Qingyuan Yang

List of Publications by Year in Descending Order

140 papers	9,053 citations	53 h-index	93 g-index
147 ext. papers	10,243 ext. citations	6.3 avg, IF	6.28 L-index

#	Paper	IF	Citations
140	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	13.1	3
139	In Silico Screening and Experimental Study of Anion-Pillared Metal-Organic Frameworks for Hydrogen Isotope Separation. *Separation and Purification Technology*, **2022**, 121286	8.3	1
138	Prediction of Methane Storage in Covalent Organic Frameworks Using Big-Data-Mining Approach. *Chinese Journal of Chemical Engineering*, **2021**, 39, 286-286	3.2	0
137	Calcium-Based Metal–Organic Framework for Efficient Capture of Sulfur Hexafluoride at Low Concentrations. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5976-5983	3.9	6
136	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	4.1	1
135	PEG-stabilized coaxial stacking of two-dimensional covalent organic frameworks for enhanced photocatalytic hydrogen evolution. *Nature Communications*, **2021**, 12, 3934	17.4	25
134	Accelerating the Selection of Covalent Organic Frameworks with Automated Machine Learning. *ACS Omega*, **2021**, 6, 17149-17161	3.9	4
133	Identifying Promising Covalent-Organic Frameworks for Decarburization and Desulfurization from Biogas via Computational Screening. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 8858-8867	8.3	5
132	Computer-Aided Discovery of MOFs with Calixarene-Analogous Microenvironment for Exceptional SF6 Capture. *Chemistry of Materials*, **2021**, 33, 5108-5114	9.6	8
131	The lncRNA ANRIL regulates endothelial dysfunction by targeting the let-7b/TGF-R1 signalling pathway. *Journal of Cellular Physiology*, **2021**, 236, 2058-2069	7	10
130	A robust calcium-based microporous metal-organic framework for efficient CH4/N2 separation. *Chemical Engineering Journal*, **2021**, 408, 127294	14.7	21
129	Probing the halogen bond donation ability of multivalent At-center in AtXn (X=Cl, Br, I; n=1, 3, 5)?H2O/H2S complexes. *Computational and Theoretical Chemistry*, **2021**, 1195, 113090	2	3
128	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	2.8	2
127	Bimetallic MOF-Derived Sulfides with Heterojunction Interfaces Synthesized for Photocatalytic Hydrogen Evolution. *Industrial & Engineering Chemistry Research*, **2021**, 60, 11439-11449	3.9	3
126	MGRNN: Structure Generation of Molecules Based on Graph Recurrent Neural Networks. *Molecular Informatics*, **2021**, 40, e2100091	3.8	1
125	Reversed C2H6/C2H4 separation in interpenetrated diamondoid coordination networks with enhanced host–guest interaction. *Separation and Purification Technology*, **2021**, 276, 119385	8.3	3
124	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	8.3	6

123	Analyzing acetylene adsorption of metal□rganic frameworks based on machine learning. *Green Energy and Environment*, **2021**,	5.7	1
122	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,	4.6	7
121	High-throughput computational screening of Cu-MOFs with open metal sites for efficient C2H2/C2H4 separation. *Green Energy and Environment*, **2020**, 5, 333-340	5.7	10
120	Highly efficient CO2 capture and conversion of a microporous acylamide functionalized rht-type metal□rganic framework. *Inorganic Chemistry Frontiers*, **2020**, 7, 1939-1948	6.8	11
119	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	14.7	20
118	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	13	8
117	MicroRNA-223-3p modulates dendritic cell function and ameliorates experimental autoimmune myocarditis by targeting the NLRP3 inflammasome. *Molecular Immunology*, **2020**, 117, 73-83	4.3	28
116	Probing Au?O and Au?P regium bonding interaction in AuX (X□=□F, Cl, Br)?RPHOH (R□=□CH3, F, CF3, NH2, CN) complexes. *Computational and Theoretical Chemistry*, **2020**, 1179, 112800	2	3
115	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	3.8	5
114	Microporous Metal-Organic Frameworks with Hydrophilic and Hydrophobic Pores for Efficient Separation of CH/N Mixture. *ACS Omega*, **2019**, 4, 14511-14516	3.9	14
113	A new type of halogen bond involving multivalent astatine: an ab initio study. *Physical Chemistry Chemical Physics*, **2019**, 21, 15310-15318	3.6	20
112	Large-Scale Screening and Design of Metal-Organic Frameworks for CH /N Separation. *Chemistry - an Asian Journal*, **2019**, 14, 3688-3693	4.5	11
111	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	3.6	15
110	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	16.4	61
109	Large-Scale Structural Refinement and Screening of Zirconium Metal-Organic Frameworks for HS/CH Separation. *ACS Applied Materials & Interfaces*, **2019**, 11, 46984-46992	9.5	10
108	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	2.6	25
107	High-throughput computational screening and design of nanoporous materials for methane storage and carbon dioxide capture. *Green Energy and Environment*, **2018**, 3, 107-119	5.7	27
106	In Silico Screening of MOFs with open copper sites for C2H2/CO2 separation. *AICHE Journal*, **2018**, 64, 4089-4096	3.6	21

105	Materials genomics-guided ab initio screening of MOFs with open copper sites for acetylene storage. *AICHE Journal*, **2018**, 64, 1389-1398	3.6	12
104	Materials genomics methods for high-throughput construction of COFs and targeted synthesis. *Nature Communications*, **2018**, 9, 5274	17.4	104
103	Ultrahigh effective H2/D2 separation in an ultramicroporous metal–organic framework material through quantum sieving. *Journal of Materials Chemistry A*, **2018**, 6, 19954-19959	13	21
102	Pebax-based composite membranes with high gas transport properties enhanced by ionic liquids for CO2 separation. *RSC Advances*, **2017**, 7, 6422-6431	3.7	61
101	Theoretical investigation of gas separation in functionalized nanoporous graphene membranes. *Applied Surface Science*, **2017**, 407, 532-539	6.7	57
100	Exploring the structure-property relationships of covalent organic frameworks for noble gas separations. *Chemical Engineering Science*, **2017**, 168, 456-464	4.4	60
99	Computational screening of covalent organic frameworks for the capture of radioactive iodine and methyl iodide. *CrystEngComm*, **2017**, 19, 4920-4926	3.3	29
98	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	9.5	78
97	Protic ionic liquid [Bim][NTf2] with strong hydrogen bond donating ability for highly efficient ammonia absorption. *Green Chemistry*, **2017**, 19, 937-945	10	104
96	Preparation of thin film nanocomposite membranes with surface modified MOF for high flux organic solvent nanofiltration. *AICHE Journal*, **2017**, 63, 1303-1312	3.6	84
95	Graphene-like Poly(triazine imide) as N2-Selective Ultrathin Membrane for Postcombustion CO2 Capture. *Journal of Physical Chemistry C*, **2016**, 120, 28782-28788	3.8	22
94	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	14.7	53
93	Rational construction of defects in a metal–organic framework for highly efficient adsorption and separation of dyes. *Chemical Engineering Journal*, **2016**, 289, 486-493	14.7	149
92	Few-layered ultrathin covalent organic framework membranes for gas separation: a computational study. *Journal of Materials Chemistry A*, **2016**, 4, 124-131	13	62
91	Two-Dimensional Covalent Triazine Framework Membrane for Helium Separation and Hydrogen Purification. *ACS Applied Materials & Interfaces*, **2016**, 8, 8694-701	9.5	96
90	Exploration of nanoporous graphene membranes for the separation of N2 from CO2: a multi-scale computational study. *Physical Chemistry Chemical Physics*, **2016**, 18, 8352-8	3.6	46
89	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	4.4	39
88	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	15.6	98

87	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	13	96
86	Mixed matrix membranes incorporated with amine-functionalized titanium-based metal-organic framework for CO2/CH4 separation. *Journal of Membrane Science*, **2015**, 478, 130-139	9.6	104
85	Synthesis of MIL-88B(Fe)/Matrimid mixed-matrix membranes with high hydrogen permselectivity. *RSC Advances*, **2015**, 5, 7253-7259	3.7	30
84	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	3.2	30
83	Computational screening of covalent organic frameworks for CH4/H2, CO2/H2 and CO2/CH4 separations. *Microporous and Mesoporous Materials*, **2015**, 210, 142-148	5.3	31
82	Recovery of acetone from aqueous solution by ZIF-7/PDMS mixed matrix membranes. *RSC Advances* , **2015**, 5, 28394-28400	3.7	29
81	An ultrastable Zr metal□rganic framework with a thiophene-type ligand containing methyl groups. *CrystEngComm*, **2015**, 17, 3586-3590	3.3	47
80	Ionic liquid functionalized multi-walled carbon nanotubes/zeolitic imidazolate framework hybrid membranes for efficient H2/CO2 separation. *Chemical Communications*, **2015**, 51, 17281-4	5.8	32
79	Molecular mechanisms for surfactant-aided oil removal from a solid surface. *Applied Surface Science* , **2015**, 359, 98-105	6.7	20
78	An in situ self-assembly template strategy for the preparation of hierarchical-pore metal-organic frameworks. *Nature Communications*, **2015**, 6, 8847	17.4	225
77	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	13	135
76	A high surface area Zr(IV)-based metal□rganic framework showing stepwise gas adsorption and selective dye uptake. *Journal of Solid State Chemistry*, **2015**, 223, 104-108	3.3	37
75	Confinement of Ionic Liquids in Nanocages: Tailoring the Molecular Sieving Properties of ZIF-8 for Membrane-Based CO2 Capture. *Angewandte Chemie - International Edition*, **2015**, 54, 15483-7	16.4	213
74	Confinement of Ionic Liquids in Nanocages: Tailoring the Molecular Sieving Properties of ZIF-8 for Membrane-Based CO2 Capture. *Angewandte Chemie*, **2015**, 127, 15703-15707	3.6	47
73	Computational study of oxygen adsorption in metal□rganic frameworks with exposed cation sites: effect of framework metal ions. *RSC Advances*, **2015**, 5, 33432-33437	3.7	21
72	Mixed-matrix membranes containing functionalized porous metal-organic polyhedrons for the effective separation of CO2-CH4 mixture. *Chemical Communications*, **2015**, 51, 4249-51	5.8	60
71	Ionic Liquid/Metal□rganic Framework Composites for H2S Removal from Natural Gas: A Computational Exploration. *Journal of Physical Chemistry C*, **2015**, 119, 3674-3683	3.8	73
70	Molecular Modeling of Gas Separation in Metal□rganic Frameworks **2015**, 295-337		1

69	Efficient capture of nitrobenzene from waste water using metal–organic frameworks. *Chemical Engineering Journal*, **2014**, 246, 142-149	14.7	141
68	The stability and defluoridation performance of MOFs in fluoride solutions. *Microporous and Mesoporous Materials*, **2014**, 185, 72-78	5.3	129
67	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, 12229-35	4	35
66	Computational exploration of a Zr-carboxylate based metal–organic framework as a membrane material for CO2 capture. *Journal of Materials Chemistry A*, **2014**, 2, 1657-1661	13	53
65	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	3.8	60
64	Computational exploration of metal–organic frameworks for CO2/CH4 separation via temperature swing adsorption. *Chemical Engineering Science*, **2014**, 120, 59-66	4.4	25
63	Guest-modulation of the mechanical properties of flexible porous metal–organic frameworks. *Journal of Materials Chemistry A*, **2014**, 2, 9691-9698	13	12
62	Revealing the structure-property relationship of covalent organic frameworks for CO2 capture from postcombustion gas: a multi-scale computational study. *Physical Chemistry Chemical Physics*, **2014**, 16, 15189-98	3.6	48
61	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	3.9	23
60	A hybrid zeolitic imidazolate framework membrane by mixed-linker synthesis for efficient CO2 capture. *Chemical Communications*, **2013**, 49, 600-2	5.8	78
59	A robust amino-functionalized titanium(iv) based MOF for improved separation of acid gases. *Chemical Communications*, **2013**, 49, 10082-4	5.8	123
58	Computational study of nanoparticle dispersion and spatial distribution in polymer matrix under oscillatory shear flow. *Langmuir*, **2013**, 29, 13932-42	4	27
57	Computational design of metal–organic frameworks for aniline recovery from aqueous solution. *CrystEngComm*, **2013**, 15, 9588	3.3	14
56	A Water Stable Metal–Organic Framework with Optimal Features for CO2 Capture. *Angewandte Chemie*, **2013**, 125, 10506-10510	3.6	59
55	A water stable metal-organic framework with optimal features for CO2 capture. *Angewandte Chemie - International Edition*, **2013**, 52, 10316-20	16.4	265
54	A new metal–organic framework with high stability based on zirconium for sensing small molecules. *Microporous and Mesoporous Materials*, **2013**, 171, 118-124	5.3	58
53	Development of computational methodologies for metal-organic frameworks and their application in gas separations. *Chemical Reviews*, **2013**, 113, 8261-323	68.1	394
52	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	13	249

51	Guest dependent pressure behavior of the flexible MIL-53(Cr): a computational exploration. *Dalton Transactions*, **2012**, 41, 3915-9	4.3	34
50	Quantum Sieving in Metal□Organic Frameworks: A Computational Study. *Industrial & Engineering Chemistry Research*, **2012**, 51, 434-442	3.9	29
49	Adsorption Behavior of Metal□Organic Frameworks for Thiophenic Sulfur from Diesel Oil. *Industrial & Engineering Chemistry Research*, **2012**, 51, 12449-12455	3.9	64
48	CH4 storage and CO2 capture in highly porous zirconium oxide based metal-organic frameworks. *Chemical Communications*, **2012**, 48, 9831-3	5.8	150
47	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		98
46	A series of isoreticular, highly stable, porous zirconium oxide based metal-organic frameworks. *Angewandte Chemie - International Edition*, **2012**, 51, 9267-71	16.4	366
45	Helium Recovery by a Cu-BTC Metal□Organic-Framework Membrane. *Industrial & Engineering Chemistry Research*, **2012**, 51, 11274-11278	3.9	51
44	A Computational Exploration of the CO Adsorption in Cation-Exchanged Faujasites. *Journal of Physical Chemistry C*, **2012**, 116, 24512-24521	3.8	9
43	Large breathing of the MOF MIL-47(VIV) under mechanical pressure: a joint experimental□modelling exploration. *Chemical Science*, **2012**, 3, 1100	9.4	149
42	Revealing the structure-property relationships of metal-organic frameworks for CO2 capture from flue gas. *Langmuir*, **2012**, 28, 12094-9	4	103
41	Large-scale computational screening of metal-organic frameworks for CH4/H2 separation. *AICHE Journal*, **2012**, 58, 2078-2084	3.6	73
40	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	3.8	44
39	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration. *Chemical Communications*, **2011**, 47, 9603-5	5.8	298
38	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	3.8	28
37	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	3.8	154
36	An evaluation of UiO-66 for gas-based applications. *Chemistry - an Asian Journal*, **2011**, 6, 3270-80	4.5	158
35	A force field for dynamic Cu-BTC metal-organic framework. *Journal of Molecular Modeling*, **2011**, 17, 227-34		46
34	Probing the dynamics of CO2 and CH4 within the porous zirconium terephthalate UiO-66(Zr): a synergic combination of neutron scattering measurements and molecular simulations. *Chemistry - A European Journal*, **2011**, 17, 8882-9	4.8	118

33	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	3.8	46
32	Hydrocarbon adsorption in the isostructural metal organic frameworks MIL-53(Cr) and MIL-47(V). *Microporous and Mesoporous Materials*, **2011**, 140, 114-119	5.3	32
31	Methane adsorption in several series of newly synthesised metal-organic frameworks: a molecular simulation study. *Molecular Simulation*, **2010**, 36, 682-692	2	11
30	Li-modified metal□organic frameworks for CO2/CH4 separation: a route to achieving high adsorption selectivity. *Journal of Materials Chemistry*, **2010**, 20, 706-714		107
29	Studies of capillary phase transitions of methane in metal-organic frameworks by gauge cell Monte Carlo simulation. *Langmuir*, **2010**, 26, 5160-6	4	7
28	Comparative Study of Separation Performance of COFs and MOFs for CH4/CO2/H2 Mixtures. *Industrial & Engineering Chemistry Research*, **2010**, 49, 2902-2906	3.9	83
27	Computational study of the effect of organic linkers on natural gas upgrading in metal□organic frameworks. *Microporous and Mesoporous Materials*, **2010**, 130, 76-82	5.3	61
26	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	2	7
25	Effects of the side pockets on gas separation in metal-organic framework Cu-BTC: a molecular simulation study. *Molecular Simulation*, **2009**, 35, 1249-1255	2	16
24	Methane diffusion mechanism in catenated metal□organic frameworks. *Molecular Simulation*, **2009**, 35, 373-380	2	7
23	Enhanced Methane Adsorption in Catenated Metal-organic Frameworks: A Molecular Simulation Study. *Chinese Journal of Chemical Engineering*, **2009**, 17, 580-584	3.2	6
22	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	3.2	40
21	Molecular simulation study of the stepped behaviors of gas adsorption in two-dimensional covalent organic frameworks. *Langmuir*, **2009**, 25, 2302-8	4	46
20	Computational Study on the Influences of Framework Charges on CO2 Uptake in Metal□Organic Frameworks. *Industrial & Engineering Chemistry Research*, **2009**, 48, 10479-10484	3.9	72
19	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	3.8	111
18	Adsorption of methane in heterometallic metal-organic frameworks with anions: a molecular simulation study. *Molecular Simulation*, **2009**, 35, 213-219	2	5
17	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	3.8	109
16	Computational Study of CO2Storage in Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2008**, 112, 1562-1569	3.8	222

15	Molecular simulation of hydrogen diffusion in interpenetrated metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2008**, 10, 3244-9	3.6	37
14	Computer Simulations of Adsorption Characteristics of Carbon Dioxide in Slit Graphite Pores. *Canadian Journal of Chemical Engineering*, **2008**, 82, 580-589	2.3	13
13	Adsorption and separation of binary mixtures in a metal-organic framework Cu-BTC: A computational study. *Separation and Purification Technology*, **2008**, 60, 30-35	8.3	122
12	Molecular simulation of separation of CO2 from flue gases in CU-BTC metal-organic framework. *AICHE Journal*, **2007**, 53, 2832-2840	3.6	218
11	Electrostatic-field-induced enhancement of gas mixture separation in metal-organic frameworks: a computational study. *ChemPhysChem*, **2006**, 7, 1417-21	3.2	137
10	Understanding hydrogen adsorption in metal-organic frameworks with open metal sites: a computational study. *Journal of Physical Chemistry B*, **2006**, 110, 655-8	3.4	194
9	Molecular simulation of carbon dioxide/methane/hydrogen mixture adsorption in metal-organic frameworks. *Journal of Physical Chemistry B*, **2006**, 110, 17776-83	3.4	466
8	Molecular simulation of adsorption and diffusion of hydrogen in metal-organic frameworks. *Journal of Physical Chemistry B*, **2005**, 109, 11862-4	3.4	242
7	Atomistic molecular dynamics simulation of liquid carbon tetrachloride confined in pillared pore materials. *Chemical Engineering Science*, **2005**, 60, 767-775	4.4	6
6	Molecular simulation of adsorption of HCFC-22 in pillared clays. *AICHE Journal*, **2005**, 51, 281-291	3.6	9
5	Molecular simulation of vapor□quid equilibria of toxic gases. *Fluid Phase Equilibria*, **2004**, 220, 1-6	2.5	7
4	Correlation and prediction of the thermal conductivity of amorphous polymers. *Fluid Phase Equilibria*, **2001**, 181, 195-202	2.5	21
3	A modified PSRK model for the prediction of the vapor□quid equilibria of asymmetric systems. *Fluid Phase Equilibria*, **2001**, 192, 103-120	2.5	9
2	A Group Contribution Model for the Prediction of the Thermal Conductivity of Polymer Melts. *Industrial & Engineering Chemistry Research*, **2001**, 40, 4151-4153	3.9	5
1	New Model for the Prediction of the Pressure Dependence of Thermal Conductivity of Polymer Melts. *Industrial & Engineering Chemistry Research*, **2001**, 40, 4000-4004	3.9	4