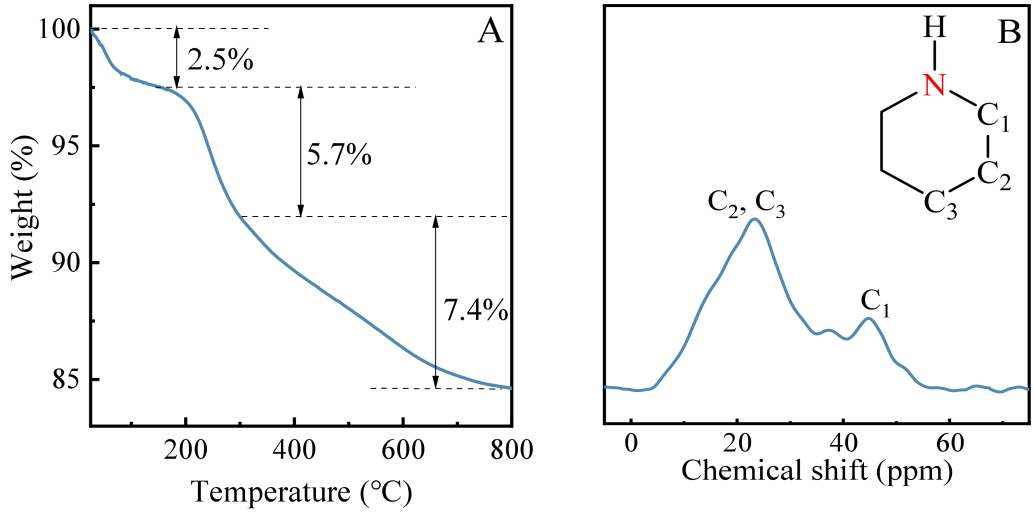
Supplementary Materials

Hydrophilic Ti-MWW for catalyzing epoxidation of allyl alcohol

Xianchen Gong[1], Jie Tuo[1], Jilong Wang[1], Xintong Li[1], Chengwei Zhai[1], Hao Xu[1,2,*], Peng Wu[1,2,*]

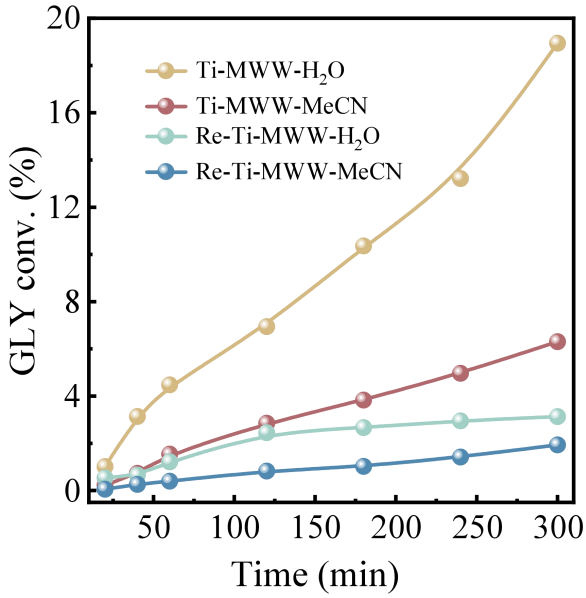
[1]Shanghai Key Laboratory of Green Chemistry and Chemical Processes, State Key Laboratory of Petroleum Molecular & Process Engineering, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai 200062, China.
[2]Institute of Eco-Chongming, Shanghai 202162, China.

[*]**Correspondence to:** Profs. Hao Xu, Peng Wu, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, State Key Laboratory of Petroleum Molecular & Process Engineering, School of Chemistry and Molecular Engineering, East China Normal University, No. 3663 North Zhongshan Road, Shanghai 200062, China. E-mail: hxu@chem.ecnu.edu.cn; pwu@chem.ecnu.edu.cn



Supplementary Figure 1. (A) TG curve and (B) ^{13}C MAS NMR spectrum of Re-Ti-MWW.

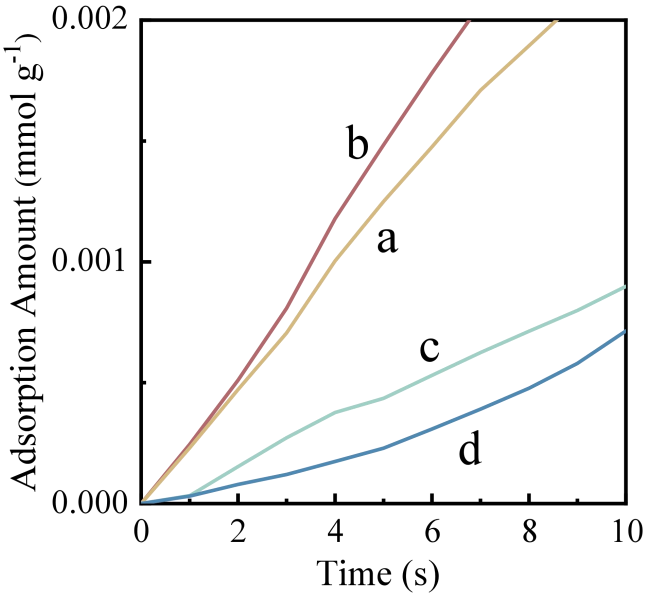
As shown in Supplementary Figure 1A, the weight loss of water (< 150 °C), organics between the layers (150-300 °C) and organics inside the pores (300-800 °C) were 2.5%, 5.7% and 7.4%, respectively, indicating that PI entered the interlayer and pores of Ti-MWW. Supplementary Figure 1B shows that the signals associated with PI molecules were detected in the range of 0-60 ppm, indicating that PI molecules were present in the Re-Ti-MWW.



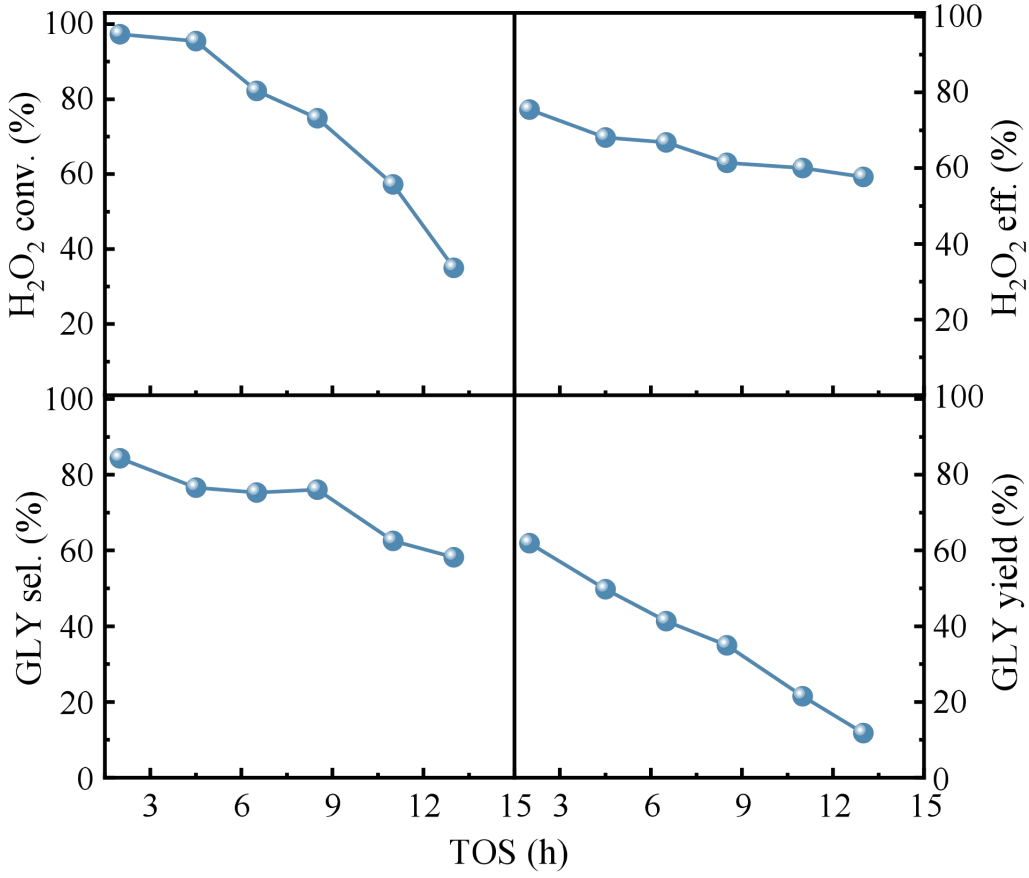
Supplementary Figure 2. GLY conversion over Ti-MWW and Re-Ti-MWW during hydrolysis of GLY in H_2O and MeCN solvents. The labels in this figure represent "sample name-solvent".

Reaction conditions: catalyst, 0.1 g; GLY, 10 mmol; Solvent, 5 mL; H_2O_2, 10 mmol; temperature, 313 K; time, 20-300 min.

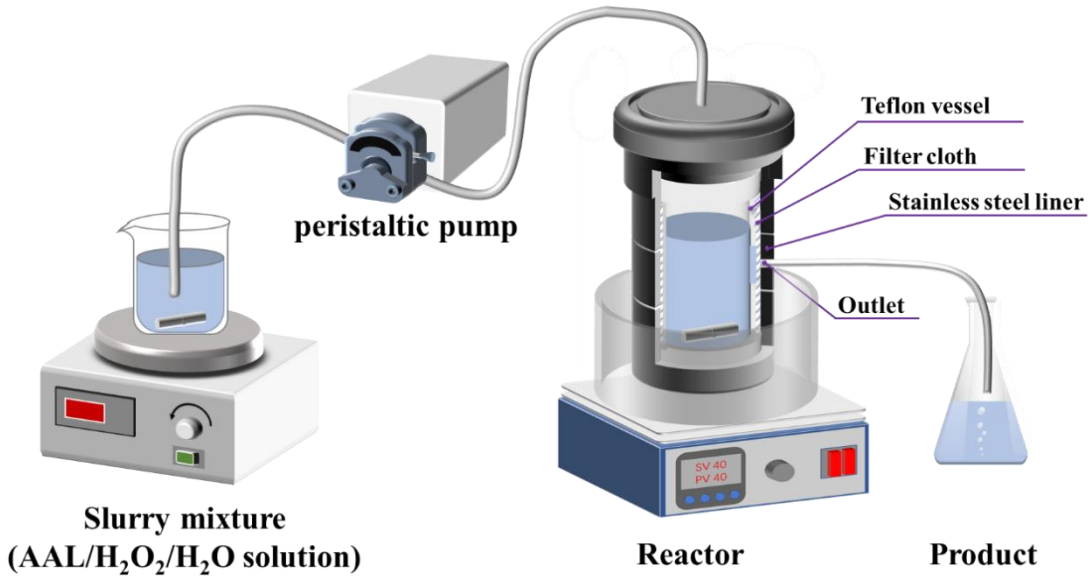
The presence of interlayer PI inhibited the hydrolysis of GLY effectively in the presence of H_2O_2 and H_2O.



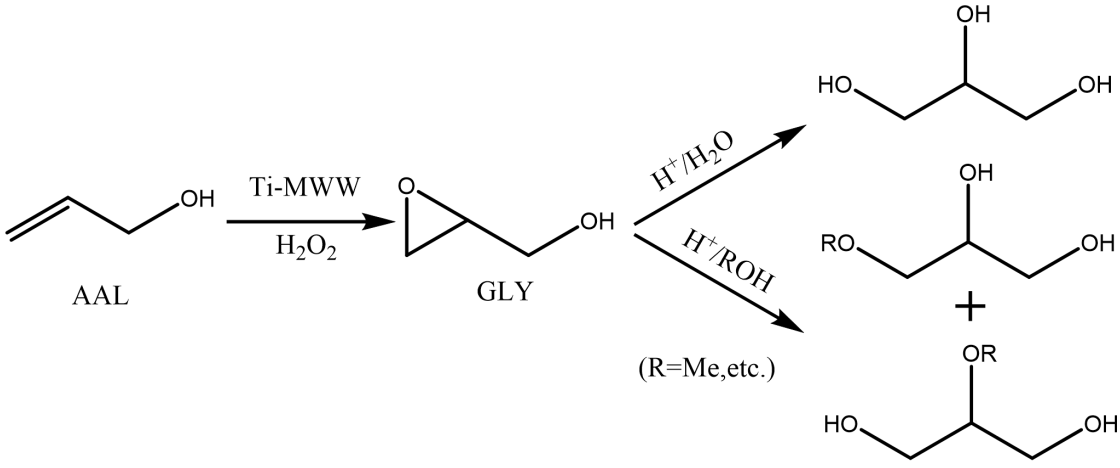
Supplementary Figure 3. Adsorption isotherms of AAL at 313 K over (a) Ti-MWW, (b) Re-Ti-MWW, (c) TS-1, and (d) Ti-MOR.



Supplementary Figure 4. The lifetime of Ti-MWW in the continuous epoxidation of AAL. Reaction conditions: catalyst, 1 g; temperature, 313 K; AAL/H_2O_2 molar ratio, 1.5; H_2O/AAL mass ratio, 4; WHSV(H_2O_2) = 0.4 h^{-1}; 500 rpm.



Supplementary Scheme 1. The schematic description of continuous slurry bed reactor for AAL epoxidation.



Supplementary Scheme 2. The main reaction and possible side-reactions of AAL epoxidation catalyzed by titanosilicate/H_2O_2 system.

Supplementary Table 1. Physicochemical properties of various titanosilicate catalysts

Sample	Si/Ti[a]	Surface area ($m^2 \cdot g^{-1}$)			Pore volume ($cm^3 \cdot g^{-1}$)		
		S_{total}[b]	S_{micro}	S_{ext}[c]	V_{total}[b]	V_{micro}[c]	V_{meso}
Ti-MWW	39	524	417	106	0.46	0.16	0.3
Re-Ti-MWW	39	149	70	79	0.38	0.03	0.35
TS-1	35	437	324	113	0.29	0.16	0.13
Ti-MOR	38	414	371	43	0.22	0.14	0.08

[a]Determined by ICP analysis;

[b]Calculated by the BET method;

[c]Calculated by the *t*-plot method.