MACADEMIA Publications

	Author	Title	Journal
1	Vermoortele et al Serre/De Vos	An amino-modified Zr-terephthalate metal-organic framework as an acid-base catalyst for cross-aldol condensation	Chem. Commun., 2011, 47, pp 1521-1523
2	Yang et al Jobic/Maurin/ Serre	Probing the dynamics of CO2 and CH4 within the porous zirconium terephthalate UiO-66(Zr): A synergic combination of neutron scattering measurements and molecular simulations	Chemistry - A European Journal, 2011, Vol 17, (32), pp 8882–8889, 28 June 2011 online
3	Llewellyn et al	Effect of dehydroxylation of the zirconium MOF UiO-66 on CO2 and CO adsorption : a combined IR, XRD, calorimetric and simulation study	Paper under Journal Review
4	Grajciar et al Nachtigall	Water adsorption on coordinatively unsaturated sites in CuBTC MOF.	J. Phys. Chem. Lett., 2010, 1(23), pp 3354–3359
5	Reinsch et al Stock	CAU-3: A new family of porous MOFs with a new Al-based brick: [Al2(OCH3)4(O2C-X-CO2)] (X=aryl)	Dalton Transactions, 2012, 41, pp 4164-4171 30 Jan 2012 online
6	Maes et al De Vos/Serre/Chang	Selective removal of N-heterocyclic aromatic contaminants from fuels by Lewis acid metal-organic frameworks	Angewandte Chemie, 2011 Apr, 123(18), pp 4296-4300 6 April 2011 online
7	Walton et al	Uptake of liquid alcohols by the flexible Fe(III) Metal-Organic Framework MIL-53 observed by time-resolved in situ X-ray diffraction	Paper published in Chem Eur J, 2011, 17(25), pp7069-7079
8	Yang et al Serre/Llewellyn/Maurin	Understanding the thermodynamic and kinetic exploration of the CO2/CH4 gas mix within the porous zirconium terepthalate UiO-66 (Zr): a joint experimental and modelling approach	Paper published in J Phy Chem C, 2011, 115 (28), pp 13768-13774
9	Reinsch et al Stock	A new aluminum-based microporous metal-organic framework: Al(BTB) (BTB = 1,3,5-benzenetrisbenzoate)	Microporous and Mesoporous Materials, 2012, 157, pp 50-55 16 June 2011 online
10	Ahnfeldt et al Stock/Serre	High-throughput and time-resolved Energy-Dispersive X-ray Diffraction study of the formation of CAU-1-(OH)2 – Microwave and Conventional Heating	Paper published in Chemistry A European Journal, 2011, 17(23), pp 6462-6468
11	Moreira et al Rodrigues	Influence of the eluent in the MIL-53(Al) selectivity for xylene isomers separation	Paper has been published in Ind. Eng. Chem. Res, 2011, 50(12), pp 7688–7695
12	Moreira et al Rodrigues	Selective liquid phase adsorption and separation of ortho-xylene with the microporous MIL-53(Al)	Paper published in Separation Sci and Tech, 2011, 46 (13), pp 1995-2003 5 July 2011 online
13	Plaza et al Rodrigues/Chang	Propylene/propane separation by vacuum swing adsorption using Cu-BTC spheres	Separation and Purification Technology, 2012, 90, pp 109-119

	Author	Title	Journal
14	Déroche et al Serre/Maurin/Jobic	Exploration of the long chain n-alkanes adsorption and diffusion in the MOF-type MIL-47 (V) material bycombining experimental and molecular simulation tools	Paper published in J Phys Chem C, 2011, 115 (28) pp13868-13876
15	Yang et al Maurin/Serre/Llewellyn	Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: A computational exploration	Paper published in Chem Commun, 2011, 47, pp 9603-9605 11 July 2011 online
16	Kurfirtova et al Chang/Cejka	High activity of iron containing metal-organic-framework in acylation of p-xylene with benzoyl chloride	Published in Catalysis Today, 2012, 179(1), pp 85-90 9 Sept 2011 online
17	Grajciar et al Nachtigall/Llewellyn/Chang	Understanding CO2 adsorption in CuBTC MOF : comparing hybrid DFT-ab initio calculations with microcalorimetry experiments.	Journal of Physical Chemistry C, 2011, 115 (36) pp 17925-17933
18	Chen et al Düren/Nachtigall	Accurate prediction of methane adsorption in a metal-organic framework with unsaturated metal sites by direct implementation of an ab-initio derived potential energy surface into GCMC simulation	Published in J Phys Chem C, 2011, 115(46) pp 23074-23080
19	Peréz and Cejka	[Cu3(BTC)2]: A Metal–Organic Framework catalyst for the Friedländer reaction	Published in ChemCatChem, 2011, 3(1) pp 157-159 21 Sept 2010 online No IC access to whole paper
20	Peréz-Mayoral et al Cejka/Gil/Nachtigall	Synthesis of quinolines via Friedlander reaction catalyzed by CuBTC MOF	Published in Dalton Transactions, 2012, 41(14), pp 4036-4044 1 Feb 2012 online
21	Dhakshinamoorthy et al Garcia	Metal-Organic-Frameworks as heterogeneous catalysts for the selective n-methylation of aromatic primary amines with dimethyl carbonate	Published in Applied Catalysis A: General, 2010, 378 (1), pp 19-25
22	Dhakshinamoorthy et al Garcia	Aerobic oxidation of thiols to disulfides using iron metal-organic frameworks as solid redox catalysts	Published in Chem. Commun., 2010, 46, pp 6476-6478
23	Maes et al De Vos	Enthalpic effects in the adsorption of alkylaromatics on the metal-organic frameworks MIL-47 and MIL-53	Published in Microporous and Mesoporous Materials, 2012, 157, pp 82-88 15 Nov 2011 online
24	Wuttke et al Serre/Chang/Daturi	Discovering the active sites for C3 separation in MIL-100(Fe) by using operando IR spectroscopy	Chemistry: A European Journal, 2012, 18(38), pp. 11959-11967 13 Aug 2012 online
25	Plaza et al Rodrigues/Chang	Separation of C3/C4 hydrocarbon mixtures by adsorption using a mesoporous iron MOF: MIL-100 (Fe)	Microporous and Mesoporous Materials, 2012 153, pp 178-190 29 Dec 2011 online
26	Biswas et al De Vos/Stock	Fuel purification, Lewis acid and aerobic oxidation catalysis performed by a microporous Co-BTT (BTT3- = 1,3,5-benzenetristetrazolate) framework having coordinatively unsaturated sites	J Materials Chemistry, 2012, 22(20), pp.10200-10209 3 Feb 2012 online

	Author	Title	Journal
27	Heymans et al De Weireld	A complete procedure for acidic gas separation by adsorption on MIL-53 (Al)	Microporous and Mesoporous Materials, 2012,154, pp 93-99 21 Oct 2011 online
28	Ahnfeldt et al Stock	Controlled modification of the inorganic and organic brick in an Albased MOF by direct and post-synthetic synthesis routes	CrystEngComm, 2012 , 14(12), pp 4126-4136 16 Feb 2012 online
29	Santos et al Rodrigues	Modelling and simulation of a SMB unit for xylene isomers separation on MIL-53(Al)	Being resubmitted
30	Reimer et al Stock	Thermal post-synthetic modification of Al-MIL-53-COOH: systematic investigation of the decarboxylation and condensation reaction	CrystEngComm, 2012, 14(12), pp 4119-4125 16 Feb 2012 online
31	Moreira et al. Serre/Rodrigues	Towards understanding the influence of ethylbenzene in p-xylene selectivity of the porous titanium amino terephthalate MIL-125(Ti): adsorption equilibrium and separation of xylene isomers	Langmuir, 2012,28, pp 3494-3502 19 Jan 2012 online
32	Moreira et al. Serre/Rodrigues/Chang	Reverse shape selectivity in liquid-phase adsorption of xylene isomers in Zirconium Terephthalate MOF UiO-66	Langmuir, 2012,28, pp 5715-5723 09 Mar 2012 online
33	Ribeiro et al. Rodrigues/Chang	Pressure swing adsorption process for the separation of nitrogen and propylene with a MOF adsorbent MIL-100 (Fe)	Separation and Purification Technology, 2013, 110, pp 101-111 14 Mar 2013 online
34	Horcajada et al Stock/Daturi/Serre/Maurin	How linker's modification controls swelling properties of highly flexible iron (III) dicarboxylates MIL-88	J Am Chem Soc, 2011, 133(44), pp17839-17847
35	Wiersum et al Daturi/Serre/Maurin/Llewellyn	An evaluation of UiO-66(Zi) for gas based applications	Chemistry An Asian Journal, 2011, 6 (12), pp 3270-3280
36	Vermoortele et al Serre/De Vos/ Stock/Düren	para-xylene-selective metal organic frameworks: a case of topology directed selectivity	J Am Chem Soc, 2011, 133 (46), pp 18526-18529
37	Dhakshinamoorthy et al Garcia	Claisen–Schmidt Condensation Catalyzed by Metal-Organic Frameworks	Adv Synthesis and Catal, 2010, 352 (4), pp 711-717 23 Feb 2010 online
38	Dhakshinamoorthy et al Garcia	Metal-organic frameworks as efficient heterogeneous catalysts for the regioselective ring opening of epoxides	Chemistry A European Journal, 2010, 16(28), pp 8530-8536 14 June 2010 Online
39	Dhakshinamoorthy et al Garcia	Atmospheric-Pressure, Liquid-Phase, Selective Aerobic Oxidation of Alkanes Catalysed by Metal–Organic Frameworks	Chemistry A European Journal, 2011, 17(22), pp 6256-6262 14 Apr 2011 online
40	Dhakshinamoorthy et al Garcia	Aerobic oxidation of benzyl amines to benzyl imines catalyzed by MOFs	ChemCatChem, 2010, 2 (11), pp 1438-1443 19 Aug 2010 online No IC access to whole article

	Author	Title	Journal
41	Dhakshinamoorthy et al Garcia	Aerobic oxidation of benzylic alcohols catalyzed by MOFS assisted by TEMPO	ACS Catal, 2011, 1(1), pp 48-53 17 Dec 2010 online
42	Dhakshinamoorthy et al Garcia	Iron(III) metal-organic frameworks as solid Lewis acids for the isomerisation of α-pinene oxide	Catalysis Science and Technology, 2012, 2, pp 324-330 23 Dec 2011 online
43	Dhakshinamoorthy et al Garcia	Metal Organic Framework as Solid Acid Catalysts for Acetalization of Aldehydes with Methanol	Adv Synthesis and Catal, 2010, 352 (17) pp 3022-3030 17 Nov 2010 online
44	Dhakshinamoorthy et al Garcia	Delineating similarities and dissimilarities in the use of metal organic frameworks and zeolites as heterogeneous catalysts for organic reactions	Dalton Trans, 2011, 40, pp. 6344-6360 24 May 2011 online
45	Dhakshinamoorthy et al Garcia	MOFs as heterogeneous catalysts for oxidation reactions	Catal Sci Technol, 2011, 1, pp 856-867 28 April 2011 online
46	Leclerc et al Serre/Daturi/Llewellyn	Infrared study of the influence of reducible iron (III) metal sites on the adsorption of CO, CO2, propane, propene and propyne in the mesoporous metal–organic framework MIL-100	Phys Chem Chem Phys, 2011, 13, pp 11748-11756 19 May 2011 online
47	Rubeš et al Nachtigall/Llewellyn	Combined theoretical and experimental investigation of CO adsorption on coordinatively unsaturated sites in CuBTC MOF	ChemPhysChem, 2012, 13, pp 488-495 13 Dec 2011 online
48	Kolokolov et al Serre/Maurin	Probing the dynamics of the porous zirconium terephthalate UiO-66(Zr) framework using 2H NMR and neutron scattering	Journal of Physical Chemistry C, 2012, 116(22), pp. 12131-12136 14 May 2012 online
49	Soubeyrand-Lenoir et al Llewellyn/Chang/Serre	How water fosters a remarkable 5-fold increase in low pressure CO2 uptake within the mesoporous MIL-100(Fe)	J Am Chem Society,2012, 134 (24), pp. 10174-10181 16 May online
50	Rives et al Jobic/Serre/Maurin	Diffusion of long chain n-alkanes in the Metal-Organic Framework MIL-47(V): A combination of neutron scattering experiments and molecular dynamics simulations	Microporous and Mesoporous Materials , 2012, 165, pp. 259-265 17 July 2012 online
51	Opanasenko et al Čejka	The effect of substrate size in the Beckmann rearrangement: MOFs vs zeolites	Catalysis Today, 2013, 204, pp. 94-100 18 Oct 2012 online
52	Moreira et al Rodrigues/Serre	Effect of ethylbenzene in p-xylene selectivity of the porous titanium amino terephthalate MIL-125 (Ti)_NH2	MicroMesoMaterials, 2012, 158, pp 229-234 29 March 2012 online
53	Guillerm *et al*. Serre/Maurin	A series of isoreticular highly stable porous Zr oxide based MOFs	Angewandte Chemie Int. Ed, 2012, 51(37), pp. 9267-9271 9 August 2012 online
54	Micek-Ilnicka and Gil	Heteropolyacid encapsulation into the MOF: influence of acid particles distribution on ethanol conversion in hybrid nanomaterials	Dalton Transactions, 2012, 41, pp. 12624-12629 24 Aug 2012 online
55	Položij et al. Čejka/Nachtigall	Theoretical investigation of the Friedländer reaction catalyzed by CuBTC: concerted effect of the adjacent Cu2+ sites	Catalysis Today, 2013, 204, pp. 101-107 24 September 2012 online

	Author	Title	Journal
56	Opanasenko et al Čejka, Nachtigall, Garcia	Comparison of the catalytic activity of MOFs and zeolites in Knoevenagel condensation	Catalysis Science & Technology, 2013, 3, pp.500-507 4 Oct 2012 online
57	Yang et al Llewellyn/ Serre	CH4 and CO2 storage in ultra-high porous zirconium oxide based metal-organic frameworks	ChemComm, 2012, 48, pp. 9831-9833 14 Aug 2012 online
58	Yang et al. Serre/Daturi/Maurin/ De Weireld	Probing the adsorption performance of the hybrid porous MIL-68 (Al): a synergic combination of experimental and modelling tools	J Materials Chemistry, 2012, 22(20), pp 10210- 10220 7 Feb 2012 online
59	Reinsch et al Gil/De Vos/Stock	Structures, sorption characteristics and nonlinear optical properties of a new series of highly stable aluminium MOFs	Chem Mater, 2013, 25(1), pp. 17-26 28 Nov 2012 online
60	Grajciar *et al.* Llewellyn/Nachtigall	Adsorption of propane and propylene on CuBTC MOF: combined theoretical and experimental investigation	J. Phys. Chem. , 2013, 117 (21) pp: 11159-11167 DOI: 10.1021/jp401600v
61	Belarbi *et al.* Chang	Adsorption and separation of n-hexane/benzene vapor mixture onto MIL-101(Cr) : An experimental and computational study	
62	Reinsch and Stock	Formation and Characterisation of Mn-MIL-100	Crystal Engineering Communications, 2013, 15, pp 544-550 1 Nov 2012 online
63	Reinsch, Marrott, Stock	The first keto-functionalized microporous Al-based metal-organic framework: [Al(OH)(O_2C-C_6H_4-CO-C_6H_4-CO_2)]	Inorganic Chemistry, 2013, 52 (4), pp 1854-1859 DOI: 10.1021/ic301961q
64	Reinsch, Waitschat, Stock	Mixed-linker MOFs with CAU-10 structure: synthesis and gas sorption characteristics	Dalton Transactions, 2013, 42 (14) pp 4840-4847 DOI: 10.1039/c3dt32355b
65	Biswas, Ahnfeldt, Stock	New functionalized flexible AL-MIL-53-X (X=-CL, -Br, -CH3, -NO2, -(OH)2) solids: syntheses, characterization, sorption and breathing behaviour	Inorganic Chemistry, 2011, 50, pp. 9518-9526 7 Sept 2011 online
66	Dhakshinamoorthy, Alvaro, Garcia	Aerobic oxidation of cycloalkenes catalyzed by iron metal organic framework containing N-hydroxyphthalimide	Journal of Catalysis, 2012, 289, pp. 259-265 30 March 2012 online
67	Dhakshinamoorthy *et al.* Serre/Daturi/Garcia	Comparison of porous iron trimesates basolite F300 and MIL-100(Fe) as heterogeneous catalysts for Lewis acid and oxidation reactions: roles of structural defects and stability	ACS Catalysis, 2012, 2, pp. 2060-2065 17 August 2012 online
68	Opanasenko, Shamzhy, Čejka	Solid acid catalysts for coumarin syntheiss by the Pechmann reaction: MOFs versus zeolites	ChemCatChem, 2013, 5(4), pp. 1024-1031 13 Aug 2012 online
69	Dan-Hardi et al Devic/Maurin/Serre/De Vos	How Interpenetration ensures rigidity and permanent porosity in a highly flexible hybrid solid	Chemistry of Materials, 2012, 24 (13), pp. 2486-2492 2 June 2012 online
70	Wiersum et al Stock/Chang/Llewellyn	Experimental screening of porous materials for high pressure gas adsorption and evaluation in gas separations: application to MOFs (MIL-100 and CAU-10)	ACS Comb Sci, 2013, 15(2), pp. 111-119 8 Jan 2013 online

	Author	Title	Journal
71	Wiersum *et al.* Serre/Llewellyn/Chang	An adsorbent performance indicator as a first step evaluation of novel sorbents for gas separations: application to Metal-Organic Frameworks	Langmuir, 2013, 29(10), pp. 3301-3309 5 Feb 2013 online
72	Nouar *et al* Daturi/Walton/Llewellyn/Serre	Tuning the breathing behaviour of MIL-53 by cation mixing	Chemical Communications, 2012, 48, pp. 10237-10239 31 Aug 2012 online
73	de Miguel *et al.* Serre/Garcia	Evidence of photoinduced charge separation in the metal-organic framework MIL-125(Ti)-NH2	ChemPhysChem, 2012, 13, pp. 3651-3654 21 Aug 2012 online
74	Reinsch *et al.* Gil/Stock	A new Al-MOF based on a unique column-shaped inorganic building unit exhibiting strongly hydrophilic sorption behaviour	Chemical Communications, 2012, 48, pp. 9486-9488 7 Aug 2012 online
75	El Osta *et al.* Walton/Stock	Crystallisation Kinetics of Metal Organic Frameworks from in situ Time-Resolved X-ray Diffraction	Powder Diffraction, 2013
76	Dhakshinamoorthy *et al.* Čejka/Garcia	Metal organic frameworks as solid catalysts in condensation reactions of carbonyl groups	Advanced Syn and Catal, 2013, 355, pp. 247-268 16 Jan 2013 online
77	Rives *et al.* Jobic/Serre/Maurin	Diffusion of Branched and Linear C_6-Alkanes in the MIL-47(V) Metal-Organic Framework.	
78	Van de Voorde *et al.* De Vos/Walton	Adsorption of N/S heterocycles in the flexible metal-organic framework MIL-53(FeIII) studied by in situ energy dispersive X-ray diffraction	PhysChemChemPhys, 2013, 15 (22), pp. 8606-8615 14 Feb 2013 online
79	Asadi *et al* Rodrigues	CO2/CH4 separation by adsorption using Nanoporous Metal organic framework Cu-BTC tablet	Chemical Engineering Technology, 2013, 36(7), pp. 1231-1239 11 June 2013 online
80	Opanasenko *et al.* Čejka/Chang/Garcia	Superior performance of MOFs over zeolites as acid solid catalysts in the Prins reaction: green synthesis of nopol	Chem Sus Chem, 2013, 6, pp. 865-871 16 April 2013 online
81	Yang *et al.* Llewellyn/Serre/Jobic/De Weireld/Maurin	Highly CO2/N2 selective water stable metal-organic framework incorporating free dual carboxylic groups into pore surface	Journal American Chem Soc
82	Rives *et al.* Jobic/Serre/Maurin	Diffusion of Xylene Isomers in the MIL-47(V) MOF Material: a Synergic Combination of Computational and Experimental Tools	J. Physical Chemistry C, 2013, 17 (12) pp 6293-6302 DOI: 10.1021/jp400507w
83	Rubeš *et al.* Nachtigall/Llewellyn	Adsorption of Propane and Propylene on CuBTC MOF: Combined theoretical and experimental investigation	J Physical Chemistry C, 2013, 117(21), pp. 11159-11167 29 April 2013 online
84	El Osta *et al.* Walton/De Vos	Liquid-phase adsorption and separation of xylene isomers by the flexible porous metal-organic framework MIL-53(Fe)	Chemistry of Materials, 2012, 24, pp. 2781-2791 5 June 2012 online
85	Ramsahye *et al.* Serre	The effect of pore shape on hydrocarbon selectivity on UiO-66(Zr) and MIL-125(Ti) metal organic frameworks: Insights from Molecular Simulations and Chromatography	Microp. Mesop. Materials

	Author	Title	Journal
86	Munn *et al.* Walton	Interaction of methanol with the flexible metal-organic framework MIL-53(Fe) observed by inelastic neutron scattering	Chemical Physics, 2013 1 June 2013 online
87	Breeze *et al.* Daturi/Walton	Isomorphous substitution in a flexible metal-organic framework: mixed-metal, mixed-valent MIL-53 type materials	Inorg. Chem., 2013, 52, pp. 8171-8182 1 July 2013 online
88	Shamzhy *et al.* Čejka	Catalytic performance of Metal-Organic-Frameworks vs. extra-large pore zeolite UTL in condensation reactions	
89	Trens *et al.* Chang	Adsorption and separation of Xylenes Isomers Vapors onto the Chromium Terephthalate-based Porous Material MIL-101(Cr). An experimental and computational study	Microp. Mesop. Materials
90	Ragon *et al.* Serre/Chang	In situ Energy-Dispersive X-ray Diffraction for the synthesis optimi-zation and scale-up of the porous zirconium terephthalate UiO-66	
91	Yang *et al*. Llewellyn/Jobic/Serre/Maurin/De Weireld	A water stable Metallic-Organic Framework with optimal features for CO2 capture	Angewandte Chemie Int. Ed, 2013, 20 June 2013 online
92	Narin *et al.* Chang/Rodrigues	Propylene/Nitrogen separation in a by-stream of the polypropylene production: from pilot test and model validation to industrial scale process design and optimization	Adsorption
93	Ragon *et al*. Serre/Devic	Influence of the nature of the organic spacer on the crystallization kinetics of the porous UiO-66(Zr) MOF type	
94	McKinlay *et al*. Daturi/De Weireld/ Serrre	Nitric Oxide Adsorption and Delivery in Flexible MIL-88(Fe) Metal-Organic Frameworks	Chemistry of Materials, 2013
95	Van de Voorde *et al*. Chang/Daturi/De Vos	N/S-heterocyclic contaminant removal from fuels by the mesoporous metal-organic framework MIL-100: the role of the metal ion	Journal of the American Chemical Society, 2013, 135(26), pp. 9849-9856 6 May 2013 online
96	Ramsahye *et al.* Serre	Impact of the flexible character of MIL-88(FeIII) dicarboxylates on the adsorption of n-alkanes.	Chemistry of Materials, 2013, 25(3), pp. 479-488 17 Jan 2013 online
97	Trens *et al*. Chang	Coadsorption of *n*-hexane and benzene vapors onto the chromium terephthalate-based porous material MIL-101(Cr) an experimental and computational study	Journal of Phys Chem C, 2012, 116, pp. 25824-25831 19 Nov 2012 online
98	*Hamon et al*	Separation of CO2–CH4 mixtures in the mesoporous MIL-100(Cr) MOF: experimental and modelling approaches	Dalton Trans., 2012, 41, 4052