Qingyuan Yang

List of Publications by Year
in descending order

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146	11,410	22132	30058
papers	citations	59	103
		h-index	g-index

147	147	147	10083
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Large-scale computational screening of metalâ€“organic frameworks for D2/H2 separation. Chinese Journal of Chemical Engineering, 2023, 54, 323-330.	1.7	3
2	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
3	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
4	Analyzing acetylene adsorption of metalâ€“organic frameworks based on machine learning. Green Energy and Environment, 2022, 7, 1062-1070.	4.7	17
5	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
6	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
7	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
8	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
9	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
10	The lncRNA ANRIL regulates endothelial dysfunction by targeting the letâ€7b/TGFâ€β²R1 signalling pathway. Journal of Cellular Physiology, 2021, 236, 2058-2069.	2.0	27
11	A robust calcium-based microporous metal-organic framework for efficient CH4/N2 separation. Chemical Engineering Journal, 2021, 408, 127294.	6.6	72
12	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
13	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
14	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
15	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
16	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
17	PEG-stabilized coaxial stacking of two-dimensional covalent organic frameworks for enhanced photocatalytic hydrogen evolution. Nature Communications, 2021, 12, 3934.	5.8	111
18	Accelerating the Selection of Covalent Organic Frameworks with Automated Machine Learning. ACS Omega, 2021, 6, 17149-17161.	1.6	18

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19	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
20	Computer-Aided Discovery of MOFs with Calixarene-Analogous Microenvironment for Exceptional SF₆ Capture. Chemistry of Materials, 2021, 33, 5108-5114.	3.2	37
21	Bimetallic MOF-Derived Sulfides with Heterojunction Interfaces Synthesized for Photocatalytic Hydrogen Evolution. Industrial & Engineering Chemistry Research, 2021, 60, 11439-11449.	1.8	18
22	MGRNN: Structure Generation of Molecules Based on Graph Recurrent Neural Networks. Molecular Informatics, 2021, 40, e2100091.	1.4	4
23	Reversed C2H6/C2H4 separation in interpenetrated diamondoid coordination networks with enhanced hostâ€“guest interaction. Separation and Purification Technology, 2021, 276, 119385.	3.9	13
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	Largeâ€Scale Screening and Design of Metalâ€“Organic Frameworks for CH₄/N₂ Separation. Chemistry - an Asian Journal, 2019, 14, 3688-3693.	1.7	24
33	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
34	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
35	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
36	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

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37	A new type of halogen bond involving multivalent astatine: an ab initio study. Physical Chemistry Chemical Physics, 2019, 21, 15310-15318.	1.3	39
38	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
39	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
40	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
41	Materials genomicsâ€guided ab initio screening of MOFs with open copper sites for acetylene storage. AICHE Journal, 2018, 64, 1389-1398.	1.8	16
42	Materials genomics methods for high-throughput construction of COFs and targeted synthesis. Nature Communications, 2018, 9, 5274.	5.8	182
43	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
44	In Silico Screening of MOFs with open copper sites for C₂H₂/CO₂ separation. AICHE Journal, 2018, 64, 4089-4096.	1.8	30
45	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
46	Theoretical investigation of gas separation in functionalized nanoporous graphene membranes. Applied Surface Science, 2017, 407, 532-539.	3.1	80
47	Exploring the structure-property relationships of covalent organic frameworks for noble gas separations. Chemical Engineering Science, 2017, 168, 456-464.	1.9	102
48	Computational screening of covalent organic frameworks for the capture of radioactive iodine and methyl iodide. CrystEngComm, 2017, 19, 4920-4926.	1.3	49
49	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
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	Two-Dimensional Covalent Triazine Framework Membrane for Helium Separation and Hydrogen Purification. ACS Applied Materials & Interfaces, 2016, 8, 8694-8701.	4.0	121
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	Synthesis of MIL-88B(Fe)/Matrimid mixed-matrix membranes with high hydrogen permselectivity. RSC Advances, 2015, 5, 7253-7259.	1.7	37
67	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
68	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
69	Recovery of acetone from aqueous solution by ZIF-7/PDMS mixed matrix membranes. RSC Advances, 2015, 5, 28394-28400.	1.7	37
70	An ultrastable Zr metalâ€“organic framework with a thiophene-type ligand containing methyl groups. CrystEngComm, 2015, 17, 3586-3590.	1.3	59
71	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
72	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

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73	Molecular mechanisms for surfactant-aided oil removal from a solid surface. Applied Surface Science, 2015, 359, 98-105.	3.1	24
74	An in situ self-assembly template strategy for the preparation of hierarchical-pore metal-organic frameworks. Nature Communications, 2015, 6, 8847.	5.8	309
75	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
76	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
77	Molecular Modeling of Gas Separation in Metalâ€“Organic Frameworks. , 2015, , 295-337.		1
78	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
79	Efficient capture of nitrobenzene from waste water using metalâ€“organic frameworks. Chemical Engineering Journal, 2014, 246, 142-149.	6.6	168
80	The stability and defluoridation performance of MOFs in fluoride solutions. Microporous and Mesoporous Materials, 2014, 185, 72-78.	2.2	165
81	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
82	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
83	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
84	Computational exploration of metalâ€“organic frameworks for CO2/CH4 separation via temperature swing adsorption. Chemical Engineering Science, 2014, 120, 59-66.	1.9	30
85	Guest-modulation of the mechanical properties of flexible porous metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	5.2	18
86	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
87	A hybrid zeolitic imidazolate framework membrane by mixed-linker synthesis for efficient CO₂capture. Chemical Communications, 2013, 49, 600-602.	2.2	83
88	A robust amino-functionalized titanium(iv) based MOF for improved separation of acid gases. Chemical Communications, 2013, 49, 10082.	2.2	135
89	Computational Study of Nanoparticle Dispersion and Spatial Distribution in Polymer Matrix under Oscillatory Shear Flow. Langmuir, 2013, 29, 13932-13942.	1.6	28
90	Computational design of metalâ€“organic frameworks for aniline recovery from aqueous solution. CrystEngComm, 2013, 15, 9588.	1.3	16

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91	A Water Stable Metalâ€“Organic Framework with Optimal Features for CO₂ Capture. Angewandte Chemie, 2013, 125, 10506-10510.	1.6	66
92	A Water Stable Metalâ€“Organic Framework with Optimal Features for CO₂ Capture. Angewandte Chemie - International Edition, 2013, 52, 10316-10320.	7.2	303
93	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
94	Development of Computational Methodologies for Metalâ€“Organic Frameworks and Their Application in Gas Separations. Chemical Reviews, 2013, 113, 8261-8323.	23.0	448
95	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
96	Guest dependent pressure behavior of the flexible MIL-53(Cr): A computational exploration. Dalton Transactions, 2012, 41, 3915-3919.	1.6	38
97	Quantum Sieving in Metalâ€“Organic Frameworks: A Computational Study. Industrial & Engineering Chemistry Research, 2012, 51, 434-442.	1.8	34
98	Adsorption Behavior of Metalâ€“Organic Frameworks for Thiophenic Sulfur from Diesel Oil. Industrial & Engineering Chemistry Research, 2012, 51, 12449-12455.	1.8	73
99	CH4 storage and CO2 capture in highly porous zirconium oxide based metalâ€“organic frameworks. Chemical Communications, 2012, 48, 9831.	2.2	180
100	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
101	A Series of Isoreticular, Highly Stable, Porous Zirconium Oxide Based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 9267-9271.	7.2	407
102	Helium Recovery by a Cu-BTC Metalâ€“Organic-Framework Membrane. Industrial & Engineering Chemistry Research, 2012, 51, 11274-11278.	1.8	62
103	A Computational Exploration of the CO Adsorption in Cation-Exchanged Faujasites. Journal of Physical Chemistry C, 2012, 116, 24512-24521.	1.5	11
104	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimentalâ€“modelling exploration. Chemical Science, 2012, 3, 1100.	3.7	176
105	Revealing the Structureâ€“Property Relationships of Metalâ€“Organic Frameworks for CO₂ Capture from Flue Gas. Langmuir, 2012, 28, 12094-12099.	1.6	110
106	Largeâ€scale computational screening of metalâ€organic frameworks for CH₄/H₂ separation. AICHE Journal, 2012, 58, 2078-2084.	1.8	91
107	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
108	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

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109	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration. Chemical Communications, 2011, 47, 9603.	2.2	345
110	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
111	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
112	An Evaluation of UiOâ€66 for Gasâ€Based Applications. Chemistry - an Asian Journal, 2011, 6, 3270-3280.	1.7	192
113	A force field for dynamic Cu-BTC metal-organic framework. Journal of Molecular Modeling, 2011, 17, 227-234.	0.8	60
114	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
115	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
116	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
117	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
118	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
119	Methane adsorption in several series of newly synthesised metal-organic frameworks: a molecular simulation study. Molecular Simulation, 2010, 36, 682-692.	0.9	12
120	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
121	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
122	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
123	Methane diffusion mechanism in catenated metalâ€"organic frameworks. Molecular Simulation, 2009, 35, 373-380.	0.9	8
124	Enhanced Methane Adsorption in Catenated Metal-organic Frameworks: A Molecular Simulation Study. Chinese Journal of Chemical Engineering, 2009, 17, 580-584.	1.7	7
125	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
126	Molecular Simulation Study of the Stepped Behaviors of Gas Adsorption in Two-Dimensional Covalent Organic Frameworks. Langmuir, 2009, 25, 2302-2308.	1.6	53

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127	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
128	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
129	Adsorption of methane in heterometallic metal-organic frameworks with anions: a molecular simulation study. Molecular Simulation, 2009, 35, 213-219.	0.9	5
130	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
131	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
132	Computational Study of CO₂ Storage in Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 1562-1569.	1.5	240
133	Molecular simulation of hydrogen diffusion in interpenetrated metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2008, 10, 3244.	1.3	40
134	Molecular simulation of separation of CO₂ from flue gases in CUâ€BTC metalâ€organic framework. AICHE Journal, 2007, 53, 2832-2840.	1.8	235
135	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
136	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
137	Electrostatic-Field-Induced Enhancement of Gas Mixture Separation in Metal-Organic Frameworks: A Computational Study. ChemPhysChem, 2006, 7, 1417-1421.	1.0	140
138	Atomistic molecular dynamics simulation of liquid carbon tetrachloride confined in pillared pore materials. Chemical Engineering Science, 2005, 60, 767-775.	1.9	6
139	Molecular simulation of adsorption of HCFC-22 in pillared clays. AICHE Journal, 2005, 51, 281-291.	1.8	9
140	Molecular Simulation of Adsorption and Diffusion of Hydrogen in Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2005, 109, 11862-11864.	1.2	276
141	Molecular simulation of vaporâ€“liquid equilibria of toxic gases. Fluid Phase Equilibria, 2004, 220, 1-6.	1.4	8
142	Computer Simulations of Adsorption Characteristics of Carbon Dioxide in Slit Graphite Pores. Canadian Journal of Chemical Engineering, 2004, 82, 580-589.	0.9	14
143	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
144	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

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145	Correlation and prediction of the thermal conductivity of amorphous polymers. Fluid Phase Equilibria, 2001, 181, 195-202.	1.4	23
146	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