Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

Catalytic Transfer Hydrogenation of Ethyl Levulinate to γ-Valerolactone over Zirconium-based Metal-Organic Frameworks

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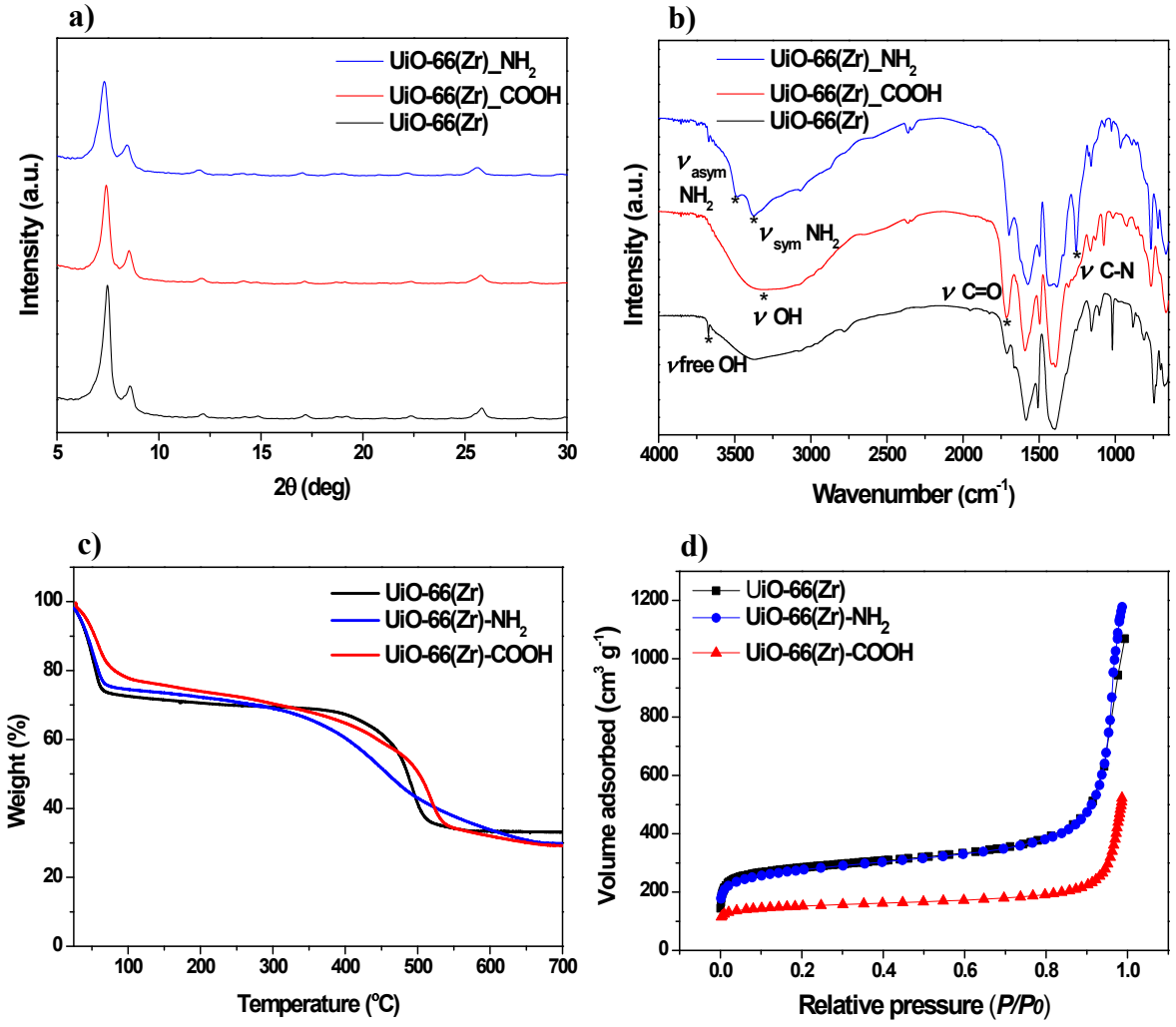


Fig. S1 a) XRD patterns, b) FTIR graphs, c) TGA curves, and d) N_2 adsorption at 77 K of UiO-66(Zr) and its functionalized analogs

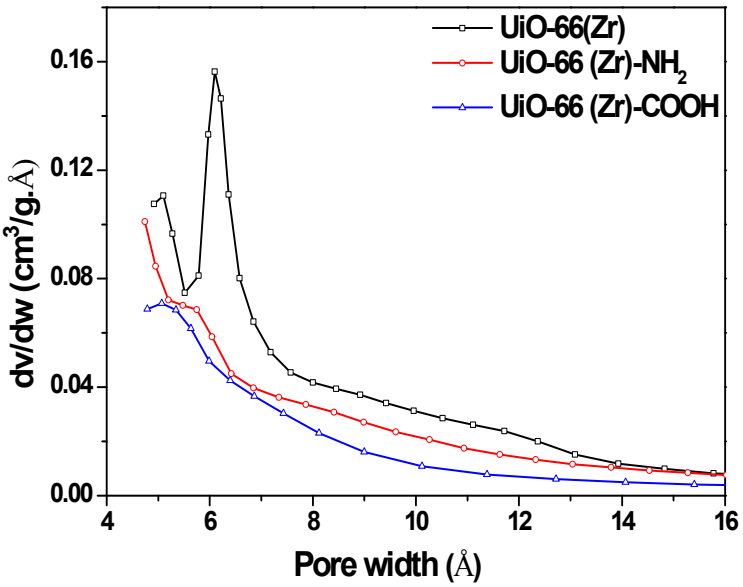


Fig. S2 Micropore size distribution of UiO-66(Zr) and its functionalized analogs calculated from Ar-sorption by using Horvath-Kawazoe method.

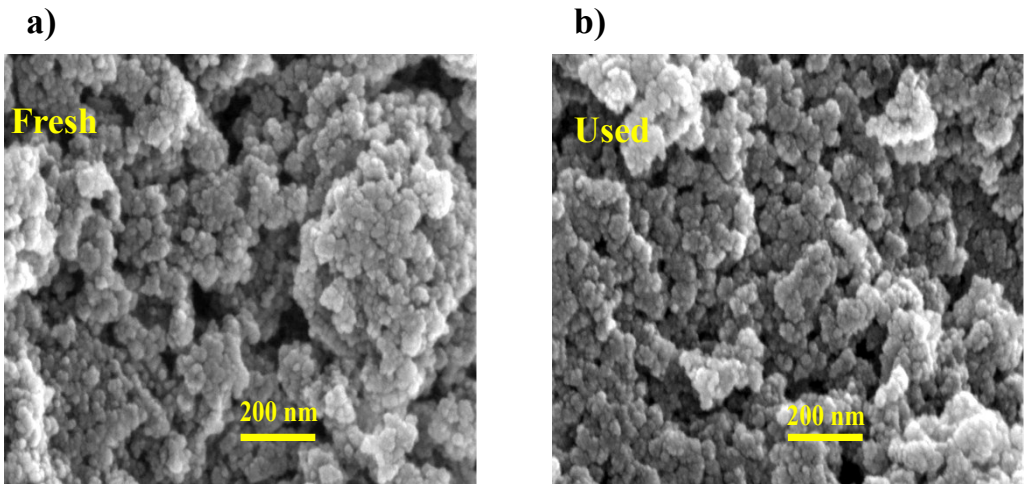
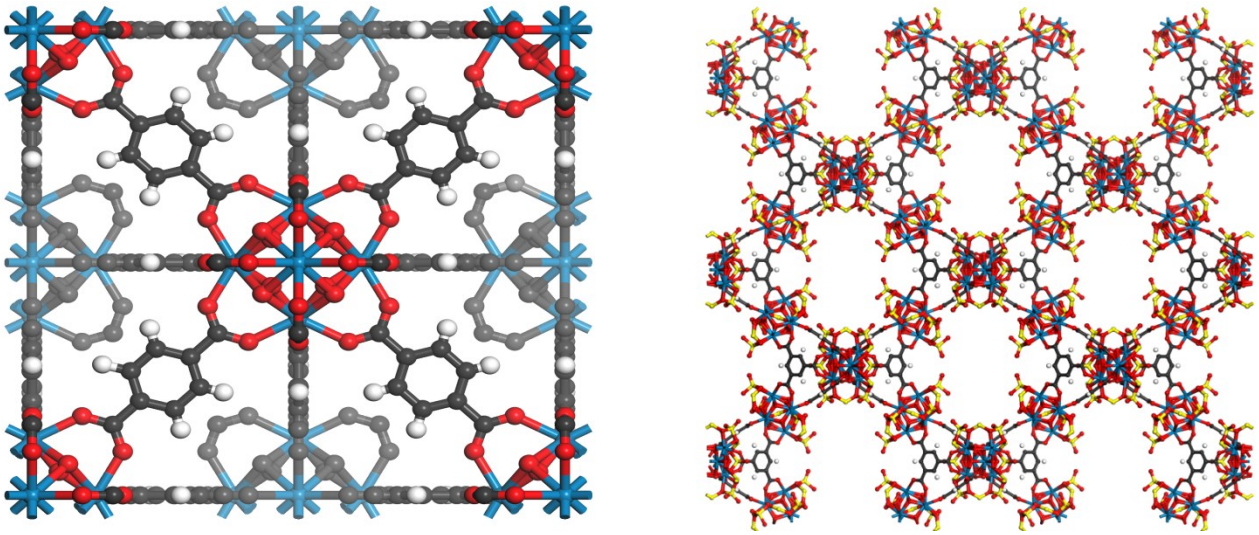


Fig. S3 SEM images of a) fresh and b) used UiO-66(Zr) catalyst .



UiO-66(Zr) **MOF-808**

Fig. S4 Representative structures of Zr-MOFs .

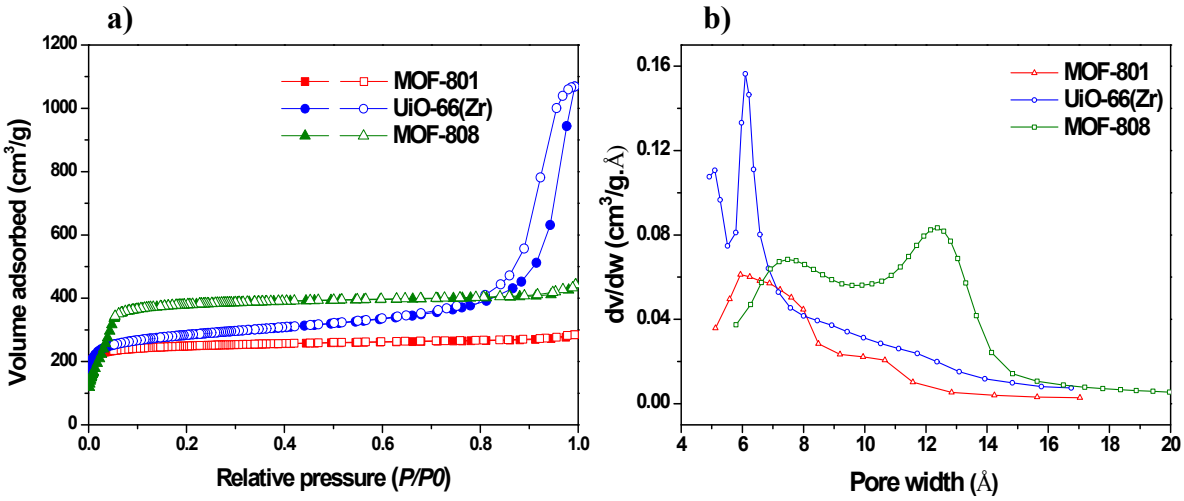


Fig. S5 a) N_2 adsorption isotherms at 77 K and b) micropore pore size distribution of Zr-MOFs calculated from Ar-sorption by using Horvath-Kawazoe method.

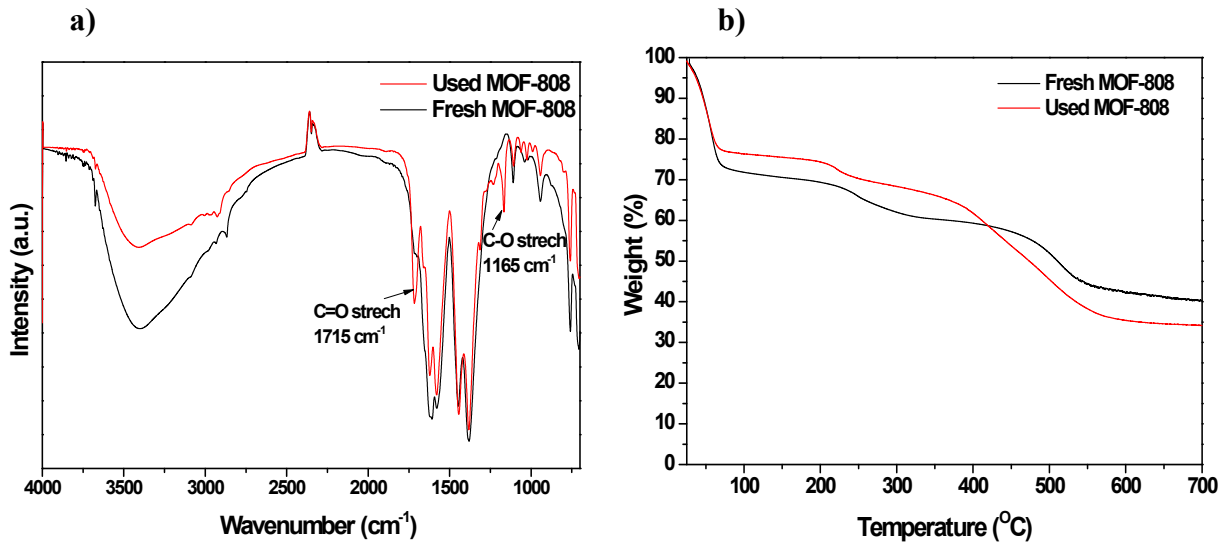


Fig.S6 a) FTIR patterns and b) TG curves of MOF-808 before and after reaction with LA at 82^{O}C.

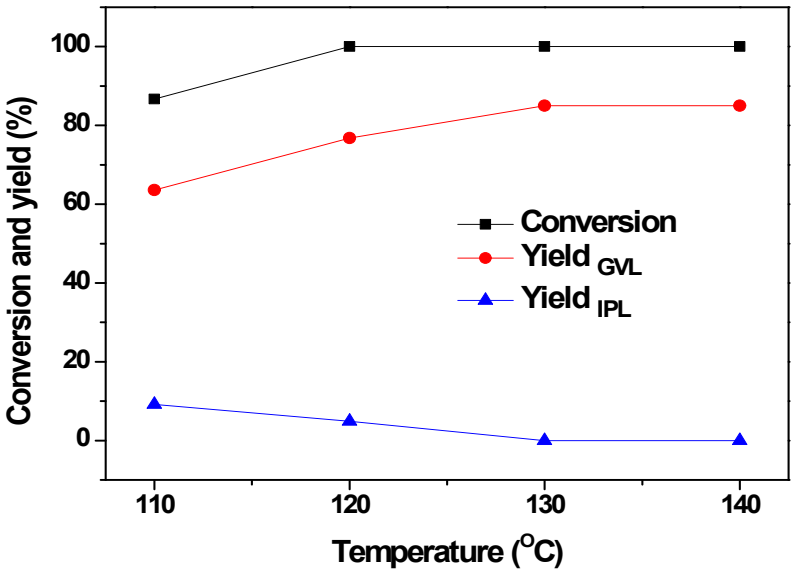


Fig.S7 Effect of reaction temperature in CTH of EL to GVL over MOF-808: Reaction conditions: EL 4 mmol, isopropanol; 400 mmol, catalyst 0.2 g, naphthalene 0.24 g, and reaction time 3 h.

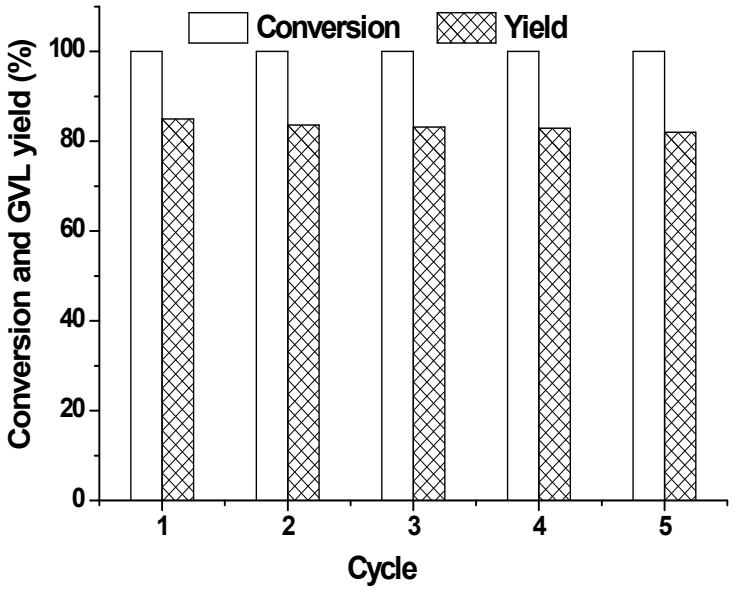


Fig. S8 Recycle test of MOF-808 catalyst. Reaction conditions**:** EL 4 mmol; isopropanol 400 mmol; catalyst 0.2 g; naphthalene 0.24 g; reaction temperature 130^{O}C; reaction time 3 h.

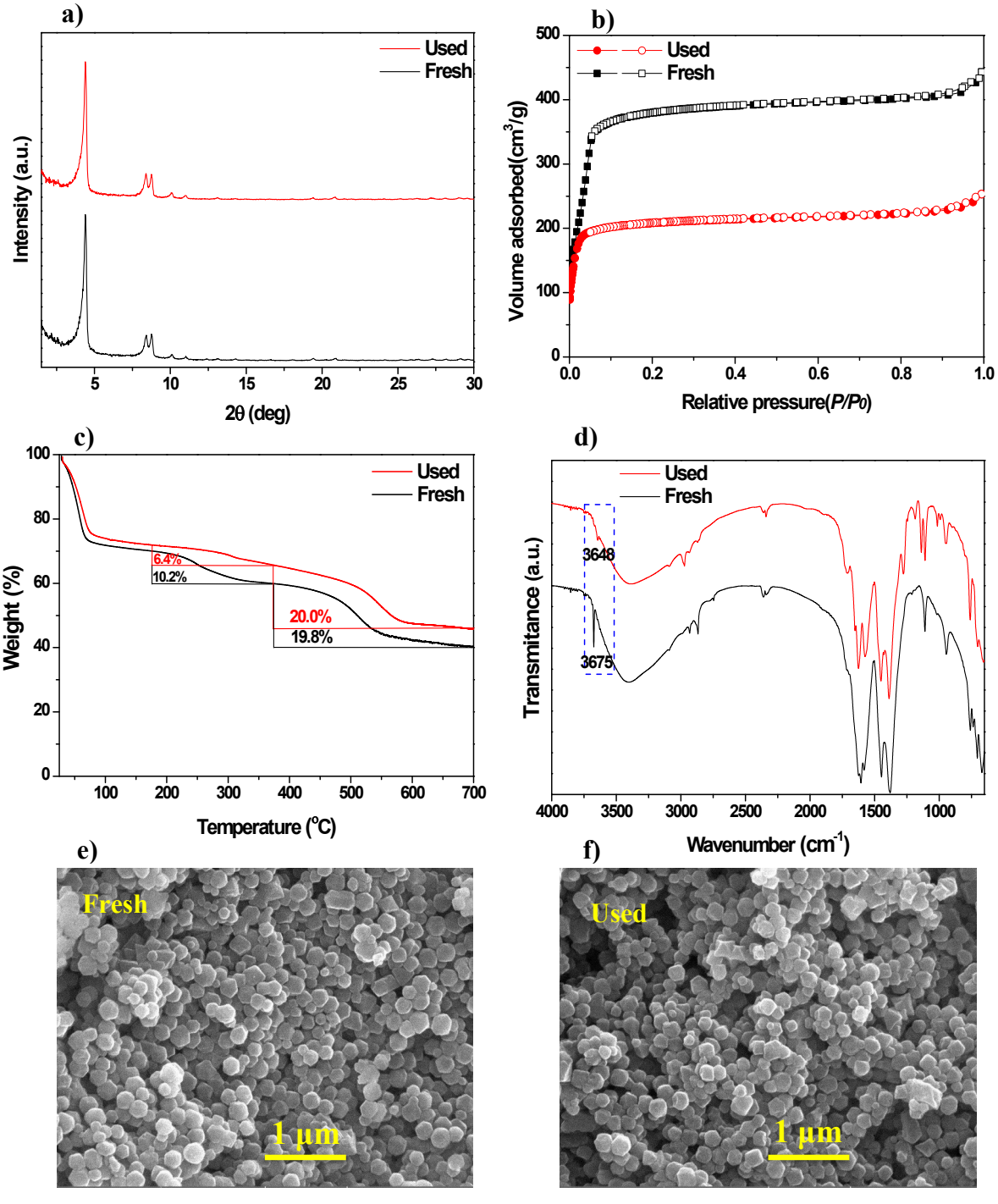

a)
Used
Fresh
Intensity (a.u.)
2θ (deg)
b)
Used
Fresh
Volume adsorbed(cm3/g)
Relative pressure(P/P0)
c)
Used
Fresh
6.4%
10.2%
20.0%
19.8%
Weight (%)
Temperature (°C)
d)
Used
Fresh
3648
3675
Transmitance (a.u.)
Wavenumber (cm-1)
e)
Fresh
1 μm
f)
Used
1 μm

Fig. S9 The characterizations of fresh and used MOF-808 after 5 cycles a) XRD pattern**,** b)N_2 adsorption-desorption isotherm at 77 K, c)TGA curves, d) FTIR patterns, and SEM images e) Fresh and f) Used

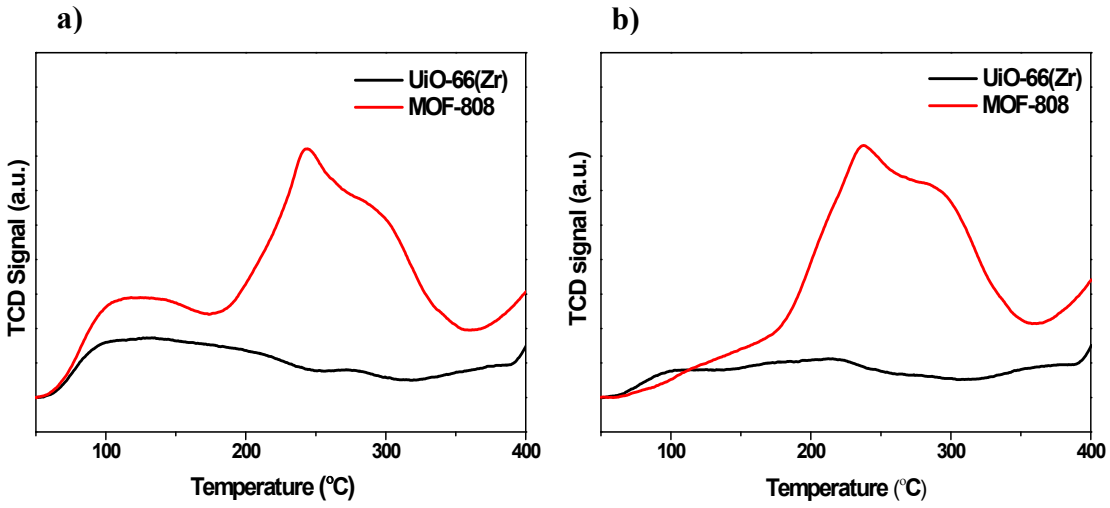


Fig.S10 a) NH_3-TPD and b) CO_2 –TPD of MOF-808(Zr) and UiO-66(Zr)

Table S1 ICP and elemental analysis of fresh and used Zr-MOFs after five recycle tests.

Catalyst	Zr (Wt.%)	C (Wt.%)	H (Wt.%)
Fresh UiO-66(Zr)	30.7	29.2	2.9
Used UiO-66(Zr)	36.5	23.3	2.7
Fresh MOF-808	32.8	22.2	3.0
Used MOF-808	36.2	21.9	2.8

Table S2 Porosity data of various catalysts (mentioned in Table 3) used for CTH of EL/LA to GVL

Entry	**Catalyst**	**S_{BET} (m^2/g)**	**PV (cm^3/g)**	**PD (nm)**	**Reference**
1	MOF-808	1450	0.44	0.74, 1.25	This study
2	UiO-66(Zr)	1046	1.65	0.6	This study
3	MOF-801	990	0.44	0.6	This study
4	ZrO_2	37	0.11	2.5, 3.7	This study
5	$ZrO(OH)_2$	250	0.19	3.8	This study
6	Zr-HBA	87.3	0.21	8	[34]
7	Zr-PhyA	215	0.42	8.5	[39]
8	Zr-Beta	474	0.27	---	[42]