Philip L Llewellyn

List of Publications by Year
in descending order

224 papers	20,999 citations	9428 76 h-index	11608 140 g-index
234 all docs	234 docs citations	234 times ranked	17132 citing authors

#	Article	IF	Citations
1	A Step in Carbon Capture from Wet Gases: Understanding the Effect of Water on CO₂ Adsorption and Diffusion in UiO-66. Journal of Physical Chemistry C, 2022, 126, 3211-3220.	1.5	12
2	Tuning the Properties of MOFâ€808 via Defect Engineering and Metal Nanoparticle Encapsulation. Chemistry - A European Journal, 2021, 27, 6804-6814.	1.7	46
3	One-pot synthesis of organic polymer functionalized mesoporous silicas. Microporous and Mesoporous Materials, 2021, 319, 111036.	2.2	7
4	Benchtop <i>In Situ</i> Measurement of Full Adsorption Isotherms by NMR. Journal of the American Chemical Society, 2021, 143, 8249-8254.	6.6	18
5	Multifunctionality of weak ferromagnetic porphyrin-based MOFs: selective adsorption in the liquid and gas phase. CrystEngComm, 2021, 23, 4205-4213.	1.3	0
6	The CO2 adsorption behavior study on activated carbon synthesized from olive waste. Journal of CO2 Utilization, 2020, 42, 101292.	3.3	31
7	Engineering micromechanics of soft porous crystals for negative gas adsorption. Chemical Science, 2020, 11, 9468-9479.	3.7	30
8	Tailoring the separation properties of flexible metal-organic frameworks using mechanical pressure. Nature Communications, 2020, 11, 1216.	5.8	88
9	Data Mining for Binary Separation Materials in Published Adsorption Isotherms. Chemistry of Materials, 2020, 32, 982-991.	3.2	16
10	Low Temperature Calorimetry Coupled with Molecular Simulations for an In-Depth Characterization of the Guest-Dependent Compliant Behavior of MOFs. Chemistry of Materials, 2020, 32, 3489-3498.	3.2	8
11	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. Nature Communications, 2019, 10, 3632.	5.8	73
12	Toward an operational methodology to identify industrial-scaled nanomaterial powders with the volume specific surface area criterion. Nanoscale Advances, 2019, 1, 3232-3242.	2.2	12
13	Vaporâ€Phase Linker Exchange of the Metalâ€"Organic Framework ZIFâ€8: A Solventâ€Free Approach to Postâ€synthetic Modification. Angewandte Chemie - International Edition, 2019, 58, 18471-18475.	7.2	42
14	Vaporâ€Phase Linker Exchange of the Metalâ€"Organic Framework ZIFâ€8: A Solventâ€Free Approach to Postâ€synthetic Modification. Angewandte Chemie, 2019, 131, 18642-18646.	1.6	14
15	Role of Structural Defects in the Adsorption and Separation of C3 Hydrocarbons in Zr-Fumarate-MOF (MOF-801). Chemistry of Materials, 2019, 31, 8413-8423.	3.2	87
16	pyGAPS: a Python-based framework for adsorption isotherm processing and material characterisation. Adsorption, 2019, 25, 1533-1542.	1.4	33
17	Nanomaterial identification of powders: comparing volume specific surface area, X-ray diffraction and scanning electron microscopy methods. Environmental Science: Nano, 2019, 6, 152-162.	2.2	12
18	Metal-organic framework crystal-glass composites. Nature Communications, 2019, 10, 2580.	5.8	97

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19	Storage of Hydrogen on Nanoporous Adsorbents. Green Energy and Technology, 2019, , 255-286.	0.4	1
20	Investigating the effect of alumina shaping on the sorption properties of promising metalâ€“organic frameworks. RSC Advances, 2019, 9, 7128-7135.	1.7	14
21	Microporous Leadâ€“Organic Framework for Selective CO₂ Adsorption and Heterogeneous Catalysis. Inorganic Chemistry, 2018, 57, 1774-1786.	1.9	31
22	A promising metalâ€“organic framework (MOF), MIL-96(Al), for CO₂ separation under humid conditions. Journal of Materials Chemistry A, 2018, 6, 2081-2090.	5.2	78
23	Metalâ€Organic Frameworks as Catalyst Supports: Influence of Lattice Disorder on Metal Nanoparticle Formation. Chemistry - A European Journal, 2018, 24, 7498-7506.	1.7	29
24	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2018, 122, 19171-19179.	1.5	52
25	Synthesis of ZIFâ€93/11 Hybrid Nanoparticles via Postâ€Synthetic Modification of ZIFâ€93 and Their Use for H₂/CO₂ Separation. Chemistry - A European Journal, 2018, 24, 11211-11219.	1.7	27
26	Study of methane and carbon dioxide adsorption capacity by synthetic nanoporous carbon based on pyrogallol-formaldehyde. International Journal of Hydrogen Energy, 2017, 42, 8905-8913.	3.8	17
27	Porous zinc and cobalt 2-nitroimidazolate frameworks with six-membered ring windows and a layered cobalt 2-nitroimidazolate polymorph. CrystEngComm, 2017, 19, 1377-1388.	1.3	6
28	Using water adsorption measurements to access the chemistry of defects in the metalâ€“organic framework UiO-66. CrystEngComm, 2017, 19, 4137-4141.	1.3	58
29	Screening the Effect of Water Vapour on Gas Adsorption Performance: Application to CO₂ Capture from Flue Gas in Metalâ€“Organic Frameworks. ChemSusChem, 2017, 10, 1543-1553.	3.6	89
30	Modeling of adsorption of CO2 in the deformed pores of MIL-53(Al). Journal of Molecular Modeling, 2017, 23, 101.	0.8	9
31	Investigating Unusual Organic Functional Groups to Engineer the Surface Chemistry of Mesoporous Silica to Tune CO₂â€“Surface Interactions. ACS Applied Materials & Interfaces, 2017, 9, 14490-14496.	4.0	2
32	Adsorptionâ€Induced Structural Phase Transformation in Nanopores. Angewandte Chemie - International Edition, 2017, 56, 16243-16246.	7.2	5
33	Adsorptionâ€Induced Structural Phase Transformation in Nanopores. Angewandte Chemie, 2017, 129, 16461-16464.	1.6	2
34	Highly Efficient Proton Conduction in a Three-Dimensional Titanium Hydrogen Phosphate. Chemistry of Materials, 2017, 29, 7263-7271.	3.2	35
35	Revisiting the Aluminum Trimesate-Based MOF (MIL-96): From Structure Determination to the Processing of Mixed Matrix Membranes for CO₂ Capture. Chemistry of Materials, 2017, 29, 10326-10338.	3.2	78
36	Hydrogen adsorption on activated carbons prepared from olive waste: effect of activation conditions on uptakes and adsorption energies. Journal of Porous Materials, 2017, 24, 1-11.	1.3	18

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37	Heterogeneous melting of methane confined in nano-pores. Journal of Chemical Physics, 2016, 145, 144704.	1.2	8
38	Observing the Effects of Shaping on Gas Adsorption in Metalâ€Organic Frameworks. European Journal of Inorganic Chemistry, 2016, 2016, 4416-4423.	1.0	40
39	Adsorption of Small Molecules in the Porous Zirconium-Based Metal Organic Framework MIL-140A (Zr): A Joint Computational-Experimental Approach. Journal of Physical Chemistry C, 2016, 120, 7192-7200.	1.5	12
40	Low temperature mechanism of adsorption of methane: Comparison between homogenous and heterogeneous pores. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 496, 86-93.	2.3	11
41	MIL-91(Ti), a small pore metalâ€“organic framework which fulfils several criteria: an upscaled green synthesis, excellent water stability, high CO₂ selectivity and fast CO₂ transport. Journal of Materials Chemistry A, 2016, 4, 1383-1389.	5.2	82
42	Mechanical energy storage performance of an aluminum fumarate metalâ€“organic framework. Chemical Science, 2016, 7, 446-450.	3.7	103
43	Thermodynamics of the structural transition in metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4274-4282.	1.6	18
44	Effect of the both texture and electrical properties of activated carbon on the CO 2 adsorption capacity. Materials Research Bulletin, 2016, 73, 130-139.	2.7	12
45	A Robust Infinite Zirconium Phenolate Building Unit to Enhance the Chemical Stability of Zr MOFs. Angewandte Chemie - International Edition, 2015, 54, 13297-13301.	7.2	116
46	Influence of Solventâ€Like Sidechains on the Adsorption of Light Hydrocarbons in Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2015, 21, 18764-18769.	1.7	32
47	Computational exploration of the gas adsorption on the iron tetracarboxylate metal-organic framework MIL-102. Molecular Simulation, 2015, 41, 1357-1370.	0.9	14
48	Functionalization of Zr-based MOFs with alkyl and perfluoroalkyl groups: the effect on the water sorption behavior. Dalton Transactions, 2015, 44, 19687-19692.	1.6	20
49	Structural Origin of Unusual CO₂ Adsorption Behavior of a Small-Pore Aluminum Bisphosphonate MOF. Journal of Physical Chemistry C, 2015, 119, 4208-4216.	1.5	63
50	The Direct Heat Measurement of Mechanical Energy Storage Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2015, 54, 4626-4630.	7.2	47
51	Metalâ€“Organic Frameworks from Divalent Metals and 1,4-Benzenedicarboxylate with Bidentate Pyridine-<i>N</i>-oxide Co-ligands. Crystal Growth and Design, 2015, 15, 891-899.	1.4	19
52	Adsorption of CO₂ on amine-functionalised MCM-41: experimental and theoretical studies. Physical Chemistry Chemical Physics, 2015, 17, 11095-11102.	1.3	93
53	Direct accessibility of mixed-metal (<scp>iii</scp>/<scp>ii</scp>) acid sites through the rational synthesis of porous metal carboxylates. Chemical Communications, 2015, 51, 10194-10197.	2.2	63
54	Methane storage in flexible metalâ€“organic frameworks with intrinsic thermal management. Nature, 2015, 527, 357-361.	13.7	817

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55	Highly Selective CO₂ Capture by Small Pore Scandium-Based Metalâ€"Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 23592-23598.	1.5	38
56	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
57	Location of CO₂during its uptake by the flexible porous metalâ€"organic framework MIL-53(Fe): a high resolution powder X-ray diffraction study. CrystEngComm, 2015, 17, 422-429.	1.3	19
58	Adsorption by Metal-Organic Frameworks. , 2014, , 565-610.		13
59	Adsorption by Metal Oxides. , 2014, , 393-465.		6
60	Adsorption by Ordered Mesoporous Materials. , 2014, , 529-564.		7
61	Effect of the ligand functionalization on the acidâ€"base properties of flexible MOFs. Microporous and Mesoporous Materials, 2014, 195, 197-204.	2.2	16
62	Conformation-Controlled Sorption Properties and Breathing of the Aliphatic Al-MOF [Al(OH)(CDC)]. Inorganic Chemistry, 2014, 53, 4610-4620.	1.9	74
63	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
64	High-Resolution N₂ Adsorption Isotherms at 77.4 K: Critical Effect of the He Used During Calibration. Journal of Physical Chemistry C, 2013, 117, 16885-16889.	1.5	22
65	A robust amino-functionalized titanium(iv) based MOF for improved separation of acid gases. Chemical Communications, 2013, 49, 10082.	2.2	135
66	A Water Stable Metalâ€"Organic Framework with Optimal Features for CO₂ Capture. Angewandte Chemie, 2013, 125, 10506-10510.	1.6	66
67	Evaluation of MIL-47(V) for CO₂-Related Applications. Journal of Physical Chemistry C, 2013, 117, 962-970.	1.5	42
68	An Adsorbent Performance Indicator as a First Step Evaluation of Novel Sorbents for Gas Separations: Application to Metalâ€"Organic Frameworks. Langmuir, 2013, 29, 3301-3309.	1.6	131
69	Experimental Screening of Porous Materials for High Pressure Gas Adsorption and Evaluation in Gas Separations: Application to MOFs (MIL-100 and CAU-10). ACS Combinatorial Science, 2013, 15, 111-119.	3.8	48
70	Adsorption of Propane and Propylene on CuBTC Metalâ€"Organic Framework: Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2013, 117, 11159-11167.	1.5	48
71	A Water Stable Metalâ€"Organic Framework with Optimal Features for CO₂ Capture. Angewandte Chemie - International Edition, 2013, 52, 10316-10320.	7.2	303
72	High pressure methane adsorption on microporous carbon monoliths prepared by olives stones. Materials Letters, 2013, 99, 184-187.	1.3	31

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73	Characterisation of MOF Materials by Thermomechanical Methods. , 2013, , .		0
74	Computational investigation of the adsorption of carbon dioxide onto zirconium oxide clusters. Journal of Molecular Modeling, 2012, 18, 4819-4830.	0.8	10
75	Acetylene and argon adsorption in a supramolecular organic zeolite. Physical Chemistry Chemical Physics, 2012, 14, 311-317.	1.3	20
76	CH4 storage and CO2 capture in highly porous zirconium oxide based metalâ€“organic frameworks. Chemical Communications, 2012, 48, 9831.	2.2	180
77	Separation of CO2â€“CH4 mixtures in the mesoporous MIL-100(Cr) MOF: experimental and modelling approaches. Dalton Transactions, 2012, 41, 4052.	1.6	78
78	How Water Fosters a Remarkable 5-Fold Increase in Low-Pressure CO₂ Uptake within Mesoporous MIL-100(Fe). Journal of the American Chemical Society, 2012, 134, 10174-10181.	6.6	198
79	Tuning the breathing behaviour of MIL-53 by cation mixing. Chemical Communications, 2012, 48, 10237.	2.2	129
80	Surface Area/Porosity, Adsorption, Diffusion. , 2012, , 853-879.		4
81	A Method for Screening the Potential of MOFs as CO₂ Adsorbents in Pressure Swing Adsorption Processes. ChemSusChem, 2012, 5, 762-776.	3.6	109
82	Effect of the organic functionalization of flexible MOFs on the adsorption of CO2. Journal of Materials Chemistry, 2012, 22, 10266.	6.7	125
83	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. ChemPhysChem, 2012, 13, 488-495.	1.0	53
84	Energyâ€Efficient Dehumidification over Hierachically Porous Metalâ€“Organic Frameworks as Advanced Water Adsorbents. Advanced Materials, 2012, 24, 806-810.	11.1	298
85	Infrared study of the influence of reducible iron(iii) metal sites on the adsorption of CO, CO2, propane, propene and propyne in the mesoporous metalâ€“organic framework MIL-100. Physical Chemistry Chemical Physics, 2011, 13, 11748.	1.3	192
86	Adsorption of Carbon Dioxide on Mesoporous Zirconia: Microcalorimetric Measurements, Adsorption Isotherm Modeling, and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2011, 115, 10097-10103.	1.5	43
87	Molecular Insight into the Adsorption and Diffusion of Water in the Versatile Hydrophilic/Hydrophobic Flexible MIL-53(Cr) MOF. Journal of Physical Chemistry C, 2011, 115, 10764-10776.	1.5	128
88	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
89	Effect of NH2 and CF3 functionalization on the hydrogen sorption properties of MOFs. Dalton Transactions, 2011, 40, 4879.	1.6	257
90	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration. Chemical Communications, 2011, 47, 9603.	2.2	345

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91	Understanding CO₂ Adsorption in CuBTC MOF: Comparing Combined DFTâ€“ab Initio Calculations with Microcalorimetry Experiments. Journal of Physical Chemistry C, 2011, 115, 17925-17933.	1.5	146
92	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
93	Why hybrid porous solids capture greenhouse gases?. Chemical Society Reviews, 2011, 40, 550-562.	18.7	603
94	A co-templating route to the synthesis of Cu SAPO STA-7, giving an active catalyst for the selective catalytic reduction of NO. Microporous and Mesoporous Materials, 2011, 146, 36-47.	2.2	44
95	An Evaluation of UiOâ€66 for Gasâ€Based Applications. Chemistry - an Asian Journal, 2011, 6, 3270-3280.	1.7	192
96	Amine-modified MCM-41 mesoporous silica for carbon dioxide capture. Microporous and Mesoporous Materials, 2011, 143, 174-179.	2.2	289
97	Using Pressure to Provoke the Structural Transition of Metalâ€“Organic Frameworks. Angewandte Chemie, 2010, 122, 7688-7691.	1.6	34
98	Controlled Reducibility of a Metalâ€“Organic Framework with Coordinatively Unsaturated Sites for Preferential Gas Sorption. Angewandte Chemie - International Edition, 2010, 49, 5949-5952.	7.2	526
99	Using Pressure to Provoke the Structural Transition of Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2010, 49, 7526-7529.	7.2	200
100	Green solvent extraction of a triblock copolymer from mesoporous silica: Application to the adsorption of carbon dioxide under static and dynamic conditions. Microporous and Mesoporous Materials, 2010, 128, 26-33.	2.2	15
101	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. Microporous and Mesoporous Materials, 2010, 135, 187-196.	2.2	129
102	Na⁺ Charge Tuning through Encapsulation of Sulfur Chromophores in Zeolite A and the Consequences in Adsorbent Properties. Journal of Physical Chemistry C, 2010, 114, 7880-7887.	1.5	8
103	Multistep N₂ Breathing in the Metalâˆ’Organic Framework Co(1,4-benzenedipyrazolate). Journal of the American Chemical Society, 2010, 132, 13782-13788.	6.6	220
104	Influence of [Mo₆Br₈F₆]^{2âˆ’}Cluster Unit Inclusion within the Mesoporous Solid MIL-101 on Hydrogen Storage Performance. Langmuir, 2010, 26, 11283-11290.	1.6	59
105	Explanation of the Adsorption of Polar Vapors in the Highly Flexible Metal Organic Framework MIL-53(Cr). Journal of the American Chemical Society, 2010, 132, 9488-9498.	6.6	185
106	Self and Transport Diffusivity of CO₂ in the Metalâˆ’Organic Framework MIL-47(V) Explored by Quasi-elastic Neutron Scattering Experiments and Molecular Dynamics Simulations. ACS Nano, 2010, 4, 143-152.	7.3	109
107	Adsorption of CO and CO₂ in Large Pore Sized Ag@SiO₂ Nanocomposite. Journal of Physical Chemistry C, 2010, 114, 22652-22658.	1.5	14
108	Adsorption of light hydrocarbons in the flexible MIL-53(Cr) and rigid MIL-47(V) metalâ€“organic frameworks: a combination of molecular simulations and microcalorimetry/gravimetry measurements. Physical Chemistry Chemical Physics, 2010, 12, 6428.	1.3	82

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109	Transport Diffusivity of CO₂ in the Highly Flexible Metalâ€“Organic Framework MILâ€53(Cr). Angewandte Chemie - International Edition, 2009, 48, 8335-8339.	7.2	109
110	Adsorption of CO2, CH4 and their binary mixture in Faujasite NaY: A combination of molecular simulations with gravimetryâ€“manometry and microcalorimetry measurements. Microporous and Mesoporous Materials, 2009, 119, 117-128.	2.2	86
111	Impregnation of vitamin E acetate on silica mesoporous phases using supercritical carbon dioxide. Journal of Supercritical Fluids, 2009, 51, 278-286.	1.6	48
112	Microporosity of carbon deposits collected in the Tore Supra tokamak probed by nitrogen and carbon dioxide adsorption. Carbon, 2009, 47, 109-116.	5.4	7
113	Co-adsorption and Separation of CO₂â^'CH₄ Mixtures in the Highly Flexible MIL-53(Cr) MOF. Journal of the American Chemical Society, 2009, 131, 17490-17499.	6.6	398
114	Complex Adsorption of Short Linear Alkanes in the Flexible Metal-Organic-Framework MIL-53(Fe). Journal of the American Chemical Society, 2009, 131, 13002-13008.	6.6	281
115	Single Crystal X-ray Diffraction Studies of Carbon Dioxide and Fuel-Related Gases Adsorbed on the Small Pore Scandium Terephthalate Metal Organic Framework, Sc₂(O₂CC₆H₄CO₂)₃. Langmuir, 2009, 25, 3618-3626.	1.6	91
116	Occurrence of Uncommon Infinite Chains Consisting of Edge-Sharing Octahedra in a Porous Metal Organic Framework-Type Aluminum Pyromellitate Al₄(OH)₈[C₁₀O₈H₂] (MIL-120): Synthesis, Structure, and Gas Sorption Properties. Chemistry of Materials, 2009, 21, 5783-5791.	3.2	102
117	On Defining a Simple Empirical Relationship to Predict the Pore Size of Mesoporous Silicas Prepared from PEO-<i>b</i>-PS Diblock Copolymers. Chemistry of Materials, 2009, 21, 48-55.	3.2	43
118	Adsorption and Diffusion of H₂ in the MOF Type Systems MIL-47(V) and MIL-53(Cr): A Combination of Microcalorimetry and QENS Experiments with Molecular Simulations. Journal of Physical Chemistry C, 2009, 113, 7802-7812.	1.5	89
119	Study of Carbon Dioxide Adsorption on Mesoporous Aminopropylsilane-Functionalized Silica and Titania Combining Microcalorimetry and in Situ Infrared Spectroscopy. Journal of Physical Chemistry C, 2009, 113, 21726-21734.	1.5	220
120	Adsorption of carbon dioxide in SAPO STA-7 and AlPO-18: Grand Canonical Monte Carlo simulations andÂmicrocalorimetry measurements. Adsorption, 2008, 14, 207-213.	1.4	41
121	Quasiâ€Elastic Neutron Scattering and Molecular Dynamics Study of Methane Diffusion in Metal Organic Frameworks MILâ€47(V) and MILâ€53(Cr). Angewandte Chemie - International Edition, 2008, 47, 6611-6615.	7.2	154
122	Silicon distribution in SAPO materials: A computational study of STA-7 Combined to 29Si MAS NMR spectroscopy. Microporous and Mesoporous Materials, 2008, 107, 268-275.	2.2	8
123	Direct synthesis of mesoporous silica presenting large and tunable pores using BAB triblock copolymers: Influence of each copolymer block on the porous structure. Microporous and Mesoporous Materials, 2008, 112, 612-620.	2.2	43
124	Amine-modified SBA-12 mesoporous silica for carbon dioxide capture: Effect of amine basicity on sorption properties. Microporous and Mesoporous Materials, 2008, 116, 358-364.	2.2	272
125	High Uptakes of CO₂ and CH₄ in Mesoporous Metalâ€"Organic Frameworks MIL-100 and MIL-101. Langmuir, 2008, 24, 7245-7250.	1.6	1,067
126	Prediction of the Conditions for Breathing of Metal Organic Framework Materials Using a Combination of X-ray Powder Diffraction, Microcalorimetry, and Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 12808-12814.	6.6	246

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127	Structural Transformations and Adsorption of Fuel-Related Gases of a Structurally Responsive Nickel Phosphonate Metalâ^'Organic Framework, Ni-STA-12. Journal of the American Chemical Society, 2008, 130, 15967-15981.	6.6	175
128	Hydrocarbon Adsorption in the Flexible Metal Organic Frameworks MIL-53(Al, Cr). Journal of the American Chemical Society, 2008, 130, 16926-16932.	6.6	244
129	Probing the Adsorption Sites for CO₂ in Metal Organic Frameworks Materials MIL-53 (Al,) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	137
130	Experimental Evidence Supported by Simulations of a Very High<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Diffusion in Metal Organic Framework Materials. Physical Review Letters, 2008, 100, 245901.	2.9	99
131	Influence of the Silicon Content and Chemical Disorder of the SAPO STA-7 Framework on the CO₂ Adsorption Mechanism:â€‰ Grand Canonical Monte Carlo Simulations Combined to Microcalorimetry Measurements. Journal of Physical Chemistry C, 2008, 112, 5048-5056.	1.5	17
132	Microcalorimetric Investigation of High-Surface-Area Mesoporous Titania Samples for CO₂ Adsorption. Langmuir, 2008, 24, 7963-7969.	1.6	17
133	A diffuse reflectance fourier transform infra-red study of carbon dioxide adsorption on silicalite-I. Journal of Chemical Technology and Biotechnology, 2007, 52, 473-480.	1.6	5
134	Characterization of Fine Grain Ba0.995Y0.005TiO3 Ceramics Obtained from Gelâ€"Precursor Nanopowder. Journal of Nanoscience and Nanotechnology, 2007, 7, 1014-1020.	0.9	0
135	On the breathing effect of a metalâ€"organic framework upon CO2 adsorption: Monte Carlo compared to microcalorimetry experiments. Chemical Communications, 2007, , 3261.	2.2	137
136	Gas Adsorption in Zeolites and Related Materials. Studies in Surface Science and Catalysis, 2007, 168, 555-XVI.	1.5	14
137	Charge distribution in metal organic framework materials: transferability to a preliminary molecular simulation study of the CO2adsorption in the MIL-53 (Al) system. Physical Chemistry Chemical Physics, 2007, 9, 1059-1063.	1.3	112
138	Evidence of CO2 molecule acting as an electron acceptor on a nanoporous metalâ€"organic-framework MIL-53 or Cr3+(OH)(O2Câ€"C6H4â€"CO2). Chemical Communications, 2007, , 3291.	2.2	117
139	Is the bet equation applicable to microporous adsorbents?. Studies in Surface Science and Catalysis, 2007, 160, 49-56.	1.5	759
140	An Explanation for the Very Large Breathing Effect of a Metalâ€"Organic Framework during CO₂ Adsorption. Advanced Materials, 2007, 19, 2246-2251.	11.1	501
141	Some aspects of thermal decomposition of NiC2O4Â·2H2O. Thermochimica Acta, 2007, 466, 57-62.	1.2	47
142	Diversity of carboxylate coordination in two novel zinc(II) cinnamate complexes. Inorganic Chemistry Communication, 2007, 10, 27-32.	1.8	30
143	Investigation of CO2 adsorption in Faujasite systems: Grand Canonical Monte Carlo and molecular dynamics simulations based on a new derived Na+â€"CO2 force field. Microporous and Mesoporous Materials, 2007, 99, 70-78.	2.2	58
144	Structural and dynamic properties of confined hydrogen isotopes (H2, HD, D2) in model porous materials: Silicalite-I, AlPO4-N family (N=5, 8, 11, 54) and MCM-41 (âˆ…=25Ã…). Microporous and Mesoporous Materials, 2007, 101, 271-278.	2.2	14

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145	Functionalised micro-/mesoporous silica for the adsorption of carbon dioxide. Microporous and Mesoporous Materials, 2007, 99, 79-85.	2.2	216
146	Diffusion of CO2 in NaY and NaX Faujasite systems: Quasi-elastic neutron scattering experiments and molecular dynamics simulations. European Physical Journal: Special Topics, 2007, 141, 127-132.	1.2	18
147	Ageing of wet-synthesized oxide powders. Journal of Thermal Analysis and Calorimetry, 2007, 88, 789-793.	2.0	8
148	Adsorption of CO2 in metal organic frameworks of different metal centres: Grand Canonical Monte Carlo simulations compared to experiments. Adsorption, 2007, 13, 461-467.	1.4	123
149	CO2 adsorption in LiY and NaY at high temperature: molecularÂsimulations compared to experiments. Adsorption, 2007, 13, 453-460.	1.4	38
150	CO2 diffusivity in LiY and NaY faujasite systems: aÂcombination of molecular dynamics simulations and quasi-elastic neutron scattering experiments. Adsorption, 2007, 13, 209-214.	1.4	11
151	Mesoporous Silica Modified with Titania:Â Structure and Thermal Stability. Chemistry of Materials, 2006, 18, 3184-3191.	3.2	65
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