Electronic Supplementary Information

Synthesis of titanium-oxo macrocyles and catalytic property for oxidative desulfurization

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Table S1. Crystal data and structure refinements summary for **Ti_{32}-BTA** and **Ti_{32}-DMBTA**.

	Ti_{32}-BTA	**Ti_{32}-DMBTA**
Empirical formula	$C_{160}H_{408}O_{188}Ti_{32}$	$C_{204}H_{456}O_{172}Ti_{32}$
Formula weight	6873.64	7194.46
Crystal system	tetragonal	monoclinic
Space group	$P4/n$	$C2/c$
a (Å)	33.635(3)	51.758(4)
b (Å)	33.635(3)	14.9948(11)
c (Å)	13.0634(12)	47.346(3)
α (°)	90	90
β (°)	90	119.823(2)
γ (°)	90	90
V (Å^3)	14779(3)	31879(4)
Z	2	4
ρ_{calcd} (g cm^{-3})	1.545	1.499
μ (mm^{-1})	0.916	0.850
F(000)	7152	15040
T (K)	100(2)	100(2)
Measured refls.	84405	150653
Independent refls.	12977	31311
R_{int}	0.0717	0.0851
GOF	1.156	1.036
R_1 [$I > 2\sigma(I)$][a]	0.1297	0.1064
wR_2 [$I > 2\sigma(I)$][b]	0.3005	0.2837

[a]$R_1 = \sum \| F_o | - | F_c \| / \sum | F_o |$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$.

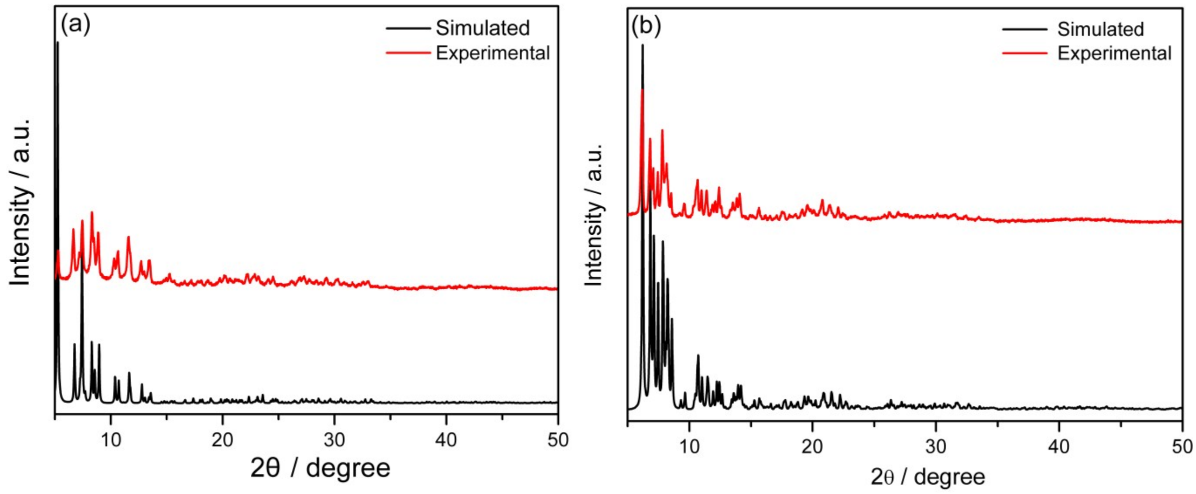

Fig. S1 XRD patterns of (a) Ti_{32}-BTA and (b) Ti_{32}-DMBTA.

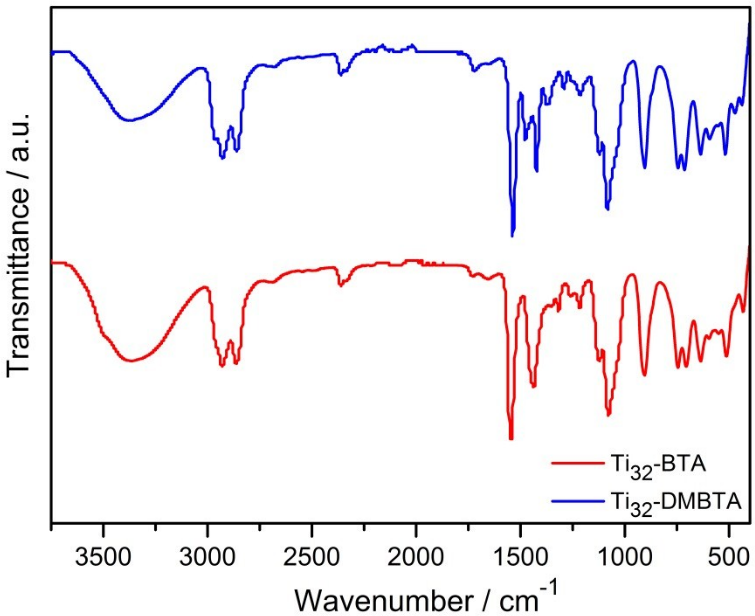

Fig. S2 FT-IR spectra of Ti_{32}-BTA and Ti_{32}-DMBTA.

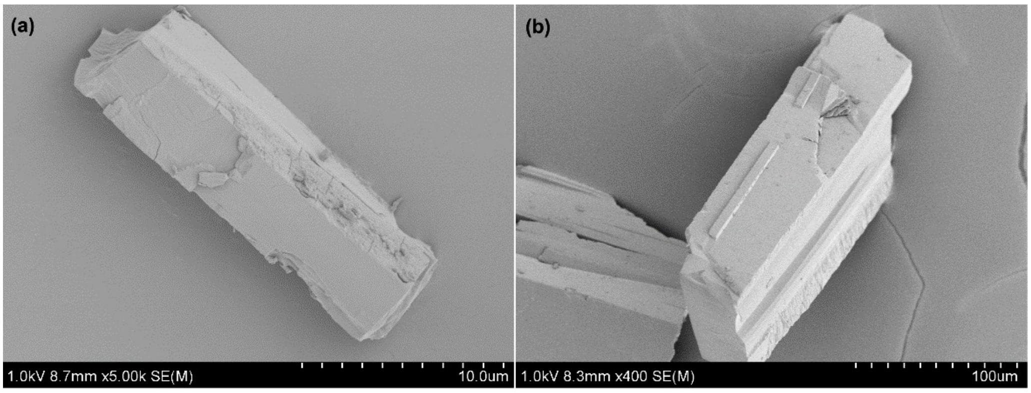

Fig. S3 SEM image of (a) Ti_{32}-BTA and (b) Ti_{32}-DMBTA.

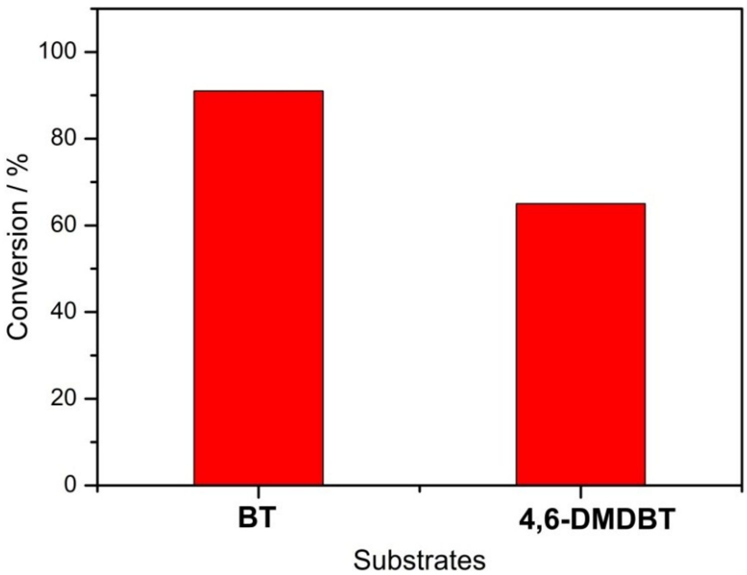

Fig. S4 Desulfurization efficiencies for BT and 4,6-DMDBT with Ti_{32}-BTA as catalyst.

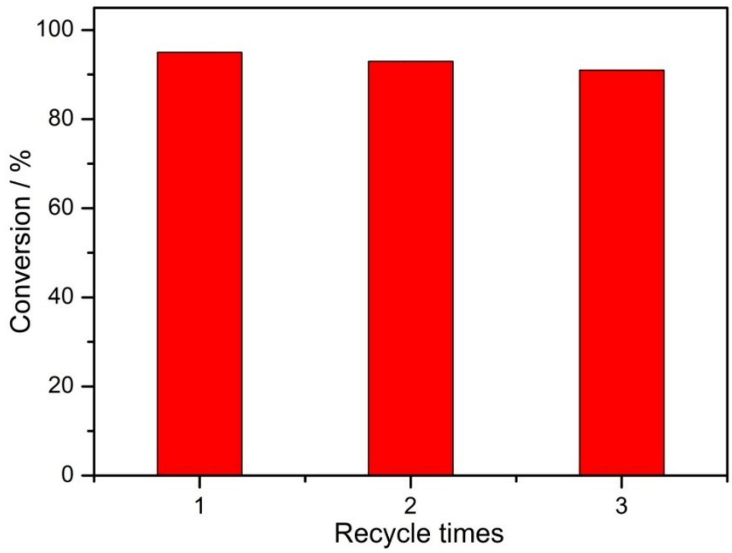

Fig. S5 Recycle tests in the oxidation of DBT with Ti_{32}-BTA as catalyst.

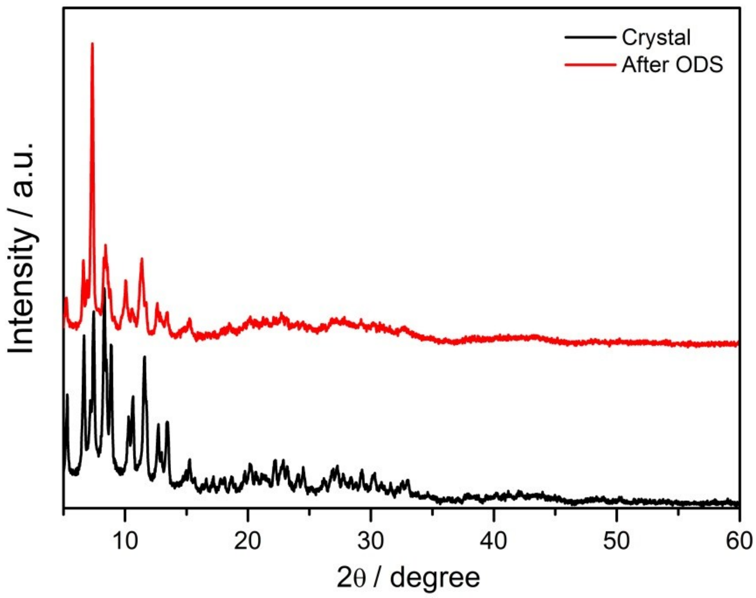

Fig. S6 XRD patterns of Ti_{32}-BTA before and after ODS reaction.

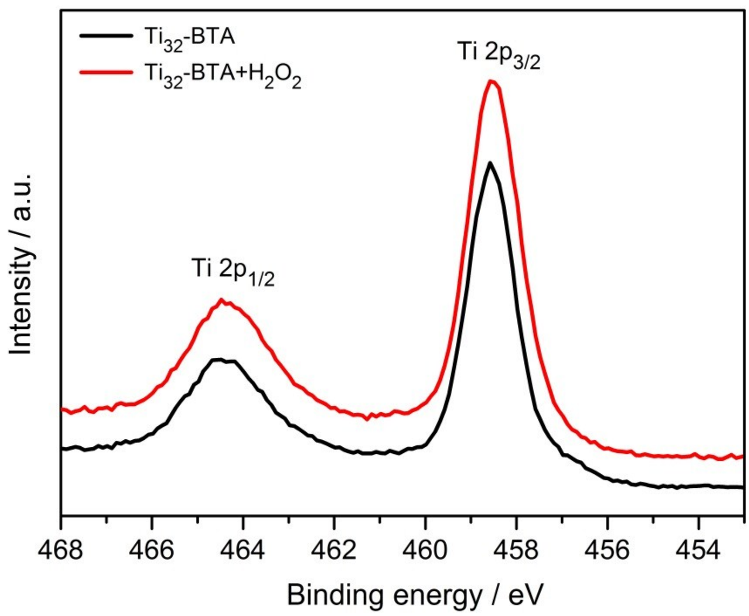

Fig. S7 Ti 2p XPS spectra of Ti_{32}-BTA before and after treated with H_2O_2.

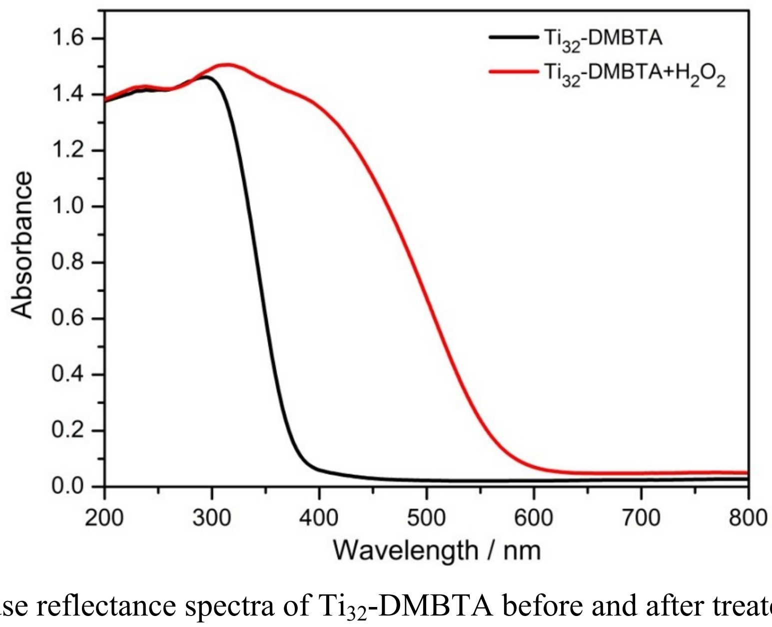

Fig. S8 Diffuse reflectance spectra of Ti_{32}-DMBTA before and after treated with H_2O_2.