Supplementary Information

Mesoporous titanosilicate nanoparticles: facile preparation and application in heterogeneous epoxidation of cyclohexene

Yanqiu Jiang,^{a,†} Yong Zhao,^{a,†} Xianzhu Xu,*,^a Kaifeng Lin*,^a and Dan Wang^b

^{*a*} MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, 150080 Harbin, China.

^b State Key Laboratory of Multi-phase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China.

[†]These authors have contributed equally to this study.

* Corresponding authors. Email: <u>linkaifeng@hit.edu.cn</u>; <u>xuxianzhu@hit.edu.cn</u>.

	$d_{100} \ (nm)^{a}$	Unit cell $(a_0, nm)^b$	Wall thickness (nm) ^c
Ti-MCM-41	3.96	4.57	1.27
Nano-MesoTS(0.18)	4.12	4.76	1.86
Nano-Ti-MCM-41	4.24	4.90	1.90

Table S1 Textural properties of the materials

^{*a*} Calculated from XRD results.

^b $a_0=2 \times d(100)/3^{1/2}$. ^c The wall thickness was calculated as: a_0 -pore size.



Scheme S1. Proposed path for the formation of mesoporous titanosilicate nanoparticles in the presence of cationic polymer.



Figure S1 XRD patterns of C-hex-Nano-Ti-MCM-41-3 (a), C-hex-Nano-Ti-MCM-41-5 (b), Nano-Ti-MCM-41-5 (c) and Nano-Ti-MCM-41-3 (d).

As we described in the main text, the material of Nano-Ti-MCM-41 was prepared as follows: under the given preparation conditions for Nano-MesoTS(1), n-hexane and aqueous H_2O_2 (30%) were added to the preparation process, obtaining a novel sample of mesoporous titanosilicate nanoparticles (Nano-Ti-MCM-41), in which molar ratio between hexane and CTAB is 2 and the value between H_2O_2 and TBOT is 238. When different molar ratios of hexane to CTAB at 3 and 5 were applied for Nano-Ti-MCM-41, obtained materials were denoted as Nano-Ti-MCM-41-3 and Nano-Ti-MCM-41-5, respectively. For comparison, other titanosilicate samples were prepared as the same procedure used for Nano-Ti-MCM-41, but without using hydrogen peroxide (C-hex-Nano-Ti-MCM-41-x), where x refers to the molar ratio of hexane to CTAB is 3 and 5.



Figure S2 ²⁹Si MAS NMR spectra of Ti-MCM-41 (A) and Nano-Ti-MCM-41 (B).