metal–organic framework with high stability based on zirconium for sensing small molecules. Microporous and Mesoporous Materials, 2013, 171, 118-124.	2.2	68
56	Computational exploration of a Zr-carboxylate based metal–organic framework as a membrane material for CO_2 capture. Journal of Materials Chemistry A, 2014, 2, 1657-1661.	5.2	68
57	A Water Stable Metal–Organic Framework with Optimal Features for CO_2 Capture. Angewandte Chemie, 2013, 125, 10506-10510.	1.6	66
58	Computational study of the effect of organic linkers on natural gas upgrading in metal–organic frameworks. Microporous and Mesoporous Materials, 2010, 130, 76-82.	2.2	65
59	Helium Recovery by a Cu-BTC Metal–Organic-Framework Membrane. Industrial & Engineering Chemistry Research, 2012, 51, 11274-11278.	1.8	62
60	Effect of exercise-based cardiac rehabilitation on anxiety and depression in patients with myocardial infarction: A systematic review and meta-analysis. Heart and Lung: Journal of Acute and Critical Care, 2019, 48, 1-7.	0.8	61
61	A force field for dynamic Cu-BTC metal-organic framework. Journal of Molecular Modeling, 2011, 17, 227-234.	0.8	60
62	An ultrastable Zr metal–organic framework with a thiophene-type ligand containing methyl groups. CrystEngComm, 2015, 17, 3586-3590.	1.3	59
63	Exploration of nanoporous graphene membranes for the separation of N_2 from CO_2: a multi-scale computational study. Physical Chemistry Chemical Physics, 2016, 18, 8352-8358.	1.3	55
64	Molecular Simulation Study of the Stepped Behaviors of Gas Adsorption in Two-Dimensional Covalent Organic Frameworks. Langmuir, 2009, 25, 2302-2308.	1.6	53
65	Effects of ionic liquid dispersion in metal-organic frameworks and covalent organic frameworks on CO2 capture: A computational study. Chemical Engineering Science, 2016, 140, 1-9.	1.9	53
66	Influence of the Organic Ligand Functionalization on the Breathing of the Porous Iron Terephthalate Metal Organic Framework Type Material upon Hydrocarbon Adsorption. Journal of Physical Chemistry C, 2011, 115, 18683-18695.	1.5	50
67	Exploration of the Long-Chain *N*-Alkanes Adsorption and Diffusion in the MOF-Type MIL-47 (V) Material by Combining Experimental and Molecular Simulation Tools. Journal of Physical Chemistry C, 2011, 115, 13868-13876.	1.5	49
68	Computational screening of covalent organic frameworks for the capture of radioactive iodine and methyl iodide. CrystEngComm, 2017, 19, 4920-4926.	1.3	49
69	Highly Selective Adsorption and Separation of Aniline/Phenol from Aqueous Solutions by Microporous MIL-53(Al): A Combined Experimental and Computational Study. Langmuir, 2014, 30, 12229-12235.	1.6	47
70	Computational screening of covalent organic frameworks for CH4/H2, CO2/H2 and CO2/CH4 separations. Microporous and Mesoporous Materials, 2015, 210, 142-148.	2.2	46
71	Construction of stable IL@MOF composite with multiple adsorption sites for efficient ammonia capture from dry and humid conditions. Chemical Engineering Journal, 2020, 401, 126106.	6.6	46
72	A high surface area Zr(IV)-based metal–organic framework showing stepwise gas adsorption and selective dye uptake. Journal of Solid State Chemistry, 2015, 223, 104-108.	1.4	44

#	ARTICLE	IF	CITATIONS
73	MicroRNA-223-3p modulates dendritic cell function and ameliorates experimental autoimmune myocarditis by targeting the NLRP3 inflammasome. Molecular Immunology, 2020, 117, 73-83.	1.0	43
74	Molecular Simulation of CO2/H2 Mixture Separation in Metal-organic Frameworks: Effect of Catenation and Electrostatic Interactions. Chinese Journal of Chemical Engineering, 2009, 17, 781-790.	1.7	42
75	Molecular simulation of hydrogen diffusion in interpenetrated metal–organic frameworks. Physical Chemistry Chemical Physics, 2008, 10, 3244.	1.3	40
76	High-throughput computational screening and design of nanoporous materials for methane storage and carbon dioxide capture. Green Energy and Environment, 2018, 3, 107-119.	4.7	40
77	A new type of halogen bond involving multivalent astatine: an *ab initio* study. Physical Chemistry Chemical Physics, 2019, 21, 15310-15318.	1.3	39
78	Guest dependent pressure behavior of the flexible MIL-53(Cr): A computational exploration. Dalton Transactions, 2012, 41, 3915-3919.	1.6	38
79	Microporous Metal–Organic Frameworks with Hydrophilic and Hydrophobic Pores for Efficient Separation of CH_4/N_2 Mixture. ACS Omega, 2019, 4, 14511-14516.	1.6	38
80	Synthesis of MIL-88B(Fe)/Matrimid mixed-matrix membranes with high hydrogen permselectivity. RSC Advances, 2015, 5, 7253-7259.	1.7	37
81	Recovery of acetone from aqueous solution by ZIF-7/PDMS mixed matrix membranes. RSC Advances, 2015, 5, 28394-28400.	1.7	37
82	Computer-Aided Discovery of MOFs with Calixarene-Analogous Microenvironment for Exceptional SF_6 Capture. Chemistry of Materials, 2021, 33, 5108-5114.	3.2	37
83	Ionic liquid functionalized multi-walled carbon nanotubes/zeolitic imidazolate framework hybrid membranes for efficient H_2/CO_2 separation. Chemical Communications, 2015, 51, 17281-17284.	2.2	36
84	Hydrocarbon adsorption in the isostructural metal organic frameworks MIL-53(Cr) and MIL-47(V). Microporous and Mesoporous Materials, 2011, 140, 114-119.	2.2	34
85	Quantum Sieving in Metal–Organic Frameworks: A Computational Study. Industrial & Engineering Chemistry Research, 2012, 51, 434-442.	1.8	34
86	Computational exploration of H2S/CH4 mixture separation using acid-functionalized UiO-66(Zr) membrane and composites. Chinese Journal of Chemical Engineering, 2015, 23, 1291-1299.	1.7	33
87	Molecular simulation study of role of polymer–particle interactions in the strain-dependent viscoelasticity of elastomers (Payne effect). Journal of Chemical Physics, 2014, 141, 104901.	1.2	31
88	Ultrahigh effective H_2/D_2 separation in an ultramicroporous metal–organic framework material through quantum sieving. Journal of Materials Chemistry A, 2018, 6, 19954-19959.	5.2	31
89	Computational exploration of metal–organic frameworks for CO2/CH4 separation via temperature swing adsorption. Chemical Engineering Science, 2014, 120, 59-66.	1.9	30
90	*In Silico* Screening of MOFs with open copper sites for C_2H_2/CO_2 separation. AICHE Journal, 2018, 64, 4089-4096.	1.8	30

#	Article	IF	Citations
91	Calcium-Based Metal–Organic Framework for Efficient Capture of Sulfur Hexafluoride at Low Concentrations. Industrial & Engineering Chemistry Research, 2021, 60, 5976-5983.	1.8	30
92	Enhancement of CO2/N2 Mixture Separation Using the Thermodynamic Stepped Behavior of Adsorption in Metal–Organic Frameworks. Journal of Physical Chemistry C, 2011, 115, 2790-2797.	1.5	28
93	Computational Study of Nanoparticle Dispersion and Spatial Distribution in Polymer Matrix under Oscillatory Shear Flow. Langmuir, 2013, 29, 13932-13942.	1.6	28
94	The lncRNA ANRIL regulates endothelial dysfunction by targeting the let‐7b/TGF‐β2R1 signalling pathway. Journal of Cellular Physiology, 2021, 236, 2058-2069.	2.0	27
95	Separation of CH_4/N_2 by an ultra‐stable metal–organic framework with the highest breakthrough selectivity. AICHE Journal, 2022, 68, .	1.8	26
96	Crystal‐State Photochromism and Dual‐Mode Mechanochromism of an Organic Molecule with Fluorescence, Room‐Temperature Phosphorescence, and Delayed Fluorescence. Angewandte Chemie, 2019, 131, 16597-16602.	1.6	25
97	Computational study of oxygen adsorption in metal–organic frameworks with exposed cation sites: effect of framework metal ions. RSC Advances, 2015, 5, 33432-33437.	1.7	24
98	Molecular mechanisms for surfactant-aided oil removal from a solid surface. Applied Surface Science, 2015, 359, 98-105.	3.1	24
99	Graphene-like Poly(triazine imide) as N_2-Selective Ultrathin Membrane for Postcombustion CO_2 Capture. Journal of Physical Chemistry C, 2016, 120, 28782-28788.	1.5	24
100	Large‐Scale Screening and Design of Metal–Organic Frameworks for CH_4/N_2 Separation. Chemistry - an Asian Journal, 2019, 14, 3688-3693.	1.7	24
101	Highly efficient CO_2 capture and conversion of a microporous acylamide functionalized *rht*-type metal–organic framework. Inorganic Chemistry Frontiers, 2020, 7, 1939-1948.	3.0	24
102	Correlation and prediction of the thermal conductivity of amorphous polymers. Fluid Phase Equilibria, 2001, 181, 195-202.	1.4	23
103	High-throughput computational screening of Cu-MOFs with open metal sites for efficient C2H2/C2H4 separation. Green Energy and Environment, 2020, 5, 333-340.	4.7	23
104	Large-Scale Structural Refinement and Screening of Zirconium Metal–Organic Frameworks for H_2S/CH_4 Separation. ACS Applied Materials & Interfaces, 2019, 11, 46984-46992.	4.0	22
105	A robust metal-organic framework with guest molecules induced splint-like pore confinement to construct propane-trap for propylene purification. Separation and Purification Technology, 2021, 279, 119656.	3.9	22
106	PtCu@Ir-PCN-222: Synergistic Catalysis of Bimetallic PtCu Nanowires in Hydrosilane-Concentrated Interspaces of an Iridium(III)–Porphyrin-Based Metal–Organic Framework. ACS Catalysis, 2022, 12, 3604-3614.	5.5	22
107	Effects of the side pockets on gas separation in metal-organic framework Cu-BTC: a molecular simulation study. Molecular Simulation, 2009, 35, 1249-1255.	0.9	18
108	Guest-modulation of the mechanical properties of flexible porous metal–organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	5.2	18

#	Article	IF	Citations
109	Accelerating the Selection of Covalent Organic Frameworks with Automated Machine Learning. ACS Omega, 2021, 6, 17149-17161.	1.6	18
110	Bimetallic MOF-Derived Sulfides with Heterojunction Interfaces Synthesized for Photocatalytic Hydrogen Evolution. Industrial & Engineering Chemistry Research, 2021, 60, 11439-11449.	1.8	18
111	Analyzing acetylene adsorption of metal–organic frameworks based on machine learning. Green Energy and Environment, 2022, 7, 1062-1070.	4.7	17
112	Computational design of metal–organic frameworks for aniline recovery from aqueous solution. CrystEngComm, 2013, 15, 9588.	1.3	16
113	Materials genomics–guided ab initio screening of MOFs with open copper sites for acetylene storage. AICHE Journal, 2018, 64, 1389-1398.	1.8	16
114	Computer Simulations of Adsorption Characteristics of Carbon Dioxide in Slit Graphite Pores. Canadian Journal of Chemical Engineering, 2004, 82, 580-589.	0.9	14
115	A Multiscale Evaluation of the Coupling Relationship between Urban Land and Carbon Emissions: A Case Study of Chongqing, China. International Journal of Environmental Research and Public Health, 2020, 17, 3416.	1.2	13
116	Quantum sieving of H_2/D_2 in MOFs: a study on the correlation between the separation performance, pore size and temperature. Journal of Materials Chemistry A, 2020, 8, 6319-6327.	5.2	13
117	Reversed C2H6/C2H4 separation in interpenetrated diamondoid coordination networks with enhanced host–guest interaction. Separation and Purification Technology, 2021, 276, 119385.	3.9	13
118	Methane adsorption in several series of newly synthesised metal-organic frameworks: a molecular simulation study. Molecular Simulation, 2010, 36, 682-692.	0.9	12
119	A Computational Exploration of the CO Adsorption in Cation-Exchanged Faujasites. Journal of Physical Chemistry C, 2012, 116, 24512-24521.	1.5	11
120	Identifying Promising Covalent-Organic Frameworks for Decarburization and Desulfurization from Biogas via Computational Screening. ACS Sustainable Chemistry and Engineering, 2021, 9, 8858-8867.	3.2	10
121	High-Throughput Computational Exploration of MOFs with Open Cu Sites for Adsorptive Separation of Hydrogen Isotopes. ACS Applied Materials & Interfaces, 2022, 14, 24980-24991.	4.0	10
122	A modified PSRK model for the prediction of the vapor–liquid equilibria of asymmetric systems. Fluid Phase Equilibria, 2001, 192, 103-120.	1.4	9
123	Molecular simulation of adsorption of HCFC-22 in pillared clays. AICHE Journal, 2005, 51, 281-291.	1.8	9
124	Silver Nanoparticles Prepared by One-Step Reaction via Reducibility of a Metal–Organic Framework to Remove the Toxic Bromine Ions. Journal of Chemical & Engineering Data, 2021, 66, 535-543.	1.0	9
125	Molecular simulation of vapor–liquid equilibria of toxic gases. Fluid Phase Equilibria, 2004, 220, 1-6.	1.4	8
126	Methane diffusion mechanism in catenated metal–organic frameworks. Molecular Simulation, 2009, 35, 373-380.	0.9	8

#	Article	IF	Citations
127	Studies of Capillary Phase Transitions of Methane in Metal–Organic Frameworks by Gauge Cell Monte Carlo Simulation. Langmuir, 2010, 26, 5160-5166.	1.6	8
128	Probing the halogen bond donation ability of multivalent At-center in AtXn (XÂ=ÂCl, Br, I; nÂ=Â1, 3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.1	8
129	Molecular simulation study of the quantum effects of hydrogen adsorption in metal-organic frameworks: influences of pore size and temperature. Molecular Simulation, 2009, 35, 748-754.	0.9	7
130	Enhanced Methane Adsorption in Catenated Metal-organic Frameworks: A Molecular Simulation Study. Chinese Journal of Chemical Engineering, 2009, 17, 580-584.	1.7	7
131	Probing Au⋯O and Au⋯P regium bonding interaction in AuX (XÂ=ÂF, Cl, Br)⋯RPHOH (RÂ=ÂCH3, F, CF3, NH2, CN) complexes. Computational and Theoretical Chemistry, 2020, 1179, 112800.	1.1	7
132	In silico screening and experimental study of anion-pillared metal-organic frameworks for hydrogen isotope separation. Separation and Purification Technology, 2022, 295, 121286.	3.9	7
133	Atomistic molecular dynamics simulation of liquid carbon tetrachloride confined in pillared pore materials. Chemical Engineering Science, 2005, 60, 767-775.	1.9	6
134	Computational Insights on the Role of Nanochannel Environment in the CO_2/CH_4 and H_2/CH_4 Separation Using Restacked Covalent Organic Framework Membranes. Journal of Physical Chemistry C, 2019, 123, 22949-22958.	1.5	6
135	Exploration of the Influences of the $PODE_3$ Additive on the Initial Pyrolysis of Diesel by ReaxFF Molecular Dynamics Simulations. Energy & Fuels, 2021, 35, 9825-9835.	2.5	6
136	A Stable Cu(I)-Based Ultramicroporous NKMOF-8-Br with High CH_4 Uptake for Efficient Separation of CH_4/N_2 Mixtures. Journal of Chemical & Engineering Data, 2022, 67, 1654-1662.	1.0	6
137	A Group Contribution Model for the Prediction of the Thermal Conductivity of Polymer Melts. Industrial & Engineering Chemistry Research, 2001, 40, 4151-4153.	1.8	5
138	Adsorption of methane in heterometallic metal-organic frameworks with anions: a molecular simulation study. Molecular Simulation, 2009, 35, 213-219.	0.9	5
139	Screening and design of COF-based mixed-matrix membrane for CH4/N2 separation. Chinese Journal of Chemical Engineering, 2022, 42, 170-177.	1.7	5
140	New Model for the Prediction of the Pressure Dependence of Thermal Conductivity of Polymer Melts. Industrial & Engineering Chemistry Research, 2001, 40, 4000-4004.	1.8	4
141	Prediction of methane storage in covalent organic frameworks using big-data-mining approach. Chinese Journal of Chemical Engineering, 2021, 39, 286-296.	1.7	4
142	MGRNN: Structure Generation of Molecules Based on Graph Recurrent Neural Networks. Molecular Informatics, 2021, 40, e2100091.	1.4	4
143	Large-scale simulations of CO2 diffusion in metal–organic frameworks with open Cu sites. Chinese Journal of Chemical Engineering, 2022, 42, 1-9.	1.7	3
144	Large-scale computational screening of metal–organic frameworks for D2/H2 separation. Chinese Journal of Chemical Engineering, 2023, 54, 323-330.	1.7	3

#	ARTICLE	IF	CITATIONS
145	Computational Study of Metal-Organic Frameworks for Removing H_2S from Natural Gas. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 41-50.	2.2	2
146	Molecular Modeling of Gas Separation in Metal–Organic Frameworks. , 2015, , 295-337.		1