

# Philip L Llewellyn

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/59610/publications.pdf>

Version: 2024-02-01

224  
papers

20,999  
citations

8172

76  
h-index

10152

140  
g-index

234  
all docs

234  
docs citations

234  
times ranked

15242  
citing authors

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

#	ARTICLE	IF	CITATIONS
19	Storage of Hydrogen on Nanoporous Adsorbents. <i>Green Energy and Technology</i> , 2019, , 255-286.	0.4	1
20	Investigating the effect of alumina shaping on the sorption properties of promising metal-organic frameworks. <i>RSC Advances</i> , 2019, 9, 7128-7135.	1.7	14
21	Microporous Lead-Organic Framework for Selective CO <sub>2</sub> Adsorption and Heterogeneous Catalysis. <i>Inorganic Chemistry</i> , 2018, 57, 1774-1786.	1.9	31
22	A promising metal-organic framework (MOF), MIL-96(Al), for CO <sub>2</sub> separation under humid conditions. <i>Journal of Materials Chemistry A</i> , 2018, 6, 2081-2090.	5.2	78
23	Metal-Organic Frameworks as Catalyst Supports: Influence of Lattice Disorder on Metal Nanoparticle Formation. <i>Chemistry - A European Journal</i> , 2018, 24, 7498-7506.	1.7	29
24	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19171-19179.	1.5	52
25	Synthesis of ZIF-11 Hybrid Nanoparticles via Post-Synthetic Modification of ZIF-90 and Their Use for H <sub>2</sub> /CO <sub>2</sub> Separation. <i>Chemistry - A European Journal</i> , 2018, 24, 11211-11219.	1.7	27
26	Study of methane and carbon dioxide adsorption capacity by synthetic nanoporous carbon based on pyrogallol-formaldehyde. <i>International Journal of Hydrogen Energy</i> , 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. <i>CrystEngComm</i> , 2017, 19, 1377-1388.	1.3	6
28	Using water adsorption measurements to access the chemistry of defects in the metal-organic framework UiO-66. <i>CrystEngComm</i> , 2017, 19, 4137-4141.	1.3	58
29	Screening the Effect of Water Vapour on Gas Adsorption Performance: Application to CO <sub>2</sub> Capture from Flue Gas in Metal-Organic Frameworks. <i>ChemSusChem</i> , 2017, 10, 1543-1553.	3.6	89
30	Modeling of adsorption of CO <sub>2</sub> in the deformed pores of MIL-53(Al). <i>Journal of Molecular Modeling</i> , 2017, 23, 101.	0.8	9
31	Investigating Unusual Organic Functional Groups to Engineer the Surface Chemistry of Mesoporous Silica to Tune CO <sub>2</sub> -Surface Interactions. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 14490-14496.	4.0	2
32	Adsorption-Induced Structural Phase Transformation in Nanopores. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16243-16246.	7.2	5
33	Adsorption-Induced Structural Phase Transformation in Nanopores. <i>Angewandte Chemie</i> , 2017, 129, 16461-16464.	1.6	2
34	Highly Efficient Proton Conduction in a Three-Dimensional Titanium Hydrogen Phosphate. <i>Chemistry of Materials</i> , 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 CO <sub>2</sub> Capture. <i>Chemistry of Materials</i> , 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. <i>Journal of Porous Materials</i> , 2017, 24, 1-11.	1.3	18

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

#	ARTICLE	IF	CITATIONS
55	Highly Selective CO <sub>2</sub> Capture by Small Pore Scandium-Based Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 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. <i>Journal of Materials Chemistry A</i> , 2015, 3, 3294-3309.	5.2	174
57	Location of CO <sub>2</sub> during its uptake by the flexible porous metal-organic framework MIL-53(Fe): a high resolution powder X-ray diffraction study. <i>CrystEngComm</i> , 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 acid-base properties of flexible MOFs. <i>Microporous and Mesoporous Materials</i> , 2014, 195, 197-204.	2.2	16
62	Conformation-Controlled Sorption Properties and Breathing of the Aliphatic Al-MOF [Al(OH)(CDC)]. <i>Inorganic Chemistry</i> , 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. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27470-27482.	1.5	84
64	High-Resolution N <sub>2</sub> Adsorption Isotherms at 77.4 K: Critical Effect of the He Used During Calibration. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16885-16889.	1.5	22
65	A robust amino-functionalized titanium(IV) based MOF for improved separation of acid gases. <i>Chemical Communications</i> , 2013, 49, 10082.	2.2	135
66	A Water Stable Metal-Organic Framework with Optimal Features for CO <sub>2</sub> Capture. <i>Angewandte Chemie</i> , 2013, 125, 10506-10510.	1.6	66
67	Evaluation of MIL-47(V) for CO <sub>2</sub> -Related Applications. <i>Journal of Physical Chemistry C</i> , 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 Metal-Organic Frameworks. <i>Langmuir</i> , 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). <i>ACS Combinatorial Science</i> , 2013, 15, 111-119.	3.8	48
70	Adsorption of Propane and Propylene on CuBTC Metal-Organic Framework: Combined Theoretical and Experimental Investigation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11159-11167.	1.5	48
71	A Water Stable Metal-Organic Framework with Optimal Features for CO <sub>2</sub> Capture. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 10316-10320.	7.2	303
72	High pressure methane adsorption on microporous carbon monoliths prepared by olives stones. <i>Materials Letters</i> , 2013, 99, 184-187.	1.3	31

#	ARTICLE	IF	CITATIONS
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	CH <sub>4</sub> storage and CO <sub>2</sub> capture in highly porous zirconium oxide based metal-organic frameworks. Chemical Communications, 2012, 48, 9831.	2.2	180
77	Separation of CO <sub>2</sub> -CH <sub>4</sub> 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 CO <sub>2</sub> 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 CO <sub>2</sub> 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 CO <sub>2</sub> . 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	Energy-Efficient Dehumidification over Hierarchically Porous Metal-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, CO <sub>2</sub> , propane, propene and propyne in the mesoporous metal-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 NH <sub>2</sub> and CF <sub>3</sub> 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

#	ARTICLE	IF	CITATIONS
91	Understanding CO <sub>2</sub> Adsorption in CuBTC MOF: Comparing Combined DFT <sup>ab Initio</sup> Calculations with Microcalorimetry Experiments. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17925-17933.	1.5	146
92	Understanding the Thermodynamic and Kinetic Behavior of the CO <sub>2</sub> /CH <sub>4</sub> Gas Mixture within the Porous Zirconium Terephthalate UiO-66(Zr): A Joint Experimental and Modeling Approach. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13768-13774.	1.5	166
93	Why hybrid porous solids capture greenhouse gases?. <i>Chemical Society Reviews</i> , 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. <i>Microporous and Mesoporous Materials</i> , 2011, 146, 36-47.	2.2	44
95	An Evaluation of UiO-66 for Gas-Based Applications. <i>Chemistry - an Asian Journal</i> , 2011, 6, 3270-3280.	1.7	192
96	Amine-modified MCM-41 mesoporous silica for carbon dioxide capture. <i>Microporous and Mesoporous Materials</i> , 2011, 143, 174-179.	2.2	289
97	Using Pressure to Provoke the Structural Transition of Metal-Organic Frameworks. <i>Angewandte Chemie</i> , 2010, 122, 7688-7691.	1.6	34
98	Controlled Reducibility of a Metal-Organic Framework with Coordinatively Unsaturated Sites for Preferential Gas Sorption. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 5949-5952.	7.2	526
99	Using Pressure to Provoke the Structural Transition of Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 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. <i>Microporous and Mesoporous Materials</i> , 2010, 128, 26-33.	2.2	15
101	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. <i>Microporous and Mesoporous Materials</i> , 2010, 135, 187-196.	2.2	129
102	Na <sup>+</sup> Charge Tuning through Encapsulation of Sulfur Chromophores in Zeolite A and the Consequences in Adsorbent Properties. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7880-7887.	1.5	8
103	Multistep N <sub>2</sub> Breathing in the Metal-Organic Framework Co(1,4-benzenedipyrazolate). <i>Journal of the American Chemical Society</i> , 2010, 132, 13782-13788.	6.6	220
104	Influence of [Mo <sub>6</sub> Br <sub>8</sub> F <sub>6</sub> ] <sup>2+</sup> Cluster Unit Inclusion within the Mesoporous Solid MIL-101 on Hydrogen Storage Performance. <i>Langmuir</i> , 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). <i>Journal of the American Chemical Society</i> , 2010, 132, 9488-9498.	6.6	185
106	Self and Transport Diffusivity of CO <sub>2</sub> in the Metal-Organic Framework MIL-47(V) Explored by Quasi-elastic Neutron Scattering Experiments and Molecular Dynamics Simulations. <i>ACS Nano</i> , 2010, 4, 143-152.	7.3	109
107	Adsorption of CO and CO <sub>2</sub> in Large Pore Sized Ag@SiO <sub>2</sub> Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22652-22658.	1.5	14
108	Adsorption of light hydrocarbons in the flexible MIL-53(Cr) and rigid MIL-47(V) metal-organic frameworks: a combination of molecular simulations and microcalorimetry/gravimetry measurements. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6428.	1.3	82

#	ARTICLE	IF	CITATIONS
109	Transport Diffusivity of CO <sub>2</sub> in the Highly Flexible Metal-Organic Framework MIL-53(Cr). <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8335-8339.	7.2	109
110	Adsorption of CO <sub>2</sub> , CH <sub>4</sub> and their binary mixture in Faujasite NaY: A combination of molecular simulations with gravimetry-manometry and microcalorimetry measurements. <i>Microporous and Mesoporous Materials</i> , 2009, 119, 117-128.	2.2	86
111	Impregnation of vitamin E acetate on silica mesoporous phases using supercritical carbon dioxide. <i>Journal of Supercritical Fluids</i> , 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. <i>Carbon</i> , 2009, 47, 109-116.	5.4	7
113	Co-adsorption and Separation of CO <sub>2</sub> and CH <sub>4</sub> Mixtures in the Highly Flexible MIL-53(Cr) MOF. <i>Journal of the American Chemical Society</i> , 2009, 131, 17490-17499.	6.6	398
114	Complex Adsorption of Short Linear Alkanes in the Flexible Metal-Organic-Framework MIL-53(Fe). <i>Journal of the American Chemical Society</i> , 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, Sc <sub>2</sub> (O <sub>2</sub> CC <sub>6</sub> H <sub>4</sub> CO) <sub>3</sub> . <i>Langmuir</i> , 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 Al <sub>4</sub> (OH) <sub>8</sub> [C <sub>10</sub> O <sub>8</sub> H <sub>2</sub> ] (MIL-120): Synthesis, Structure, and Gas Sorption Properties. <i>Chemistry of Materials</i> , 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. <i>Chemistry of Materials</i> , 2009, 21, 48-55.	3.2	43
118	Adsorption and Diffusion of H <sub>2</sub> in the MOF Type Systems MIL-47(V) and MIL-53(Cr): A Combination of Microcalorimetry and QENS Experiments with Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 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. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21726-21734.	1.5	220
120	Adsorption of carbon dioxide in SAPO STA-7 and AlPO-18: Grand Canonical Monte Carlo simulations and microcalorimetry measurements. <i>Adsorption</i> , 2008, 14, 207-213.	1.4	41
121	Quasi-Elastic Neutron Scattering and Molecular Dynamics Study of Methane Diffusion in Metal Organic Frameworks MIL-47(V) and MIL-53(Cr). <i>Angewandte Chemie - International Edition</i> , 2008, 47, 6611-6615.	7.2	154
122	Silicon distribution in SAPO materials: A computational study of STA-7 Combined to <sup>29</sup> Si MAS NMR spectroscopy. <i>Microporous and Mesoporous Materials</i> , 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. <i>Microporous and Mesoporous Materials</i> , 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. <i>Microporous and Mesoporous Materials</i> , 2008, 116, 358-364.	2.2	272
125	High Uptakes of CO <sub>2</sub> and CH <sub>4</sub> in Mesoporous Metal-Organic Frameworks MIL-100 and MIL-101. <i>Langmuir</i> , 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. <i>Journal of the American Chemical Society</i> , 2008, 130, 12808-12814.	6.6	246

#	ARTICLE	IF	CITATIONS
127	Structural Transformations and Adsorption of Fuel-Related Gases of a Structurally Responsive Nickel Phosphonate Metal-Organic Framework, Ni-STA-12. <i>Journal of the American Chemical Society</i> , 2008, 130, 15967-15981.	6.6	175
128	Hydrocarbon Adsorption in the Flexible Metal Organic Frameworks MIL-53(Al, Cr). <i>Journal of the American Chemical Society</i> , 2008, 130, 16926-16932.	6.6	244
129	Probing the Adsorption Sites for CO <sub>2</sub> in Metal Organic Frameworks Materials MIL-53 (Al). <i>Journal of Physical Chemistry B</i> , 2008, 112, 15743-15751.	1.5	187
130	Experimental Evidence Supported by Simulations of a Very High Hydrogen Diffusion in Metal Organic Framework Materials. <i>Physical Review Letters</i> , 2008, 100, 245901.	2.9	99
131	Influence of the Silicon Content and Chemical Disorder of the SAPO STA-7 Framework on the CO <sub>2</sub> Adsorption Mechanism: Grand Canonical Monte Carlo Simulations Combined to Microcalorimetry Measurements. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5048-5056.	1.5	17
132	Microcalorimetric Investigation of High-Surface-Area Mesoporous Titania Samples for CO <sub>2</sub> Adsorption. <i>Langmuir</i> , 2008, 24, 7963-7969.	1.6	17
133	A diffuse reflectance fourier transform infra-red study of carbon dioxide adsorption on silicalite-I. <i>Journal of Chemical Technology and Biotechnology</i> , 2007, 52, 473-480.	1.6	5
134	Characterization of Fine Grain Ba <sub>0.995</sub> Y <sub>0.005</sub> TiO <sub>3</sub> Ceramics Obtained from Gel-Precursor Nanopowder. <i>Journal of Nanoscience and Nanotechnology</i> , 2007, 7, 1014-1020.	0.9	0
135	On the breathing effect of a metal-organic framework upon CO <sub>2</sub> adsorption: Monte Carlo compared to microcalorimetry experiments. <i>Chemical Communications</i> , 2007, , 3261.	2.2	137
136	Gas Adsorption in Zeolites and Related Materials. <i>Studies in Surface Science and Catalysis</i> , 2007, 168, 555-XVI.	1.5	14
137	Charge distribution in metal organic framework materials: transferability to a preliminary molecular simulation study of the CO <sub>2</sub> adsorption in the MIL-53 (Al) system. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1059-1063.	1.3	112
138	Evidence of CO <sub>2</sub> molecule acting as an electron acceptor on a nanoporous metal-organic-framework MIL-53 or Cr <sup>3+</sup> (OH)(O <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> ). <i>Chemical Communications</i> , 2007, , 3291.	2.2	117
139	Is the bet equation applicable to microporous adsorbents?. <i>Studies in Surface Science and Catalysis</i> , 2007, 160, 49-56.	1.5	759
140	An Explanation for the Very Large Breathing Effect of a Metal-Organic Framework during CO <sub>2</sub> Adsorption. <i>Advanced Materials</i> , 2007, 19, 2246-2251.	11.1	501
141	Some aspects of thermal decomposition of NiC <sub>2</sub> O <sub>4</sub> ·2H <sub>2</sub> O. <i>Thermochimica Acta</i> , 2007, 466, 57-62.	1.2	47
142	Diversity of carboxylate coordination in two novel zinc(II) cinnamate complexes. <i>Inorganic Chemistry Communication</i> , 2007, 10, 27-32.	1.8	30
143	Investigation of CO <sub>2</sub> adsorption in Faujasite systems: Grand Canonical Monte Carlo and molecular dynamics simulations based on a new derived Na <sup>+</sup> CO <sub>2</sub> force field. <i>Microporous and Mesoporous Materials</i> , 2007, 99, 70-78.	2.2	58
144	Structural and dynamic properties of confined hydrogen isotopes (H <sub>2</sub> , HD, D <sub>2</sub> ) in model porous materials: Silicalite-I, AlPO <sub>4</sub> -N family (N=5, 8, 11, 54) and MCM-41 (n=25). <i>Microporous and Mesoporous Materials</i> , 2007, 101, 271-278.	2.2	14

#	ARTICLE	IF	CITATIONS
145	Functionalised micro-/mesoporous silica for the adsorption of carbon dioxide. <i>Microporous and Mesoporous Materials</i> , 2007, 99, 79-85.	2.2	216
146	Diffusion of CO <sub>2</sub> in NaY and NaX Faujasite systems: Quasi-elastic neutron scattering experiments and molecular dynamics simulations. <i>European Physical Journal: Special Topics</i> , 2007, 141, 127-132.	1.2	18
147	Ageing of wet-synthesized oxide powders. <i>Journal of Thermal Analysis and Calorimetry</i> , 2007, 88, 789-793.	2.0	8
148	Adsorption of CO <sub>2</sub> in metal organic frameworks of different metal centres: Grand Canonical Monte Carlo simulations compared to experiments. <i>Adsorption</i> , 2007, 13, 461-467.	1.4	123
149	CO <sub>2</sub> adsorption in LiY and NaY at high temperature: molecular simulations compared to experiments. <i>Adsorption</i> , 2007, 13, 453-460.	1.4	38
150	CO <sub>2</sub> diffusivity in LiY and NaY faujasite systems: a combination of molecular dynamics simulations and quasi-elastic neutron scattering experiments. <i>Adsorption</i> , 2007, 13, 209-214.	1.4	11
151	Mesoporous Silica Modified with Titania: Structure and Thermal Stability. <i>Chemistry of Materials</i> , 2006, 18, 3184-3191.	3.2	65
152	Synthesis of MIL-102, a Chromium Carboxylate Metal-Organic Framework, with Gas Sorption Analysis. <i>Journal of the American Chemical Society</i> , 2006, 128, 14889-14896.	6.6	229
153	Thermal Stability and Thermodynamic Properties of Hybrid Proton-Conducting Polyaryl Etherketones. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15817-15823.	1.2	49
154	Molecular Dynamics Simulation of the Cation Motion upon Adsorption of CO <sub>2</sub> in Faujasite Zeolite Systems. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14372-14378.	1.2	58
155	CO <sub>2</sub> adsorption in alkali cation exchanged Y faujasites: A quantum chemical study compared to experiments. <i>Chemical Physics Letters</i> , 2006, 426, 387-392.	1.2	62
156	Simulation of the adsorption properties of CH <sub>4</sub> in faujasites up to high pressure: Comparison with microcalorimetry. <i>Microporous and Mesoporous Materials</i> , 2006, 89, 96-102.	2.2	25
157	Sol-gel synthesis and characterization of Ce doped-BaTiO <sub>3</sub> . <i>Journal of the European Ceramic Society</i> , 2006, 26, 3241-3246.	2.8	66
158	MIL-96, a Porous Aluminum Trimesate 3D Structure Constructed from a Hexagonal Network of 18-Membered Rings and 1/3-Oxo-Centered Trinuclear Units. <i>Journal of the American Chemical Society</i> , 2006, 128, 10223-10230.	6.6	386
159	Hydrogen Storage in the Giant-Pore Metal-Organic Frameworks MIL-100 and MIL-101. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 8227-8231.	7.2	716
160	How Hydration Drastically Improves Adsorption Selectivity for CO <sub>2</sub> over CH <sub>4</sub> in the Flexible Chromium Terephthalate MIL-53. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7751-7754.	7.2	412
161	Adsorption of argon and nitrogen in X-faujasites: relationships for understanding the interactions with monovalent and divalent cations. <i>Microporous and Mesoporous Materials</i> , 2005, 79, 53-59.	2.2	34
162	Zinc(II)-benzoate complexes immobilised in mesoporous silica host. <i>Microporous and Mesoporous Materials</i> , 2005, 83, 125-135.	2.2	25

#	ARTICLE	IF	CITATIONS
163	Gas adsorption microcalorimetry and modelling to characterise zeolites and related materials. <i>Comptes Rendus Chimie</i> , 2005, 8, 283-302.	0.2	124
164	Do the Differential Enthalpies of Adsorption Vary Between 77 K and 302 K? An Experimental Case Study of Argon and Nitrogen on Two Faujasite Type Zeolites. <i>Adsorption</i> , 2005, 11, 73-78.	1.4	9
165	Adsorption of Non Polar and Quadrupolar Gases in Siliceous Faujasite: Molecular Simulations and Experiments. <i>Adsorption</i> , 2005, 11, 331-336.	1.4	39
166	Nitrogen Adsorption on Divalent Cation Substituted X-Faujasites: Microcalorimetry and Monte Carlo Simulation. <i>Adsorption</i> , 2005, 11, 343-347.	1.4	2
167	Growth Mode of Hydrogen in Mesoporous MCM-41. <i>Adsorption and Neutron Scattering Coupled Studies</i> . <i>Adsorption</i> , 2005, 11, 679-684.	1.4	4
168	Constant transformation rate thermal analysis of $\text{HGdP}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ . <i>Journal of Thermal Analysis and Calorimetry</i> , 2005, 82, 783-789.	2.0	6
169	Influence of Extra-Framework Cations on the Adsorption Properties of X-Faujasite Systems: $\hat{\text{A}}$ Microcalorimetry and Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 125-129.	1.2	83
170	Different Adsorption Behaviors of Methane and Carbon Dioxide in the Isotypic Nanoporous Metal Terephthalates MIL-53 and MIL-47. <i>Journal of the American Chemical Society</i> , 2005, 127, 13519-13521.	6.6	1,005
171	Adsorption Mechanism of Carbon Dioxide in Faujasites: Grand Canonical Monte Carlo Simulations and Microcalorimetry Measurements. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16084-16091.	1.2	185
172	Argon and Nitrogen Adsorption in Disordered Nanoporous Carbons: $\hat{\text{A}}$ Simulation and Experiment. <i>Langmuir</i> , 2005, 21, 4431-4440.	1.6	56
173	A Zn(II)-Coordination Polymer Formed by Benzoate and 3-Pyridinemethanol Ligands: Synthesis, Spectroscopic Properties, Crystal Structure and Kinetics of Thermal Decomposition. <i>Journal of Coordination Chemistry</i> , 2004, 57, 87-96.	0.8	17
174	Calorimetry by immersion into liquid nitrogen and liquid argon: a better way to determine the internal surface area of micropores. <i>Journal of Colloid and Interface Science</i> , 2004, 277, 383-386.	5.0	3
175	Preparation and Electrical Properties of Dense Ceramics with NASICON Composition Sintered at Reduced Temperatures. <i>Journal of Electroceramics</i> , 2004, 13, 817-823.	0.8	13
176	Comparing the Basic Phenomena Involved in Three Methods of Pore-size Characterization: Gas Adsorption, Liquid Intrusion and Thermoporometry. <i>Particle and Particle Systems Characterization</i> , 2004, 21, 128-137.	1.2	21
177	Preparation, characterisation and crystal structure of two zinc(II) benzoate complexes with pyridine-based ligands nicotinamide and methyl-3-pyridylcarbamate. <i>Inorganica Chimica Acta</i> , 2004, 357, 2049-2059.	1.2	56
178	A comparison between melting-solidification and capillary condensation hysteresis in mesoporous materials: application to the interpretation of thermoporometry data. <i>Thermochimica Acta</i> , 2004, 421, 11-18.	1.2	48
179	Anomalous adsorption behavior observed during the characterization of a polystyrene film prepared on a mesoporous material. <i>Journal of Colloid and Interface Science</i> , 2004, 275, 48-52.	5.0	1
180	Modeling of pore wall amorphous structures: influence of wall heterogeneity on the mechanism of adsorption. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2004, 241, 137-142.	2.3	34

#	ARTICLE	IF	CITATIONS
181	Emanation thermal analysis study of synthetic gibbsite. <i>Journal of Thermal Analysis and Calorimetry</i> , 2003, 71, 773-782.	2.0	18
182	SCTA and Adsorbents. <i>Journal of Thermal Analysis and Calorimetry</i> , 2003, 72, 1099-1101.	2.0	5
183	Synthesis of Bi <sub>2</sub> O <sub>3</sub> by controlled transformation rate thermal analysis: a new route for this oxide?. <i>Solid State Ionics</i> , 2003, 157, 163-169.	1.3	73
184	Monte Carlo simulations of krypton adsorption in nanopores: Influence of pore-wall heterogeneity on the adsorption mechanism. <i>Low Temperature Physics</i> , 2003, 29, 880-882.	0.2	20
185	Characterising the porous structure of Egyptian mortars using thermoporometry, mercury intrusion porometry and gas adsorption manometry. <i>Studies in Surface Science and Catalysis</i> , 2002, 144, 435-441.	1.5	1
186	Assessing microporosity by immersion microcalorimetry into liquid nitrogen or liquid argon. <i>Studies in Surface Science and Catalysis</i> , 2002, , 171-176.	1.5	9
187	Complementarity of microcalorimetry, manometry and gravimetry in the study of gas adsorption by microporous solids up to 50bar. <i>Studies in Surface Science and Catalysis</i> , 2002, , 723-729.	1.5	3
188	Sorption of ammonia gas on the solid ion conductor Cu(i)Br. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 802-805.	1.3	10
189	Controlled Rate Thermal Analysis of kaolinite dehydroxylation: effect of water vapour pressure on the mechanism. <i>Thermochimica Acta</i> , 2002, 390, 123-132.	1.2	38
190	In situ surfactant removal from MCM-type mesostructures by ozone treatment. <i>Journal of Materials Chemistry</i> , 2001, 11, 589-593.	6.7	45
191	Use of sample controlled thermal analysis to liberate the micropores of aluminophosphate AlPO <sub>4</sub> -11: evidence of template evaporation. <i>Journal of Materials Chemistry</i> , 2001, 11, 1300-1304.	6.7	16
192	Investigation of the mechanism of the surfactant removal from a mesoporous alumina prepared in the presence of sodium dodecylsulfate. <i>Microporous and Mesoporous Materials</i> , 2001, 44-45, 195-201.	2.2	46
193	Characterisation of microporous materials by adsorption microcalorimetry. <i>Membrane Science and Technology</i> , 2000, , 213-230.	0.5	7
194	Low temperature constant rate thermodesorption as a tool to characterise porous solids. <i>Thermochimica Acta</i> , 2000, 360, 77-83.	1.2	11
195	Glass transition, freezing and melting of liquids confined in the mesoporous silicate MCM-41. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1999, 79, 1847-1855.	0.6	36
196	Thermal Methods in the Synthesis of New Ordered Mesoporous Adsorbents. <i>Magyar Árvad Kémlemlények</i> , 1999, 56, 261-266.	1.4	12
197	Calcination of the MCM-41 mesophase: mechanism of surfactant thermal degradation and evolution of the porosity. <i>Journal of Materials Chemistry</i> , 1999, 9, 2843-2849.	6.7	91
198	Deintercalation process of fluorinated carbon fibres. II. Kinetic study and reaction mechanisms. <i>Carbon</i> , 1998, 36, 1199-1205.	5.4	12

#	ARTICLE	IF	CITATIONS
199	Microcalorimetric Study of Argon, Nitrogen, and Carbon Monoxide Adsorption on Mesoporous Vycor Glass. <i>Journal of Colloid and Interface Science</i> , 1998, 206, 527-531.	5.0	14
200	Study of Gypsum Dehydration by Controlled Transformation Rate Thermal Analysis (CRTA). <i>Journal of Solid State Chemistry</i> , 1998, 139, 37-44.	1.4	46
201	Ozone treatment for the removal of surfactant to form MCM-41 type materials. <i>Chemical Communications</i> , 1998, , 2203-2204.	2.2	82
202	Deintercalation Process of Fluorinated Carbon Fibres. Part I - Controlled Rate Evolved Gas Analysis. <i>Molecular Crystals and Liquid Crystals</i> , 1998, 310, 111-118.	0.3	7
203	Multiple Features of a Porous Structure as Assessed from the Hysteresis of Nitrogen Adsorption/Desorption: Case Study of the Formation of UO <sub>3</sub> from UO <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O. <i>Langmuir</i> , 1998, 14, 4217-4221.	1.6	14
204	Controlled transformation rate thermal analysis: an inverse method allowing the characterisation of the thermal behaviour of polyphosphate glasses. <i>High Temperatures - High Pressures</i> , 1998, 30, 575-580.	0.3	7
205	Kinetic Study by Controlled-Transformation Rate Thermal Analysis of the Dehydroxylation of Kaolinite. <i>Clay Minerals</i> , 1998, 33, 269-276.	0.2	5
206	Dehydroxylation mechanisms of polyphosphate glasses in relation to temperature and pressure. <i>Journal of Non-Crystalline Solids</i> , 1997, 222, 415-421.	1.5	24
207	Characterization of polyphosphate glasses preparation using CRTA. <i>Journal of Theoretical Biology</i> , 1997, 49, 1171-1178.	0.8	10
208	Investigation of the dehydration of Y-TZP gels by Controlled transformation Rate Thermal Analysis. <i>Solid State Ionics</i> , 1997, 95, 23-28.	1.3	5
209	Preparation of reactive nickel oxide by the controlled thermolysis of hexahydrated nickel nitrate. <i>Solid State Ionics</i> , 1997, 101-103, 1293-1298.	1.3	21
210	Thermodynamic and structural properties of physisorbed phases within the model mesoporous adsorbent M41S (pore diameter 2.5 nm). <i>Surface Science</i> , 1996, 352-354, 468-474.	0.8	34
211	Water Sorption on Mesoporous Aluminosilicate MCM-41. <i>Langmuir</i> , 1995, 11, 574-577.	1.6	179
212	Effect of pore size on adsorbate condensation and hysteresis within a potential model adsorbent: M41S. <i>Microporous Materials</i> , 1994, 3, 345-349.	1.6	146
213	Quasi-equilibrium adsorption gravimetry of water on MFI- and FER™-type zeolites and on an AFI-type aluminophosphate. <i>Journal of Thermal Analysis</i> , 1994, 42, 855-867.	0.7	9
214	A microcalorimetric comparison of the effect of n-alkane preadsorption on the adsorption of argon and nitrogen on Silicalite-I. <i>Journal of Thermal Analysis</i> , 1994, 41, 1343-1356.	0.7	3
215	MCM-41 and related materials as media for controlled polymerization processes. <i>Studies in Surface Science and Catalysis</i> , 1994, 84, 2013-2020.	1.5	68
216	Effect of T(III) zoning in MFI-type zeolites on the adsorption isotherm and differential enthalpies of adsorption at 77 K. <i>Langmuir</i> , 1994, 10, 570-575.	1.6	9

#	ARTICLE	IF	CITATIONS
217	On the physisorption isotherm of the MFI-type zeolites: The high-pressure hysteresis. <i>Microporous Materials</i> , 1993, 1, 247-256.	1.6	18
218	Adsorption by MFI-type zeolites examined by isothermal microcalorimetry and neutron diffraction. 2. Nitrogen and carbon monoxide. <i>Langmuir</i> , 1993, 9, 1852-1856.	1.6	120
219	Adsorption by MFI-type zeolites examined by isothermal microcalorimetry and neutron diffraction. 1. Argon, krypton, and methane. <i>Langmuir</i> , 1993, 9, 1846-1851.	1.6	122
220	Adsorption of Argon, Methane, Nitrogen, Carbon Monoxide and Water Vapour on Sepiolite and Alpo4-5 as Studied by Isothermal Microcalorimetry. <i>Studies in Surface Science and Catalysis</i> , 1993, , 235-242.	1.5	6
221	Evaluation of the n-nonane preadsorption method with a well characterized model adsorbent: Silicalite-I. <i>Pure and Applied Chemistry</i> , 1993, 65, 2157-2167.	0.9	13
222	A microcalorimetric comparison of the adsorption of various gases on two microporous adsorbents: a model aluminophosphate and a natural clay. <i>Thermochimica Acta</i> , 1992, 204, 79-88.	1.2	26
223	A microcalorimetric study of the different states of argon and nitrogen adsorbed AT 77 K on silicalite-I and ZSM-5. <i>Journal of Thermal Analysis</i> , 1992, 38, 683-692.	0.7	17
224	Adsorption Methodology. , 0, , 575-605.		1