

Philip L Llewellyn

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	High Uptakes of CO ₂ and CH ₄ in Mesoporous Metal-Organic Frameworks MIL-100 and MIL-101. <i>Langmuir</i> , 2008, 24, 7245-7250.	1.6	1,067
2	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
3	Methane storage in flexible metal-organic frameworks with intrinsic thermal management. <i>Nature</i> , 2015, 527, 357-361.	13.7	817
4	Is the bet equation applicable to microporous adsorbents?. <i>Studies in Surface Science and Catalysis</i> , 2007, 160, 49-56.	1.5	759
5	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
6	Why hybrid porous solids capture greenhouse gases?. <i>Chemical Society Reviews</i> , 2011, 40, 550-562.	18.7	603
7	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
8	An Explanation for the Very Large Breathing Effect of a Metal-Organic Framework during CO ₂ Adsorption. <i>Advanced Materials</i> , 2007, 19, 2246-2251.	11.1	501
9	How Hydration Drastically Improves Adsorption Selectivity for CO ₂ over CH ₄ in the Flexible Chromium Terephthalate MIL-53. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7751-7754.	7.2	412
10	Co-adsorption and Separation of CO ₂ and CH ₄ Mixtures in the Highly Flexible MIL-53(Cr) MOF. <i>Journal of the American Chemical Society</i> , 2009, 131, 17490-17499.	6.6	398
11	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
12	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration. <i>Chemical Communications</i> , 2011, 47, 9603.	2.2	345
13	A Water Stable Metal-Organic Framework with Optimal Features for CO ₂ Capture. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 10316-10320.	7.2	303
14	Energy-Efficient Dehumidification over Hierarchically Porous Metal-Organic Frameworks as Advanced Water Adsorbents. <i>Advanced Materials</i> , 2012, 24, 806-810.	11.1	298
15	Amine-modified MCM-41 mesoporous silica for carbon dioxide capture. <i>Microporous and Mesoporous Materials</i> , 2011, 143, 174-179.	2.2	289
16	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
17	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
18	Effect of NH ₂ and CF ₃ functionalization on the hydrogen sorption properties of MOFs. <i>Dalton Transactions</i> , 2011, 40, 4879.	1.6	257

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19	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
20	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
21	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
22	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
23	Multistep N ₂ Breathing in the Metal-Organic Framework Co(1,4-benzenedipyrzolate). <i>Journal of the American Chemical Society</i> , 2010, 132, 13782-13788.	6.6	220
24	Functionalised micro-/mesoporous silica for the adsorption of carbon dioxide. <i>Microporous and Mesoporous Materials</i> , 2007, 99, 79-85.	2.2	216
25	Using Pressure to Provoke the Structural Transition of Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7526-7529.	7.2	200
26	How Water Fosters a Remarkable 5-Fold Increase in Low-Pressure CO ₂ Uptake within Mesoporous MIL-100(Fe). <i>Journal of the American Chemical Society</i> , 2012, 134, 10174-10181.	6.6	198
27	Infrared study of the influence of reducible iron(III) metal sites on the adsorption of CO, CO ₂ , propane, propene and propyne in the mesoporous metal-organic framework MIL-100. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11748.	1.3	192
28	An Evaluation of UiO-66 for Gas-Based Applications. <i>Chemistry - an Asian Journal</i> , 2011, 6, 3270-3280.	1.7	192
29	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
30	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
31	CH ₄ storage and CO ₂ capture in highly porous zirconium oxide based metal-organic frameworks. <i>Chemical Communications</i> , 2012, 48, 9831.	2.2	180
32	Water Sorption on Mesoporous Aluminosilicate MCM-41. <i>Langmuir</i> , 1995, 11, 574-577.	1.6	179
33	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
34	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
35	Understanding the Thermodynamic and Kinetic Behavior of the CO ₂ /CH ₄ 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
36	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

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37	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
38	Understanding CO ₂ Adsorption in CuBTC MOF: Comparing Combined DFTâ€‘ab Initio Calculations with Microcalorimetry Experiments. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17925-17933.	1.5	146
39	On the breathing effect of a metalâ€‘organic framework upon CO ₂ adsorption: Monte Carlo compared to microcalorimetry experiments. <i>Chemical Communications</i> , 2007, , 3261.	2.2	137
40	Probing the Adsorption Sites for CO ₂ in Metal Organic Frameworks Materials MIL-53 (Al). <i>Journal of Physical Chemistry C</i> , 2011, 115, 10764-10776.	1.5	137
41	A robust amino-functionalized titanium(iv) based MOF for improved separation of acid gases. <i>Chemical Communications</i> , 2013, 49, 10082.	2.2	135
42	An Adsorbent Performance Indicator as a First Step Evaluation of Novel Sorbents for Gas Separations: Application to Metalâ€‘Organic Frameworks. <i>Langmuir</i> , 2013, 29, 3301-3309.	1.6	131
43	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. <i>Microporous and Mesoporous Materials</i> , 2010, 135, 187-196.	2.2	129
44	Tuning the breathing behaviour of MIL-53 by cation mixing. <i>Chemical Communications</i> , 2012, 48, 10237.	2.2	129
45	Molecular Insight into the Adsorption and Diffusion of Water in the Versatile Hydrophilic/Hydrophobic Flexible MIL-53(Cr) MOF. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10764-10776.	1.5	128
46	Effect of the organic functionalization of flexible MOFs on the adsorption of CO ₂ . <i>Journal of Materials Chemistry</i> , 2012, 22, 10266.	6.7	125
47	Gas adsorption microcalorimetry and modelling to characterise zeolites and related materials. <i>Comptes Rendus Chimie</i> , 2005, 8, 283-302.	0.2	124
48	Adsorption of CO ₂ 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
49	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
50	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
51	Evidence of CO ₂ molecule acting as an electron acceptor on a nanoporous metalâ€‘organic-framework MIL-53 or Cr ₃ (OH)(O ₂ Câ€‘C ₆ H ₄ â€‘CO ₂). <i>Chemical Communications</i> , 2007, , 3291.	2.2	117
52	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
53	Charge distribution in metal organic framework materials: transferability to a preliminary molecular simulation study of the CO ₂ adsorption in the MIL-53 (Al) system. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1059-1063.	1.3	112
54	Transport Diffusivity of CO ₂ in the Highly Flexible Metalâ€‘Organic Framework MILâ€‘53(Cr). <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8335-8339.	7.2	109

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55	Self and Transport Diffusivity of CO ₂ in the Metal-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
56	A Method for Screening the Potential of MOFs as CO ₂ Adsorbents in Pressure Swing Adsorption Processes. ChemSusChem, 2012, 5, 762-776.	3.6	109
57	Mechanical energy storage performance of an aluminum fumarate metal-organic framework. Chemical Science, 2016, 7, 446-450.	3.7	103
58	Occurrence of Uncommon Infinite Chains Consisting of Edge-Sharing Octahedra in a Porous Metal Organic Framework-Type Aluminum Pyromellitate Al ₄ (OH) ₈ [C ₁₀ O ₈ H ₂] (MIL-120): Synthesis, Structure, and Gas Sorption Properties. Chemistry of Materials, 2009, 21, 5783-5791.	3.2	102
59	Experimental Evidence Supported by Simulations of a Very High Diffusion in Metal Organic Framework Materials. Physical Review Letters, 2008, 100, 245901.	2.9	99
60	Metal-organic framework crystal-glass composites. Nature Communications, 2019, 10, 2580.	5.8	97
61	Adsorption of CO ₂ on amine-functionalised MCM-41: experimental and theoretical studies. Physical Chemistry Chemical Physics, 2015, 17, 11095-11102.	1.3	93
62	Calcination of the MCM-41 mesophase: mechanism of surfactant thermal degradation and evolution of the porosity. Journal of Materials Chemistry, 1999, 9, 2843-2849.	6.7	91
63	Single Crystal X-ray Diffraction Studies of Carbon Dioxide and Fuel-Related Gases Adsorbed on the Small Pore Scandium Terephthalate Metal Organic Framework, Sc ₂ (O ₂ CC ₆ H ₄ CO ₂) ₃ . Langmuir, 2009, 25, 3618-3626.	1.6	91
64	Adsorption and Diffusion of H ₂ 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
65	Screening the Effect of Water Vapour on Gas Adsorption Performance: Application to CO ₂ Capture from Flue Gas in Metal-Organic Frameworks. ChemSusChem, 2017, 10, 1543-1553.	3.6	89
66	Tailoring the separation properties of flexible metal-organic frameworks using mechanical pressure. Nature Communications, 2020, 11, 1216.	5.8	88
67	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
68	Adsorption of CO ₂ , CH ₄ and their binary mixture in Faujasite NaY: A combination of molecular simulations with gravimetry-manometry and microcalorimetry measurements. Microporous and Mesoporous Materials, 2009, 119, 117-128.	2.2	86
69	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
70	Influence of Extra-Framework Cations on the Adsorption Properties of X-Faujasite Systems: A Microcalorimetry and Molecular Simulations. Journal of Physical Chemistry B, 2005, 109, 125-129.	1.2	83
71	Ozone treatment for the removal of surfactant to form MCM-41 type materials. Chemical Communications, 1998, , 2203-2204.	2.2	82
72	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. Physical Chemistry Chemical Physics, 2010, 12, 6428.	1.3	82

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73	MIL-91(Ti), a small pore metal-organic framework which fulfils several criteria: an upscaled green synthesis, excellent water stability, high CO ₂ selectivity and fast CO ₂ transport. <i>Journal of Materials Chemistry A</i> , 2016, 4, 1383-1389.	5.2	82
74	Separation of CO ₂ -CH ₄ mixtures in the mesoporous MIL-100(Cr) MOF: experimental and modelling approaches. <i>Dalton Transactions</i> , 2012, 41, 4052.	1.6	78
75	Revisiting the Aluminum Trimesate-Based MOF (MIL-96): From Structure Determination to the Processing of Mixed Matrix Membranes for CO ₂ Capture. <i>Chemistry of Materials</i> , 2017, 29, 10326-10338.	3.2	78
76	A promising metal-organic framework (MOF), MIL-96(Al), for CO ₂ separation under humid conditions. <i>Journal of Materials Chemistry A</i> , 2018, 6, 2081-2090.	5.2	78
77	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
78	Synthesis of Bi ₂ O ₃ by controlled transformation rate thermal analysis: a new route for this oxide?. <i>Solid State Ionics</i> , 2003, 157, 163-169.	1.3	73
79	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. <i>Nature Communications</i> , 2019, 10, 3632.	5.8	73
80	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
81	Sol-gel synthesis and characterization of Ce doped-BaTiO ₃ . <i>Journal of the European Ceramic Society</i> , 2006, 26, 3241-3246.	2.8	66
82	A Water Stable Metal-Organic Framework with Optimal Features for CO ₂ Capture. <i>Angewandte Chemie</i> , 2013, 125, 10506-10510.	1.6	66
83	Mesoporous Silica Modified with Titania: Structure and Thermal Stability. <i>Chemistry of Materials</i> , 2006, 18, 3184-3191.	3.2	65
84	Structural Origin of Unusual CO ₂ Adsorption Behavior of a Small-Pore Aluminum Bisphosphonate MOF. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4208-4216.	1.5	63
85	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
86	CO ₂ 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
87	Influence of [Mo ₆ Br ₈ F ₆] ²⁺ Cluster Unit Inclusion within the Mesoporous Solid MIL-101 on Hydrogen Storage Performance. <i>Langmuir</i> , 2010, 26, 11283-11290.	1.6	59
88	Molecular Dynamics Simulation of the Cation Motion upon Adsorption of CO ₂ in Faujasite Zeolite Systems. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14372-14378.	1.2	58
89	Investigation of CO ₂ adsorption in Faujasite systems: Grand Canonical Monte Carlo and molecular dynamics simulations based on a new derived Na ⁺ -CO ₂ force field. <i>Microporous and Mesoporous Materials</i> , 2007, 99, 70-78.	2.2	58
90	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

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91	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
92	Argon and Nitrogen Adsorption in Disordered Nanoporous Carbons: A Simulation and Experiment. <i>Langmuir</i> , 2005, 21, 4431-4440.	1.6	56
93	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. <i>ChemPhysChem</i> , 2012, 13, 488-495.	1.0	53
94	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
95	Influence of the Organic Ligand Functionalization on the Breathing of the Porous Iron Terephthalate Metal-Organic Framework Type Material upon Hydrocarbon Adsorption. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18683-18695.	1.5	50
96	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
97	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
98	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
99	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
100	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
101	Some aspects of thermal decomposition of NiC ₂ O ₄ ·2H ₂ O. <i>Thermochimica Acta</i> , 2007, 466, 57-62.	1.2	47
102	The Direct Heat Measurement of Mechanical Energy Storage Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 4626-4630.	7.2	47
103	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
104	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
105	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
106	In situ surfactant removal from MCM-type mesostructures by ozone treatment. <i>Journal of Materials Chemistry</i> , 2001, 11, 589-593.	6.7	45
107	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
108	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

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109	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
110	Adsorption of Carbon Dioxide on Mesoporous Zirconia: Microcalorimetric Measurements, Adsorption Isotherm Modeling, and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10097-10103.	1.5	43
111	Evaluation of MIL-47(V) for CO ₂ -Related Applications. <i>Journal of Physical Chemistry C</i> , 2013, 117, 962-970.	1.5	42
112	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
113	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
114	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
115	Adsorption of Non Polar and Quadrupolar Gases in Siliceous Faujasite: Molecular Simulations and Experiments. <i>Adsorption</i> , 2005, 11, 331-336.	1.4	39
116	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
117	CO ₂ adsorption in LiY and NaY at high temperature: molecular simulations compared to experiments. <i>Adsorption</i> , 2007, 13, 453-460.	1.4	38
118	Highly Selective CO ₂ Capture by Small Pore Scandium-Based Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23592-23598.	1.5	38
119	Class 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
120	Highly Efficient Proton Conduction in a Three-Dimensional Titanium Hydrogen Phosphate. <i>Chemistry of Materials</i> , 2017, 29, 7263-7271.	3.2	35
121	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
122	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
123	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
124	Using Pressure to Provoke the Structural Transition of Metal-Organic Frameworks. <i>Angewandte Chemie</i> , 2010, 122, 7688-7691.	1.6	34
125	pyGAPS: a Python-based framework for adsorption isotherm processing and material characterisation. <i>Adsorption</i> , 2019, 25, 1533-1542.	1.4	33
126	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

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127	High pressure methane adsorption on microporous carbon monoliths prepared by olives stones. <i>Materials Letters</i> , 2013, 99, 184-187.	1.3	31
128	Microporous Lead-Organic Framework for Selective CO ₂ Adsorption and Heterogeneous Catalysis. <i>Inorganic Chemistry</i> , 2018, 57, 1774-1786.	1.9	31
129	The CO ₂ adsorption behavior study on activated carbon synthesized from olive waste. <i>Journal of CO₂ Utilization</i> , 2020, 42, 101292.	3.3	31
130	Diversity of carboxylate coordination in two novel zinc(II) cinnamate complexes. <i>Inorganic Chemistry Communication</i> , 2007, 10, 27-32.	1.8	30
131	Engineering micromechanics of soft porous crystals for negative gas adsorption. <i>Chemical Science</i> , 2020, 11, 9468-9479.	3.7	30
132	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
133	Synthesis of ZIF-11 Hybrid Nanoparticles via Post-Synthetic Modification of ZIF-93 and Their Use for H ₂ /CO ₂ Separation. <i>Chemistry - A European Journal</i> , 2018, 24, 11211-11219.	1.7	27
134	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
135	Zinc(II)-benzoate complexes immobilised in mesoporous silica host. <i>Microporous and Mesoporous Materials</i> , 2005, 83, 125-135.	2.2	25
136	Simulation of the adsorption properties of CH ₄ in faujasites up to high pressure: Comparison with microcalorimetry. <i>Microporous and Mesoporous Materials</i> , 2006, 89, 96-102.	2.2	25
137	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
138	High-Resolution N ₂ 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
139	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
140	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
141	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
142	Acetylene and argon adsorption in a supramolecular organic zeolite. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 311-317.	1.3	20
143	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
144	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

#	ARTICLE	IF	CITATIONS
145	Location of CO ₂ 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
146	On the physisorption isotherm of the MFI-type zeolites: The high-pressure hysteresis. <i>Microporous Materials</i> , 1993, 1, 247-256.	1.6	18
147	Emanation thermal analysis study of synthetic gibbsite. <i>Journal of Thermal Analysis and Calorimetry</i> , 2003, 71, 773-782.	2.0	18
148	Diffusion of CO ₂ 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
149	Thermodynamics of the structural transition in metal-organic frameworks. <i>Dalton Transactions</i> , 2016, 45, 4274-4282.	1.6	18
150	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
151	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
152	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
153	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
154	Influence of the Silicon Content and Chemical Disorder of the SAPO STA-7 Framework on the CO ₂ 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
155	Microcalorimetric Investigation of High-Surface-Area Mesoporous Titania Samples for CO ₂ Adsorption. <i>Langmuir</i> , 2008, 24, 7963-7969.	1.6	17
156	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
157	Use of sample controlled thermal analysis to liberate the micropores of aluminophosphate AlPO ₄ -11: evidence of template evaporation. <i>Journal of Materials Chemistry</i> , 2001, 11, 1300-1304.	6.7	16
158	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
159	Data Mining for Binary Separation Materials in Published Adsorption Isotherms. <i>Chemistry of Materials</i> , 2020, 32, 982-991.	3.2	16
160	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
161	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
162	Multiple Features of a Porous Structure as Assessed from the Hysteresis of Nitrogen Adsorption-Desorption: Case Study of the Formation of UO ₃ from UO ₂ (NO ₃) ₂ ·6H ₂ O. <i>Langmuir</i> , 1998, 14, 4217-4221.	1.6	14

#	ARTICLE	IF	CITATIONS
163	Gas Adsorption in Zeolites and Related Materials. <i>Studies in Surface Science and Catalysis</i> , 2007, 168, 555-XVI.	1.5	14
164	Structural and dynamic properties of confined hydrogen isotopes (H ₂ , HD, D ₂) in model porous materials: Silicalite-I, AlPO ₄ -N family (N=5, 8, 11, 54) and MCM-41 (̂...=25Å...). <i>Microporous and Mesoporous Materials</i> , 2007, 101, 271-278.	2.2	14
165	Adsorption of CO and CO ₂ in Large Pore Sized Ag@SiO ₂ Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22652-22658.	1.5	14
166	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
167	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
168	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
169	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
170	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
171	Adsorption by Metal-Organic Frameworks. , 2014, , 565-610.		13
172	Deintercalation process of fluorinated carbon fibres-II. Kinetic study and reaction mechanisms. <i>Carbon</i> , 1998, 36, 1199-1205.	5.4	12
173	Thermal Methods in the Synthesis of New Ordered Mesoporous Adsorbents. <i>Magyar Árvad Kémlemlenyek</i> , 1999, 56, 261-266.	1.4	12
174	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
175	Effect of the both texture and electrical properties of activated carbon on the CO ₂ adsorption capacity. <i>Materials Research Bulletin</i> , 2016, 73, 130-139.	2.7	12
176	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
177	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
178	A Step in Carbon Capture from Wet Gases: Understanding the Effect of Water on CO ₂ Adsorption and Diffusion in UiO-66. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3211-3220.	1.5	12
179	Low temperature constant rate thermodesorption as a tool to characterise porous solids. <i>Thermochimica Acta</i> , 2000, 360, 77-83.	1.2	11
180	CO ₂ 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

#	ARTICLE	IF	CITATIONS
181	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
182	Characterization of polyphosphate glasses preparation using CRTA. <i>Journal of Theoretical Biology</i> , 1997, 49, 1171-1178.	0.8	10
183	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
184	Computational investigation of the adsorption of carbon dioxide onto zirconium oxide clusters. <i>Journal of Molecular Modeling</i> , 2012, 18, 4819-4830.	0.8	10
185	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
186	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
187	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
188	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
189	Modeling of adsorption of CO ₂ in the deformed pores of MIL-53(Al). <i>Journal of Molecular Modeling</i> , 2017, 23, 101.	0.8	9
190	Ageing of wet-synthesized oxide powders. <i>Journal of Thermal Analysis and Calorimetry</i> , 2007, 88, 789-793.	2.0	8
191	Silicon distribution in SAPO materials: A computational study of STA-7 Combined to ²⁹ Si MAS NMR spectroscopy. <i>Microporous and Mesoporous Materials</i> , 2008, 107, 268-275.	2.2	8
192	Na ⁺ 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
193	Heterogeneous melting of methane confined in nano-pores. <i>Journal of Chemical Physics</i> , 2016, 145, 144704.	1.2	8
194	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
195	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
196	Characterisation of microporous materials by adsorption microcalorimetry. <i>Membrane Science and Technology</i> , 2000, , 213-230.	0.5	7
197	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
198	Adsorption by Ordered Mesoporous Materials. , 2014, , 529-564.		7

#	ARTICLE	IF	CITATIONS
199	One-pot synthesis of organic polymer functionalized mesoporous silicas. <i>Microporous and Mesoporous Materials</i> , 2021, 319, 111036.	2.2	7
200	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
201	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
202	Constant transformation rate thermal analysis of HGdP2O7·3H2O. <i>Journal of Thermal Analysis and Calorimetry</i> , 2005, 82, 783-789.	2.0	6
203	Adsorption by Metal Oxides. , 2014, , 393-465.		6
204	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
205	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
206	SCTA and Adsorbents. <i>Journal of Thermal Analysis and Calorimetry</i> , 2003, 72, 1099-1101.	2.0	5
207	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
208	Adsorption-Induced Structural Phase Transformation in Nanopores. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16243-16246.	7.2	5
209	Kinetic Study by Controlled-Transformation Rate Thermal Analysis of the Dehydroxylation of Kaolinite. <i>Clay Minerals</i> , 1998, 33, 269-276.	0.2	5
210	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
211	Surface Area/Porosity, Adsorption, Diffusion. , 2012, , 853-879.		4
212	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
213	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
214	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
215	Nitrogen Adsorption on Divalent Cation Substituted X-Faujasites: Microcalorimetry and Monte Carlo Simulation. <i>Adsorption</i> , 2005, 11, 343-347.	1.4	2
216	Investigating Unusual Organic Functional Groups to Engineer the Surface Chemistry of Mesoporous Silica to Tune CO ₂ Surface Interactions. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 14490-14496.	4.0	2

#	ARTICLE	IF	CITATIONS
217	Adsorption-Induced Structural Phase Transformation in Nanopores. <i>Angewandte Chemie</i> , 2017, 129, 16461-16464.	1.6	2
218	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
219	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
220	Adsorption Methodology. , 0, , 575-605.		1
221	Storage of Hydrogen on Nanoporous Adsorbents. <i>Green Energy and Technology</i> , 2019, , 255-286.	0.4	1
222	Characterization of Fine Grain Ba _{0.995} Y _{0.005} TiO ₃ Ceramics Obtained from Gel-Precursor Nanopowder. <i>Journal of Nanoscience and Nanotechnology</i> , 2007, 7, 1014-1020.	0.9	0
223	Characterisation of MOF Materials by Thermomechanical Methods. , 2013, , .		0
224	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