

Electronic Supplementary Material (ESI) for New Journal of Chemistry

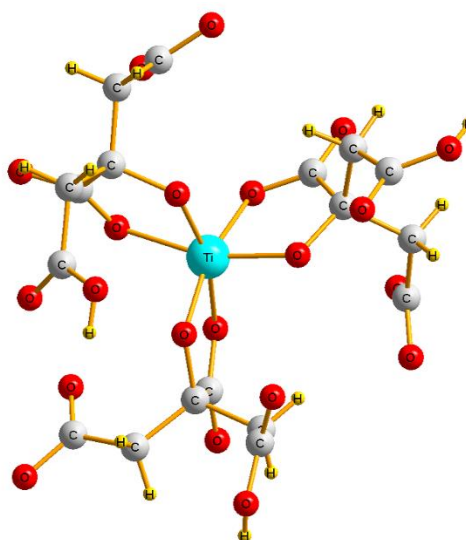
Ti functionalized hierarchical-pore UiO-66(Zr/Ti) catalyst for the transesterification of phenyl acetate and dimethyl carbonate

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Scheme S1 ORTEP structure of the anion structure of Ti-Citrate with the atom-labeling

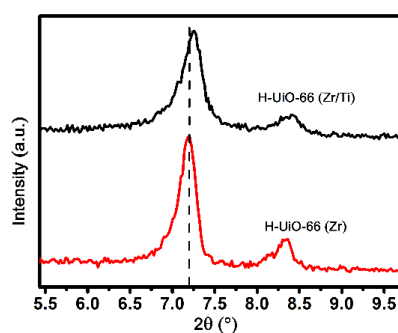


Fig. S1 The enlargement of the 2θ region from 5.5° to 10° in Fig. 1 (a)

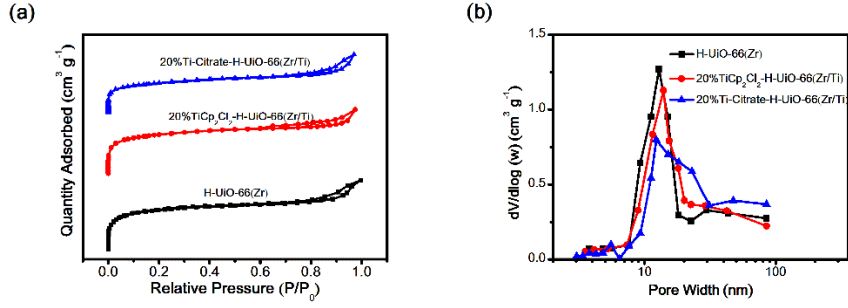


Fig. S2 (a) N₂ adsorption-desorption isotherms at 77K and (b) mesopore size distribution of Ti functionalized H-UiO-66(Zr/Ti) prepared with different Ti source

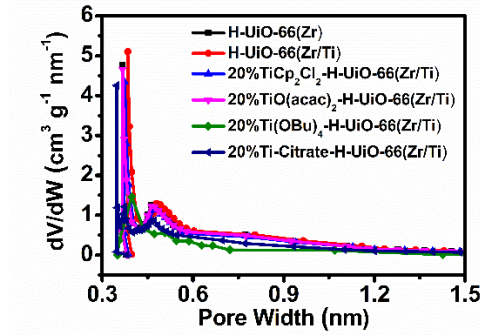


Fig. S3 micropore size distribution of synthesized samples

Table S1 XPS data for the Ti^{IV} distribution in the samples

Sample	octahedral coordinated Ti ^{IV} (%)	tetrahedral coordinated Ti ^{IV} (%)
H-UiO-66(Zr)	-	-
H-UiO-66(Zr/Ti)	72.5	27.5
20%TiCp ₂ Cl ₂ -H-UiO-66(Zr/Ti)	36.6	63.4
20%TiO(acac) ₂ -H-UiO-66(Zr/Ti)	30.9	69.1
20%Ti(OBu) ₄ -H-UiO-66(Zr/Ti)	18.8	81.2
20%Ti-Citrate-H-UiO-66(Zr/Ti)	53.12	46.88

Table S2 XPS data for the Ti^{IV} content in the sample

Sample	Ti (at%)	octahedral coordinated Ti ^{IV} (at%)	tetrahedral coordinated Ti ^{IV} (at%)	Zr (at%)	Surface octahedral coordinated Ti/Zr molar ratios
H-UiO-66(Zr)	-	-	-	6.47	-
H-UiO-66(Zr/Ti)	3.83	2.78	1.05	6.12	0.45
20%TiCp ₂ Cl ₂ -H-UiO-66(Zr/Ti)	6.42	2.35	4.07	5.13	0.46
20%TiO(acac) ₂ -H-UiO-66(Zr/Ti)	7.14	2.21	4.93	5.40	0.45
20%Ti(OBu) ₄ -H-UiO-66(Zr/Ti)	14.47	2.72	11.75	5.44	0.50
20%Ti-Citrate-H-UiO-66(Zr/Ti)	4.93	2.62	2.31	4.66	0.56

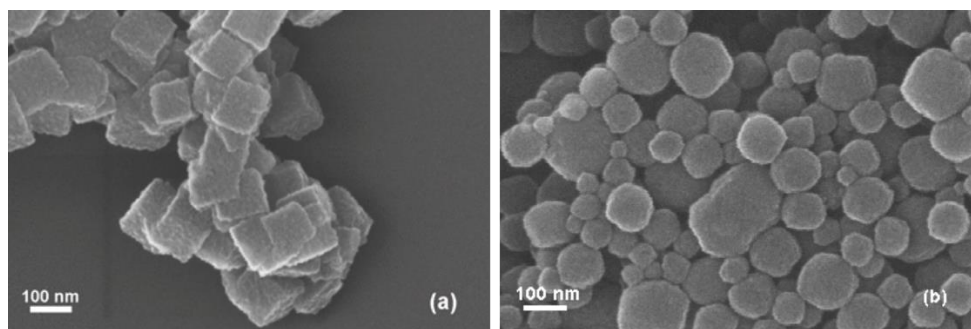


Fig. S4 SEM images of (a) UiO-66(Zr), (b) H-UiO-66(Zr)

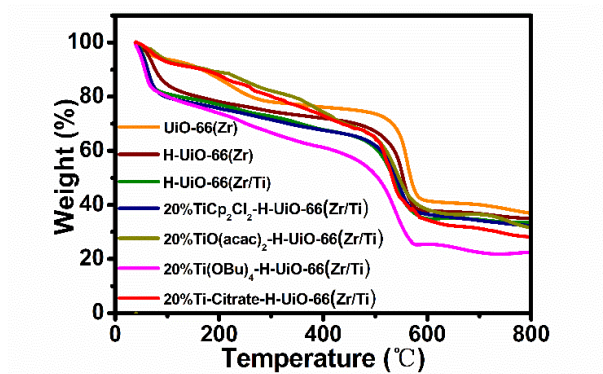


Fig. S5 TG curve of the synthesized samples

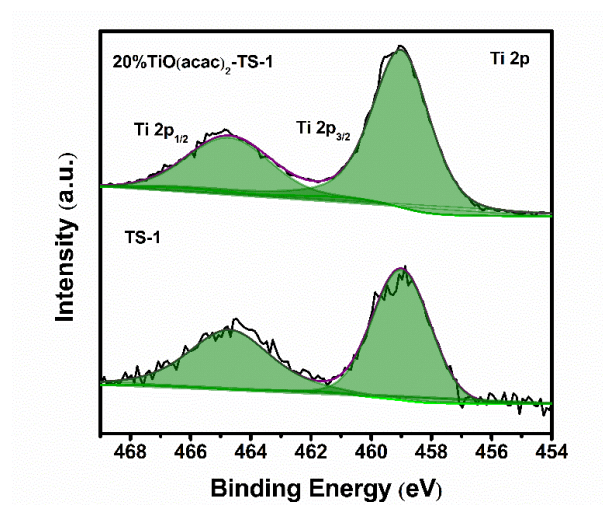


Fig. S6 Ti 2p XPS spectra of TS-1 and 20%TiO(acac)₂-TS-1

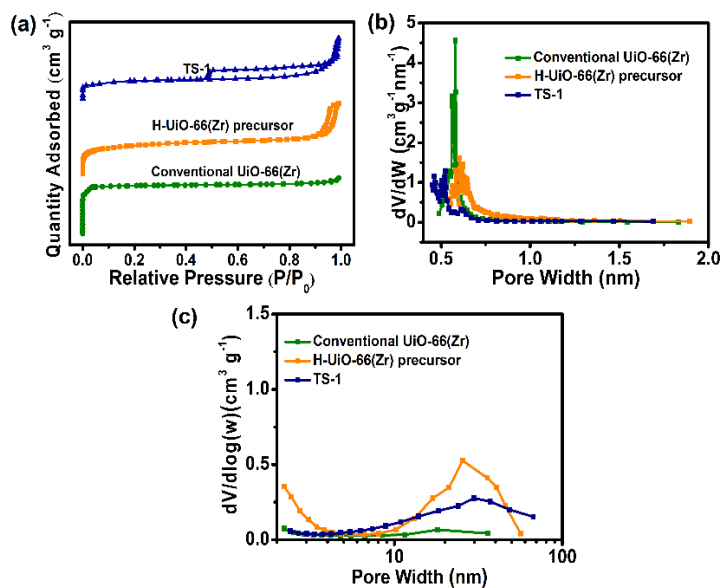


Fig. S7 (a) N₂ adsorption-desorption isotherms at 77K; (b) mesopore size distributions and (c) micropore size distribution of conventional UiO-66(Zr/Ti), H-UiO-66(Zr) precursor and TS-1

Table S3 XPS data for the Ti^{IV} content in TS-1 and 20%TiO(acac)₂-TS-1

Sample	Ti (at%)	octahedral coordinated Ti ^{IV} (at%)	tetrahedral coordinated Ti ^{IV} (at%)	Si (at%)	Surface Ti/Si molar ratios
TS-1	0.84	0	1.14	28.84	0.029
20%TiO(acac) ₂ -TS-1	2.52	0	2.52	27.93	0.09

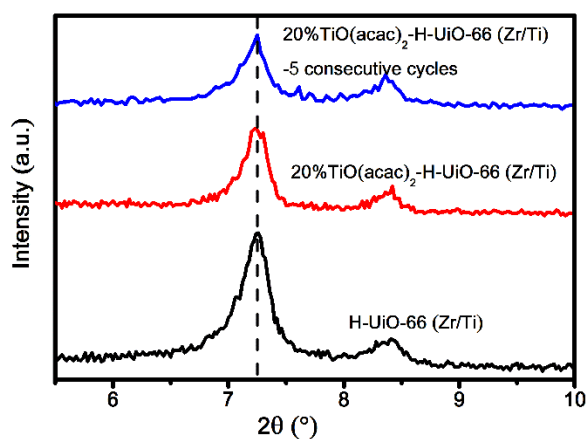


Fig S8 The enlargement of the 2θ region from 6° to 10.5° in Fig. 7 (a)