Qingyuan Yang

List of Publications by Year
in descending order

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146 papers	11,410 citations	22099 59 h-index	30010 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 Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2006, 110, 17776-17783.	1.2	503
2	Development of Computational Methodologies for Metalâ€"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 Metalâ€"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 Metalâ€"Organic Framework with Optimal Features for CO₂ 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 ZIFâ€8 for Membraneâ€Based CO₂ 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 Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2005, 109, 11862-11864.	1.2	276
10	Computational Study of CO₂ Storage in Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 1562-1569.	1.5	240
11	Molecular simulation of separation of CO₂ from flue gases in CUâ€BTC metalâ€organic framework. AICHE Journal, 2007, 53, 2832-2840.	1.8	235
12	Rational construction of defects in a metalâ€"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 Metalâ^'Organic Frameworks with Open Metal Sites:Â A Computational Study. Journal of Physical Chemistry B, 2006, 110, 655-658.	1.2	204
14	An Evaluation of UiOâ€66 for Gasâ€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 metalâ€"organic frameworks. Chemical Communications, 2012, 48, 9831.	2.2	180
17	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimentalâ€"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

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19	Efficient capture of nitrobenzene from waste water using metalâ€“organic frameworks. Chemical Engineering Journal, 2014, 246, 142-149.	6.6	168
20	Understanding the Thermodynamic and Kinetic Behavior of the CO₂/CH₄ 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][NTf₂] 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 CO₂ and CH₄ within the Porous Zirconium Terephthalate UiOâ€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 ZIFâ€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 Metalâ^'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 metalâ€“organic frameworks for CO₂/CH₄separation: 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

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37	Revealing the Structureâ€“Property Relationships of Metalâ€“Organic Frameworks for CO₂ 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 CO₂ separation. RSC Advances, 2017, 7, 6422-6431.	1.7	100
40	High-Flux Graphene Oxide Membranes Intercalated by Metalâ€“Organic Framework with Highly Selective Separation of Aqueous Organic Solution. ACS Applied Materials & Interfaces, 2017, 9, 1710-1718.	4.0	96
41	Crystalâ€“State Photochromism and Dualâ€Mode Mechanochromism of an Organic Molecule with Fluorescence, Roomâ€Temperature Phosphorescence, and Delayed Fluorescence. Angewandte Chemie - International Edition, 2019, 58, 16445-16450.	7.2	96
42	Largeâ€scale computational screening of metalâ€organic frameworks for CH₄/H₂ separation. AIChE Journal, 2012, 58, 2078-2084.	1.8	91
43	Comparative Study of Separation Performance of COFs and MOFs for CH₄/CO₂/H₂ Mixtures. Industrial & Engineering Chemistry Research, 2010, 49, 2902-2906.	1.8	88
44	Ionic Liquid/Metalâ€“Organic Framework Composites for H₂S 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 CO₂capture. 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 CO₂ Uptake in Metalâ€Organic Frameworks. Industrial & Engineering Chemistry Research, 2009, 48, 10479-10484.	1.8	76
50	Adsorption Behavior of Metalâ€“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 metalâ€“organic polyhedrons for the effective separation of CO₂â€“CH₄ mixture. Chemical Communications, 2015, 51, 4249-4251.	2.2	72
52	Enhancing CO 2 adsorption and separation ability of Zr(IV)-based metalâ€“organic frameworks through ligand functionalization under the guidance of the quantitative structureâ€“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 structureâ€“property relationship of covalent organic frameworks for CO₂ capture from postcombustion gas: a multi-scale computational study. Physical Chemistry Chemical Physics, 2014, 16, 15189-15198.	1.3	69

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55	A new metalâ€“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 metalâ€“organic framework as a membrane material for CO₂capture. Journal of Materials Chemistry A, 2014, 2, 1657-1661.	5.2	68
57	A Water Stable Metalâ€“Organic Framework with Optimal Features for CO₂ Capture. Angewandte Chemie, 2013, 125, 10506-10510.	1.6	66
58	Computational study of the effect of organic linkers on natural gas upgrading in metalâ€“organic frameworks. Microporous and Mesoporous Materials, 2010, 130, 76-82.	2.2	65
59	Helium Recovery by a Cu-BTC Metalâ€“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 metalâ€“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 N₂ from CO₂: 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 metalâ€“organic framework showing stepwise gas adsorption and selective dye uptake. Journal of Solid State Chemistry, 2015, 223, 104-108.	1.4	44

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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 metalâ€“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 Metalâ€“Organic Frameworks with Hydrophilic and Hydrophobic Pores for Efficient Separation of CH₄/N₂ 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 SF₆ 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 H₂/CO₂ 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 Metalâ€“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 polymerâ€“particle interactions in the strain-dependent viscoelasticity of elastomers (Payne effect). Journal of Chemical Physics, 2014, 141, 104901.	1.2	31
88	Ultrahigh effective H₂/D₂ separation in an ultramicroporous metalâ€“organic framework material through quantum sieving. Journal of Materials Chemistry A, 2018, 6, 19954-19959.	5.2	31
89	Computational exploration of metalâ€“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 C₂H₂/CO₂ separation. AICHE Journal, 2018, 64, 4089-4096.	1.8	30

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91	Calcium-Based Metalâ€“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 Metalâ^'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 letâ€7b/TGFâ€Î²R1 signalling pathway. Journal of Cellular Physiology, 2021, 236, 2058-2069.	2.0	27
95	Separation of<scp>CH₄</scp>/<scp>N₂</scp>by an ultraâ€stable metalâ€“organic framework with the highest breakthrough selectivity. AICHE Journal, 2022, 68, .	1.8	26
96	Crystalâ€State Photochromism and Dualâ€Mode Mechanochromism of an Organic Molecule with Fluorescence, Roomâ€Temperature Phosphorescence, and Delayed Fluorescence. Angewandte Chemie, 2019, 131, 16597-16602.	1.6	25
97	Computational study of oxygen adsorption in metalâ€“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 N₂-Selective Ultrathin Membrane for Postcombustion CO₂ Capture. Journal of Physical Chemistry C, 2016, 120, 28782-28788.	1.5	24
100	Largeâ€Scale Screening and Design of Metalâ€“Organic Frameworks for CH₄/N₂ Separation. Chemistry - an Asian Journal, 2019, 14, 3688-3693.	1.7	24
101	Highly efficient CO₂ capture and conversion of a microporous acylamide functionalized rht-type metalâ€“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 Metalâ€“Organic Frameworks for H₂S/CH₄ 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)â€“Porphyrin-Based Metalâ€“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 metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	5.2	18

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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 metalâ€“organic frameworks based on machine learning. Green Energy and Environment, 2022, 7, 1062-1070.	4.7	17
112	Computational design of metalâ€“organic frameworks for aniline recovery from aqueous solution. CrystEngComm, 2013, 15, 9588.	1.3	16
113	Materials genomicsâ€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 H₂/D₂ 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 hostâ€“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 vaporâ€“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 Metalâ€“Organic Framework to Remove the Toxic Bromine Ions. Journal of Chemical & Engineering Data, 2021, 66, 535-543.	1.0	9
125	Molecular simulation of vaporâ€“liquid equilibria of toxic gases. Fluid Phase Equilibria, 2004, 220, 1-6.	1.4	8
126	Methane diffusion mechanism in catenated metalâ€“organic frameworks. Molecular Simulation, 2009, 35, 373-380.	0.9	8

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127	Studies of Capillary Phase Transitions of Methane in Metalâ"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 Auâ‹¯O and Auâ‹¯P regium bonding interaction in AuX (XÂ=ÂF, Cl, Br)â‹¯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 CO₂/CH₄ and H₂/CH₄ 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 PODE₃ 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 CH₄ Uptake for Efficient Separation of CH₄/N₂ 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 metalâ€“organic frameworks with open Cu sites. Chinese Journal of Chemical Engineering, 2022, 42, 1-9.	1.7	3
144	Large-scale computational screening of metalâ€“organic frameworks for D2/H2 separation. Chinese Journal of Chemical Engineering, 2023, 54, 323-330.	1.7	3

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145	Computational Study of Metal-Organic Frameworks for Removing H₂S from Natural Gas. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 41-50.	2.2	2
146	Molecular Modeling of Gas Separation in Metalâ€“Organic Frameworks. , 2015, , 295-337.		1