Electronic Supplementary Information

Highly selective self-condensation of cyclic ketones using MOF encapsulating phosphotungstic acid for renewable high-density fuel

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Table S1. Composition and physicochemical properties of PTA@MIL-100. [a]: the volume of small cage; [b]: the volume of large cage.

The mass of PTA added (g)	W (wt%)	Cr/Fe (wt%)	PTA (wt%)	PTA/Cage	S_{BET} (m^2/g)	V_{total} (cm^3/g)	$V^{[a]}$ (cm^3/g)	$V^{[b]}$ (cm^3/g)
0 (Cr)	-	-	-	-	1525	1.338	0.145	0.163
3.600g (Cr)	16.25	9.13	21.2	1.0	758	0.348	0.048	0.044
0 (Fe)	-	-	-	-	1223	0.872	0.121	0.119
2.730g (Fe)	17.79	11.25	23.2	1.1	737	0.440	0.051	0.045

Figure S1. The volume of small and large cage in PTA@MIL-101.

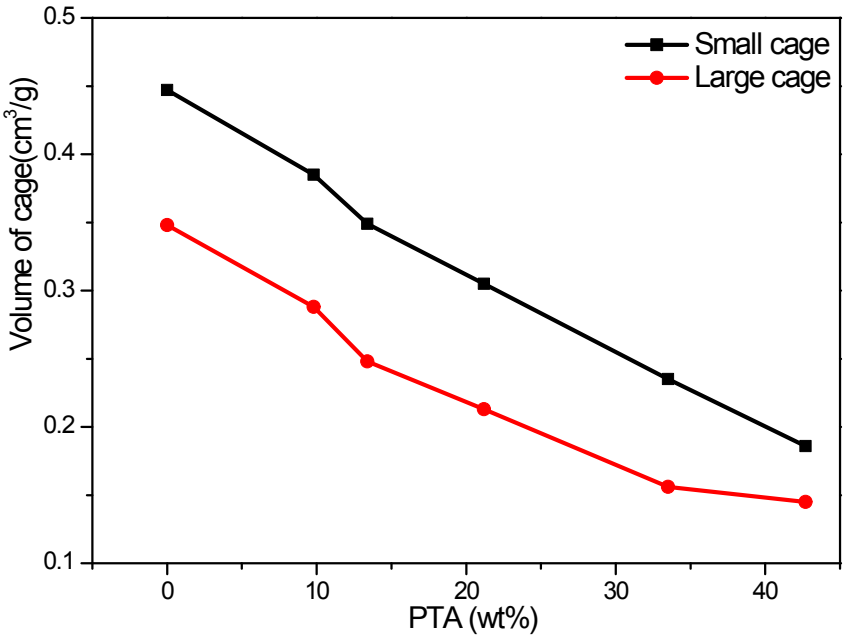

Figure S2. X-ray diffraction patterns of PTA@MIL-100.

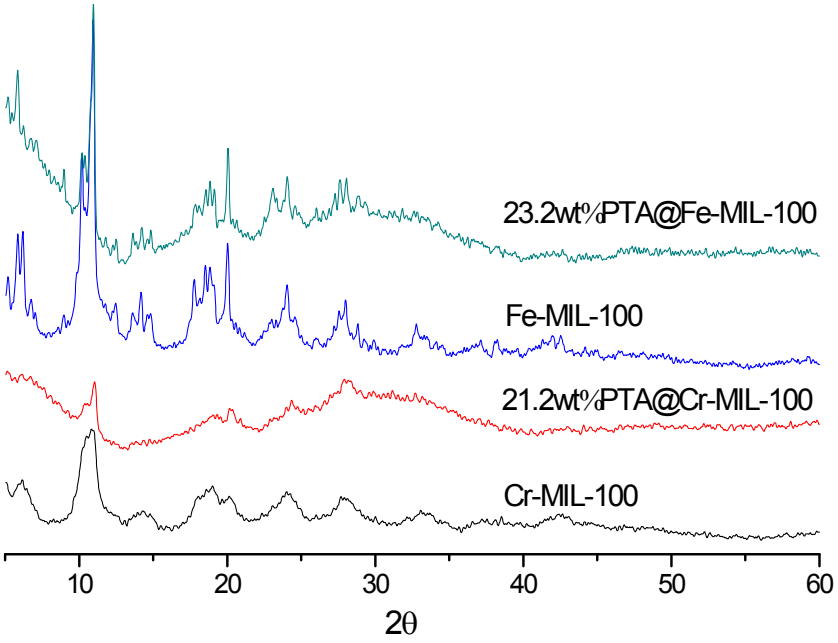

Figure S3. N_2 adsorption isotherms and the pore size distribution of (a) Cr-MIL-100, (b) 21.2wt%PTA@Cr-MIL-100, (c) Fe-MIL-100 and (d) 23.2wt%PTA@Fe-MIL-100.

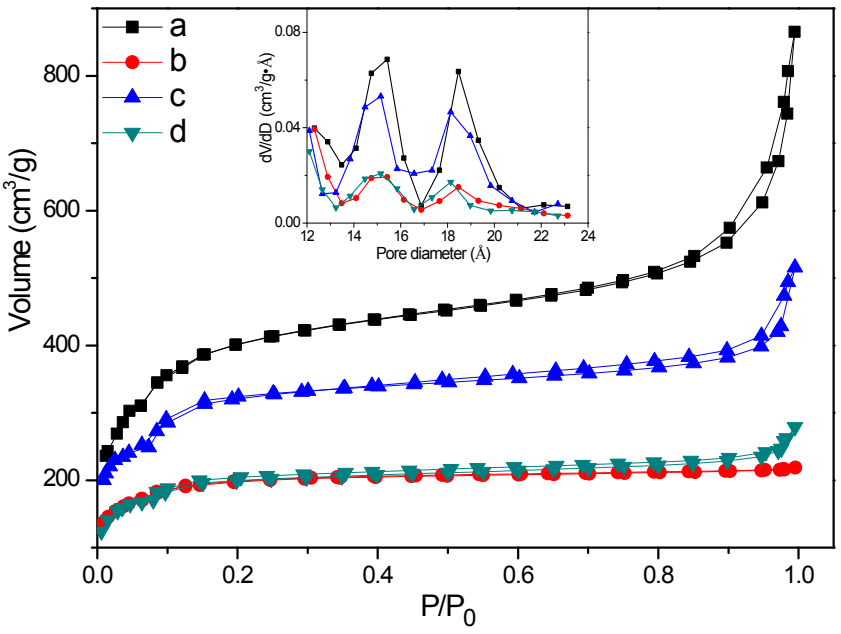

Figure S4. Activity and selectivity of MOF catalysts in cyclopentanone self-condensation.

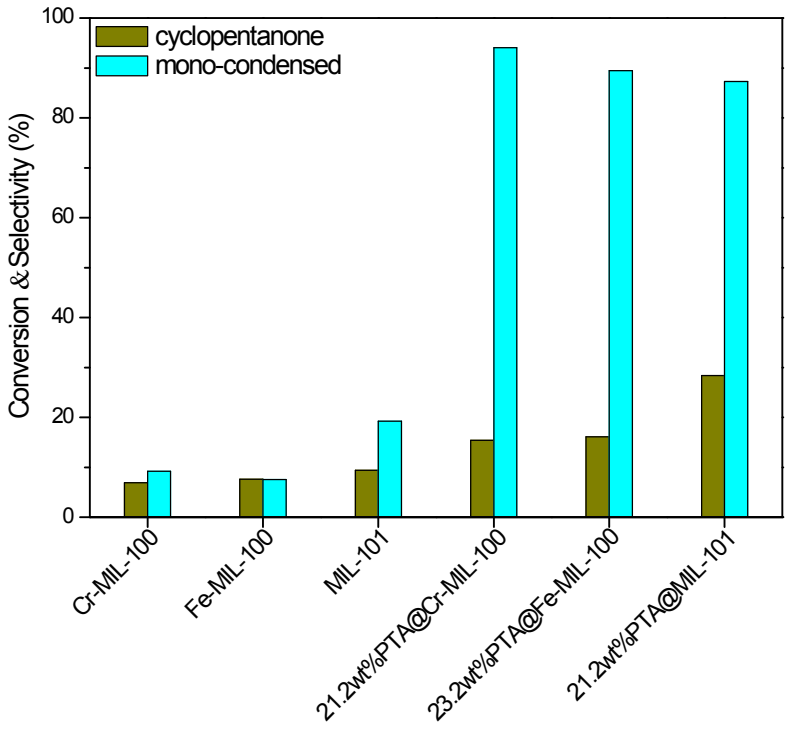

Figure S5. Product distribution of cyclohexanone self-condensation using PTA and 21.2wt%PTA@MIL-101.

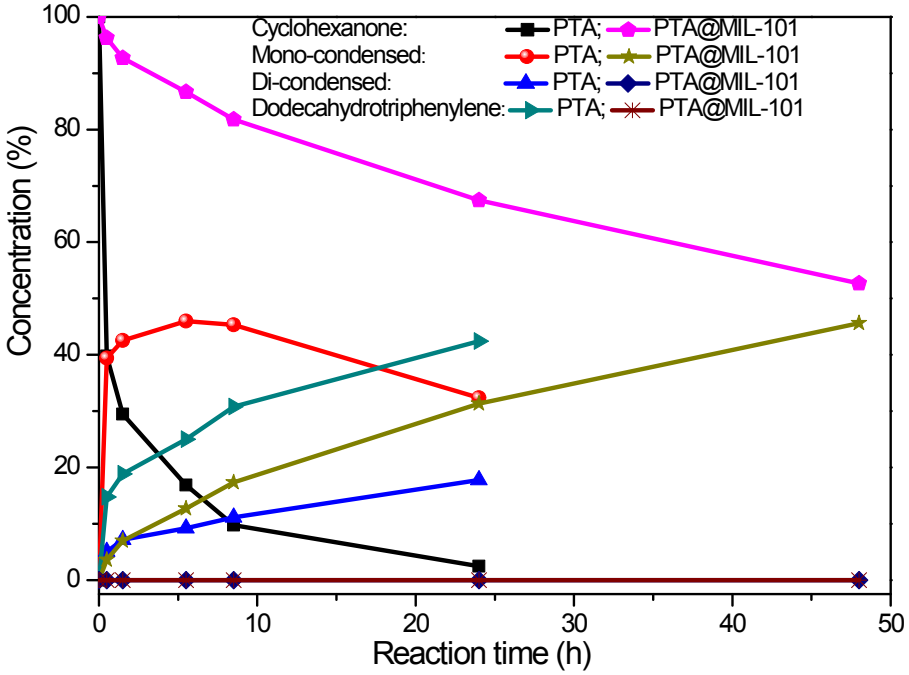

Figure S6. Activity and selectivity of cycloheptanone self-condensation using PTA and 13.4wt%PTA@MIL-101.

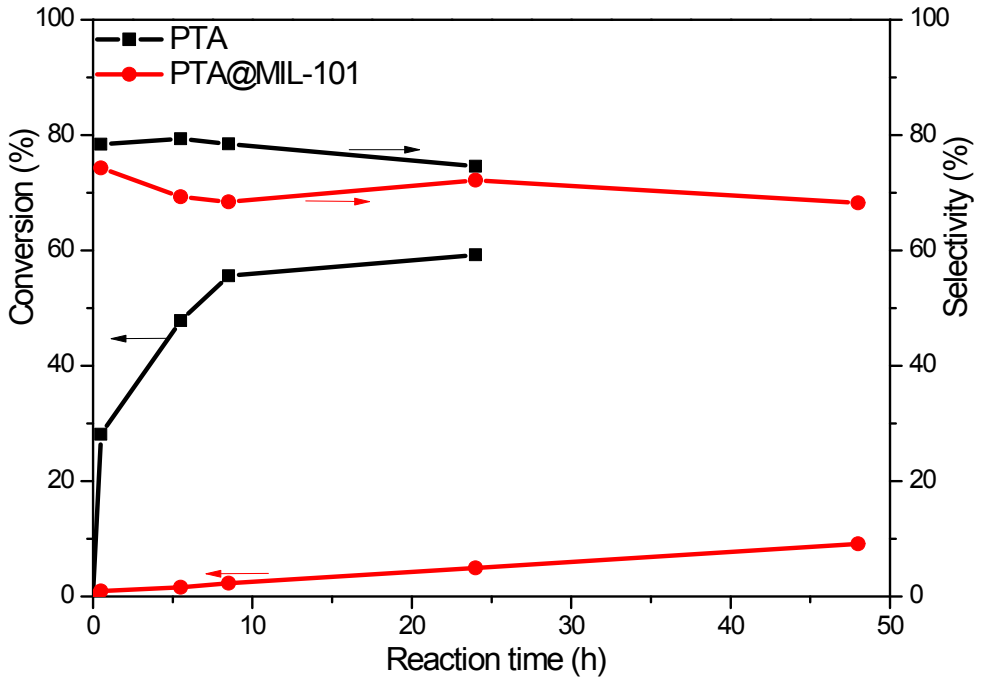

Figure S7. Fast hot catalyst filtration test in cyclopentanone self-condensation using 42.7wt%PTA@MIL-101.

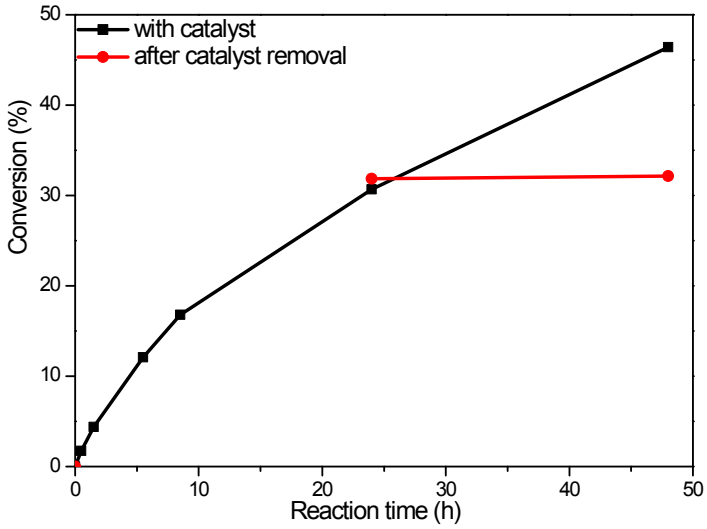

Figure S8. UV-vis spectra of $PW_{12}O_{40}^{3-}$ dissolved from PTA and 42.7wt%PTA@MIL-101 in (A) water and (B) cyclopentanone.

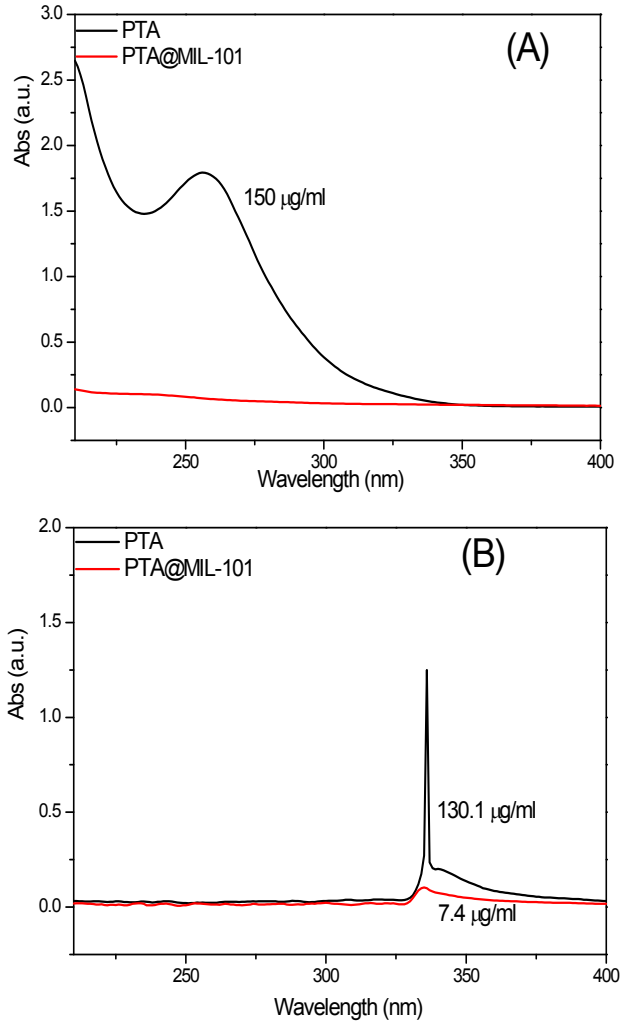

Figure S9. Photographs of 42.7wt%PTA@MIL-101 before and after 5 catalytic runs.

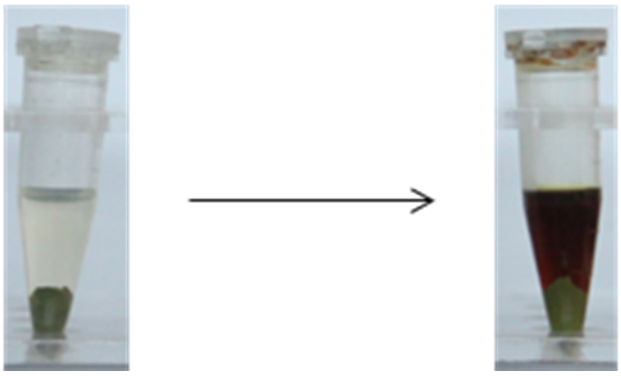

Figure S10. XRD patterns of 42.7wt%PTA@MIL-101 before and after 5 catalytic runs.