

Using molecular simulation to characterise metal–organic applications

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Citation Report

#	ARTICLE	IF	CITATIONS
5	Preferred Hydrogen Adsorption Sites in Various MOFs—A Comparative Computational Study. ChemPhysChem, 2009, 10, 2647-2657.	2.1	75
6	Mixed-ligand coordination polymers constructed from flexible 2,2'-biphenyldicarboxylate and rigid isomeric bipyridines. Polyhedron, 2009, 28, 2997-3004.	2.2	4
7	Novel 3-dimensional sixfold interpenetrating diamondoid networks of copper(I) coordination polymers of polypyridyl ligands — Syntheses, characterization and crystal structures. Inorganic Chemistry Communication, 2009, 12, 1227-1230.	3.9	14
8	Two-Dimensional Networks of Lanthanide Cubane-Shaped Dumbbells. Inorganic Chemistry, 2009, 48, 11748-11754.	4.0	67
9	An Ab Initio Force Field for Predicting Hydrogen Storage in IRMOF Materials. Journal of Physical Chemistry C, 2009, 113, 21815-21824.	3.1	47
10	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. CrystEngComm, 2009, 11, 2272.	2.6	217
11	Heats of Adsorption for Seven Gases in Three Metal-Organic Frameworks: Systematic Comparison of Experiment and Simulation. Langmuir, 2009, 25, 7383-7388.	3.5	212
12	Studies of Capillary Phase Transitions of Methane in Metal-Organic Frameworks by Gauge Cell Monte Carlo Simulation. Langmuir, 2010, 26, 5160-5166.	3.5	8
13	Comment on Comparative Molecular Simulation Study of CO ₂ /N ₂ and CH ₄ /N ₂ Separation in Zeolites and Metal-Organic Frameworks. Langmuir, 2010, 26, 2975-2978.	3.5	39
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18	Molecular simulations of very high pressure hydrogen storage using metal-organic frameworks. Microporous and Mesoporous Materials, 2010, 135, 178-186.	4.4	21
19	New Microporous Materials for Acetylene Storage and C ₂ H ₂ /CO ₂ Separation: Insights from Molecular Simulations. ChemPhysChem, 2010, 11, 2220-2229.	2.1	118
20	A High Heat of Adsorption for Hydrogen in Magnesium Formate. ChemSusChem, 2010, 3, 758-761.	6.8	27
21	Can Metal-Organic Framework Materials Play a Useful Role in Large-Scale Carbon Dioxide Separations?. ChemSusChem, 2010, 3, 879-891.	6.8	556
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25	Metal-Organic Frameworks with Exceptionally High Methane Uptake: Where and How is Methane Stored?. <i>Chemistry - A European Journal</i> , 2010, 16, 5205-5214.	3.3	227
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28	In silico screening of zeolite membranes for CO ₂ capture. <i>Journal of Membrane Science</i> , 2010, 360, 323-333.	8.2	280
29	Homoleptic silver-bis(pyridine) coordination polymers: [Ag(L1) ₂](PF ₆), [Ag(L1) ₂](SbF ₆), [Ag(L1) ₂](BF ₄), [Ag(L2)](PF ₆), and [Ag(L3)1.5](CF ₃ SO ₃)(H ₂ O) ₂ {L1=(4-py)-CHN-C ₁₀ H ₆ -NCH-(4-py); L2=(2-py)-CHN-C ₁₀ H ₆ -NCH-(2-py); L3=(3-py)-CHN-C ₁₄ H ₁₂ -NCH-(3-py)}. <i>Polyhedron</i> , 2010, 29, 2731-2738.	2.2	23
30	Atomistic theoretical models for nanoporous hybrid materials. <i>Microporous and Mesoporous Materials</i> , 2010, 129, 304-318.	4.4	46
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