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Screening of metal-organic frameworks for carbon dioxide capture from flue gas using a combined experimental and modeling approach

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#	Paper	IF	Citations
784	Molecular Design of Zirconium Tetrazolate MetalOrganic Frameworks for CO2 Capture.		
783	Interaction of Acid Gases SO2 and NO2 with Coordinatively Unsaturated Metal Organic Frameworks: MMOF-74 (M = Zn, Mg, Ni, Co).		
782	Thiophene Separation with Silver-Doped Cu-BTC MetalOrganic Framework for Deep Desulfurization.		
781	MetalOrganic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H2 and CO2 Gas Adsorption and Catalytic Studies.		
780	Potassium and Zeolitic Structure Modified Ultra-microporous Adsorbent Materials from a Renewable Feedstock with Favorable Surface Chemistry for CO2 Capture.		
779	Controlling Pore Shape and Size of Interpenetrated Anion-Pillared Ultramicroporous Materials Enables Molecular Sieving of CO2 Combined with Ultrahigh Uptake Capacity.		
778	Predicting Product Distribution of Propene Dimerization in Nanoporous Materials.		
777	Occupancy Dependency of MaxwellStefan Diffusivities in Ordered Crystalline Microporous Materials.		
776	A Partially Fluorinated, Water-Stable Cu(II)MOF Derived via Transmetalation: Significant Gas Adsorption with High CO2 Selectivity and Catalysis of Biginelli Reactions.		
775	Enhancement of CO2 Uptake and Selectivity in a MetalOrganic Framework by the Incorporation of Thiophene Functionality.		
774	Hydrogen storage and carbon dioxide capture in an iron-based sodalite-type metalorganic framework (Fe-BTT) discovered via high-throughput methods. <i>Chemical Science</i> , <b>2010</b> , 1, 184	9.4	261
773	Understanding gas separation in metalorganic frameworks using computer modeling. <b>2010</b> , 20, 10308		76
772	High-surface-area carbon molecular sieves for selective CO(2) adsorption. <b>2010</b> , 3, 974-81		282
771	Can metal-organic framework materials play a useful role in large-scale carbon dioxide separations?. <b>2010</b> , 3, 879-91		518
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769	Highly selective CO2 capture by a flexible microporous metal-organic framework (MMOF) material. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 13951-4	4.8	152
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767	De novo synthesis of a metal-organic framework material featuring ultrahigh surface area and gas storage capacities. <b>2010</b> , 2, 944-8		1350
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765	Highly selective carbon dioxide sorption in an organic molecular porous material. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 12200-2	16.4	268
764	Mixed-Matrix Membrane Hollow Fibers of Cu <sub>3</sub> (BTC) <sub>2</sub> MOF and Polyimide for Gas Separation and Adsorption. <b>2010</b> , 49, 12605-12612		184
763	Dense and homogeneous coatings of CPO-27-M type metal-organic frameworks on alumina substrates. <i>CrystEngComm</i> , <b>2010</b> , 12, 3768	3.3	27
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743	Site-Specific CO <sub>2</sub> Adsorption and Zero Thermal Expansion in an Anisotropic Pore Network. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 24915-24919	3.8	124
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4 <sup>15</sup>	Amine-modified Mg-MOF-74/CPO-27-Mg membrane with enhanced H <sub>2</sub> /CO <sub>2</sub> separation. <b>2015</b> , 124, 27-36		114
4 <sup>14</sup>	Tuning metal sites of DABCO MOF for gas purification at ambient conditions. <i>Microporous and Mesoporous Materials</i> , <b>2015</b> , 201, 277-285	5.3	61
4 <sup>13</sup>	Water interactions in metal organic frameworks. <i>CrystEngComm</i> , <b>2015</b> , 17, 247-260	3.3	120
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4 <sup>08</sup>	Remarkable Improvement in the Mechanical Properties and CO <sub>2</sub> Uptake of MOFs Brought About by Covalent Linking to Graphene. <b>2016</b> , 55, 7857-61		49



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327	Conjugated Microporous Polycarbazole Networks as Precursors for Nitrogen-Enriched Microporous Carbons for CO <sub>2</sub> Storage and Electrochemical Capacitors. <b>2017</b> , 29, 4885-4893		109
326	A new methyl-embedded (3,3,6)-connected tbt-type metal-organic framework exhibiting high H <sub>2</sub> adsorption property. <i>CrystEngComm</i> , <b>2017</b> , 19, 3094-3097	3.3	
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322	Theoretical study of carbon dioxide adsorption and diffusion in MIL-127(Fe) metal organic framework. <b>2017</b> , 491, 118-125		9
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319	Adsorption and diffusion of carbon dioxide on the metal-organic framework CuBTB. <b>2017</b> , 167, 10-17		16
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3 <sup>16</sup>	Effects of water vapor and trace gas impurities in flue gas on CO <sub>2</sub> capture in zeolitic imidazolate frameworks: The significant role of functional groups. <b>2017</b> , 200, 244-251		47
3 <sup>15</sup>	New Luminescent Three-Dimensional Zn(II)/Cd(II)-Based Metal-Organic Frameworks Showing High H <sub>2</sub> Uptake and CO <sub>2</sub> Selectivity Capacity. <b>2017</b> , 17, 2059-2065		31
3 <sup>14</sup>	Development of a Cambridge Structural Database Subset: A Collection of Metal-Organic Frameworks for Past, Present, and Future. <b>2017</b> , 29, 2618-2625		499
3 <sup>13</sup>	Increased Electric Conductivity upon I Uptake and Gas Sorption in a Pillar-Layered Metal-Organic Framework. <b>2017</b> , 82, 716-720		18
3 <sup>12</sup>	Separation characteristics as a selection criteria of CO <sub>2</sub> adsorbents. <i>Journal of CO<sub>2</sub> Utilization</i> , <b>2017</b> , 17, 69-79	7.6	16
3 <sup>11</sup>	Fine-Tuning of the Carbon Dioxide Capture Capability of Diamine-Grafted Metal-Organic Framework Adsorbents Through Amine Functionalization. <b>2017</b> , 10, 541-550		69
3 <sup>10</sup>	Assembly of anion-controlled cadmium(II) coordination polymers from the use of 2-acetyl-pyridyl-isonicotinoylhydrazone. <b>2017</b> , 457, 150-159		9
3 <sup>09</sup>	Two Li-Zn Cluster-Based Metal-Organic Frameworks: Strong H <sub>2</sub> /CO Binding and High Selectivity to CO. <b>2017</b> , 56, 705-708		17
3 <sup>08</sup>	Surface modifications of carbonaceous materials for carbon dioxide adsorption: A review. <b>2017</b> , 71, 214-234		76
3 <sup>07</sup>	An In-Depth Structural Study of the Carbon Dioxide Adsorption Process in the Porous Metal-Organic Frameworks CPO-27-M. <b>2017</b> , 10, 1710-1719		24
3 <sup>06</sup>	Systems Design and Economic Analysis of Direct Air Capture of CO <sub>2</sub> through Temperature Vacuum Swing Adsorption Using MIL-101(Cr)-PEI-800 and mmen-Mg <sub>2</sub> (dobpdc) MOF Adsorbents. <b>2017</b> , 56, 750-764		71
3 <sup>05</sup>	A (3,6)-Connected Metal-Organic Framework with pyr Topology and Highly Selective CO <sub>2</sub> Adsorption. <b>2017</b> , 17, 16-18		14
3 <sup>04</sup>	Integrated adsorbent-process optimization for carbon capture and concentration using vacuum swing adsorption cycles. <b>2017</b> , 63, 2987-2995		28
3 <sup>03</sup>	Highly selective adsorption of p-xylene over other C aromatic hydrocarbons by Co-CUK-1: a combined experimental and theoretical assessment. <b>2017</b> , 46, 16096-16101		14
3 <sup>02</sup>	Carbon dioxide capture by planar (AlN) clusters (n=3-5). <b>2017</b> , 23, 288		1
3 <sup>01</sup>	Enhanced Selectivity for CO Adsorption on Mesoporous Silica with Alkali Metal Halide Due to Electrostatic Field: A Molecular Simulation Approach. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 31683-31690	9.5	9
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297	Liquid Adsorption of Organic Compounds on Hematite (FeO) Using ReaxFF. <b>2017</b> , 33, 11257-11263		16
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295	Thin film composite membranes functionalized with montmorillonite and hydrotalcite nanosheets for CO <sub>2</sub> /N <sub>2</sub> separation. <i>Separation and Purification Technology</i> , <b>2017</b> , 189, 128-137	8.3	22
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