Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information for

Zn supported on titania-doped mesoporous silicate MCM-41 as efficient catalysts for acetylene hydration

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1. Catalyst characterizations

The synthesised Ti-doped MCM-41 mesoporous supports and their respective Zn catalysts were characterised by a serious of techniques. Fourier-transform infrared spectroscopy (FTIR): IS10 FT-IR spectrometer with wavelength range of 500-4000 cm^{-1}. X-ray diffractometry (XRD): Bruker D8 advanced X-ray diffractometer. Transmission electron microscopy (TEM): a JEM 2010 electron microscope. X-ray photoelectron spectroscopy (XPS): an Axis Ultra spectrometer with a monochromatised Al-Kα X-ray source. Brunauer–Emmett–Teller (BET): a Micromeritics ASAP 2020. Temperature-programmed desorption (TPD): an AutoChem 2720 instrument. Thermogravimetric (TG) analysis: over the temperature range of 50-1000°C with the heating rate of 20°C/min and a nitrogen flow rate of 10 mL/min. UV–VIS spectra: a Hitachi UH4150 solid state UV–VIS spectrophotometer.

2. Performance evaluation

The catalytic performance was tested in the fixed-bed glass microreactor for the hydration of acetylene. Firstly, in order to eliminate the air atmosphere of the reactor, the nitrogen was continued to purge for 30 min. Then, when the temperature of reactor reached to 240 °C, the reactant water was injected the reactor for 0.5 h by using a peristaltic pump. Else, the other reactant acetylene was poured into the system to react with water. Finally, the reaction products were detected by the gas chromatograph (GC-2014C).

Table S1 Surface atomic composition (%) of Ti-MCM-x, as determined by XPS.

Samples	**Composition (At %)**			**Binding Energy (eV)**					
	Ti	**Si**	**O**	**Ti $2p_{1/2}$**	**Ti $2p_{3/2}$**	**Ti $2p_{1/2}$**	**Ti $2p_{3/2}$**	**O 1s**	**Si 2p**
Ti-MCM-40	0.6	28.46	61.37	466.0	460.3	464.8	459.4	533.6, 530.5	104.3
Ti-MCM-30	1.03	28.71	64.09	465.5	459.8	464.6	459.1	533.4, 530.5	104.1
Ti-MCM-20	1.54	28.9	63.74	465.5	459.6	464.4	458.9	533.3, 530.5	104.0
Ti-MCM-10	2.24	28.93	65.38	465.3	459.6	464.1	458.9	533.4, 530.5	104.2
Ti-MCM-5	5.29	23.5	63.07	465.1	459.5	464.0	458.8	533.0, 530.5	103.6

Table S2 Pore structure parameters and acidity of NH_3 for Zn/Ti-MCM-x.

Samples	Surface area (m^2 g^{-1})	Pore volume (cm^3 g^{-1})	Pore size (nm)	Acidity(μmol NH_3/g)	Brønsted acidity (μmol/gcat)	Lewis acidity (μmol/gcat)
Zn/MCM	619.45	0.48	3.42	11.29	3.97	7.32
Zn/Ti-MCM-40	509.13	0.39	3.33	8.24	1.48	6.76
Zn/Ti-MCM-30	365.67	0.32	3.24	10.18	2.34	7.84
Zn/Ti-MCM-20	291.89	0.23	3.01	11.52	2.10	9.42
Zn/Ti-MCM-10	282.34	0.21	2.95	20.75	2.57	18.18
Zn/Ti-MCM-5	161.43	0.19	2.48	30.40	4.11	26.29

Table S3 The binding energy of elements for the fresh Zn/Ti-MCM-x, as determined by XPS.

Samples	Binding Energy (eV)							
	Ti $2p_{1/2}$	Ti $2p_{3/2}$	Ti $2p_{1/2}$	Ti $2p_{3/2}$	Zn^{-1} $2p_{3/2}$	Zn^{-2} $2p_{3/2}$	O 1s	Si 2p
Zn/Ti-MCM-40	465.5	459.9	464.6	459.1	1023.0	1023.7	532.9, 530.4	103.6
Zn/Ti-MCM-30	465.5	460.3	464.6	459.4	1023.1	1023.9	533.3, 530.4	104.0
Zn/Ti-MCM-20	465.2	459.6	464.6	459.0	1023.1	1023.8	533.0, 530.4	103.7
Zn/Ti-MCM-10	465.6	459.7	464.3	459.1	1023.0	1023.7	533.1, 530.4	103.7
Zn/Ti-MCM-5	465.0	459.3	463.9	458.7	1022.5	1023.1	532.7, 530.4	103.3

Table S4 The binding energy of elements for the spent Zn/Ti-MCM-x, as determined by XPS.

Sample	Binding Energy (eV)							
	Ti $2p_{1/2}$	Ti $2p_{3/2}$	Ti $2p_{1/2}$	Ti $2p_{3/2}$	Zn $2p_{3/2}^{-1}$	Zn $2p_{3/2}^{-2}$	O 1s	Si 2p
S-Zn/Ti-MCM-40	464.8	459.5	464.1	458.7	1022.6	1023.3	532.8, 530.2	103.6
S-Zn/Ti-MCM-30	464.9	459.5	464.4	458.9	1022.8	1023.5	533.0, 530.2	103.7
S-Zn/Ti-MCM-20	465.1	459.6	464.6	459.0	1022.9	1023.6	533.2, 530.2	103.9
S-Zn/Ti-MCM-10	465.2	459.3	464.4	458.7	1022.4	1023.0	533.0, 530.2	103.7
S-Zn/Ti-MCM-5	465.1	459.0	464.2	458.6	1022.3	1022.7	532.9, 530.2	103.7

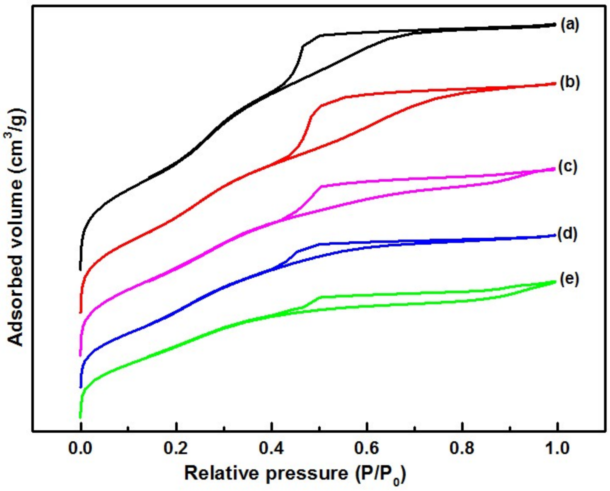


Fig. S1 N_2 adsorption–desorption isotherms of Ti-doped MCM-41 mesoporous materials (a) Ti-MCM-40, (b) Ti-MCM-30, (c) Ti-MCM-20, (d) Ti-MCM-10, (e) Ti-MCM-5.

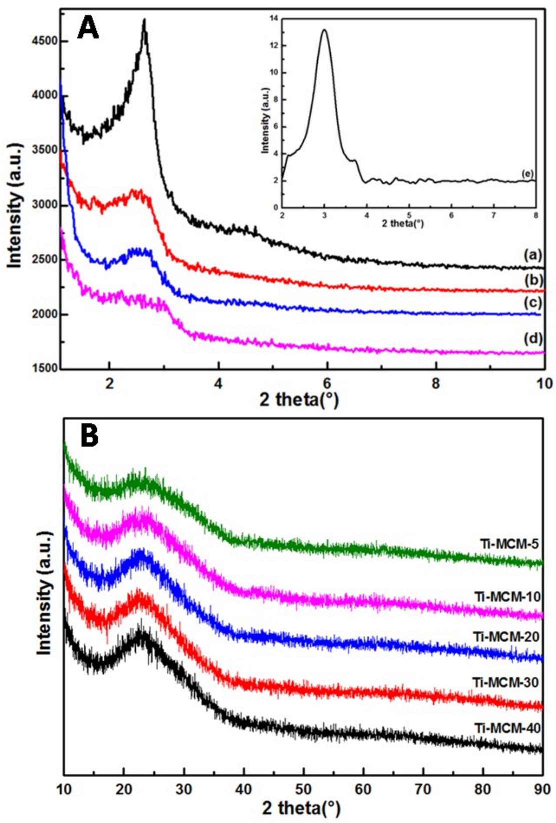


Fig. S2 Small- and Wide-angel XRD patterns of Ti-doped MCM-41 mesoporous materials(a) Ti-MCM-40, (b) Ti-MCM-30, (c) Ti-MCM-20, (d) Ti-MCM-10, (e) Ti-MCM-5.

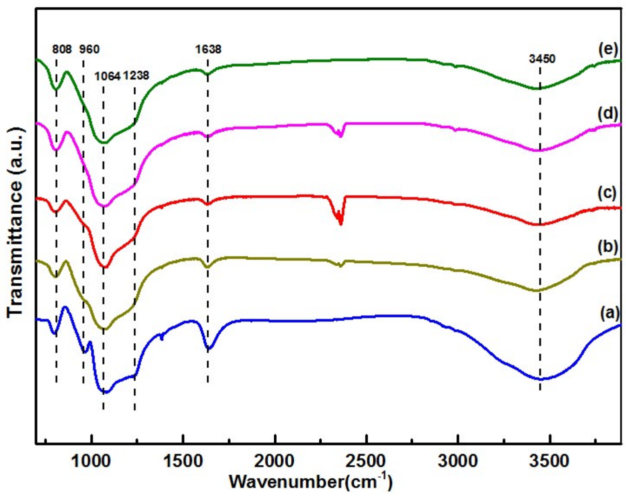


Fig. S3 FT-IR spectra of Ti-doped MCM-41 mesoporous materials (a) Ti-MCM-40, (b) Ti-MCM-30, (c) Ti-MCM-20, (d) Ti-MCM-10, (e) Ti-MCM-5.

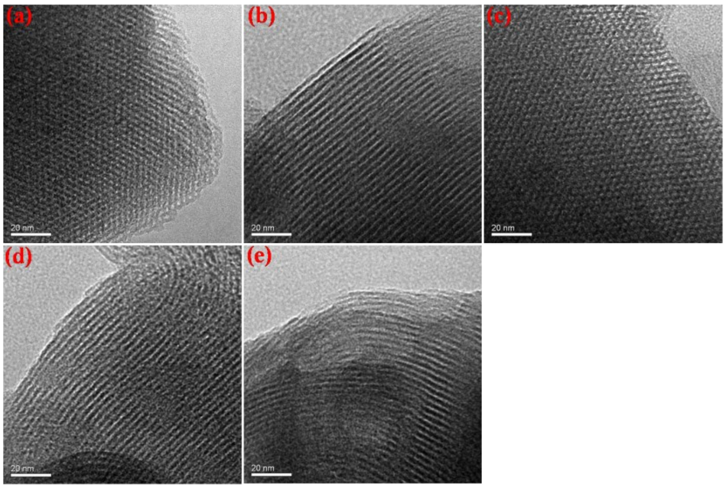


Fig. S4 TEM images of Ti-doped MCM-41 mesoporous materials (a) Ti-MCM-40, (b) Ti-MCM-30, (c) Ti-MCM-20, (d) Ti-MCM-10, (e) Ti-MCM-5.

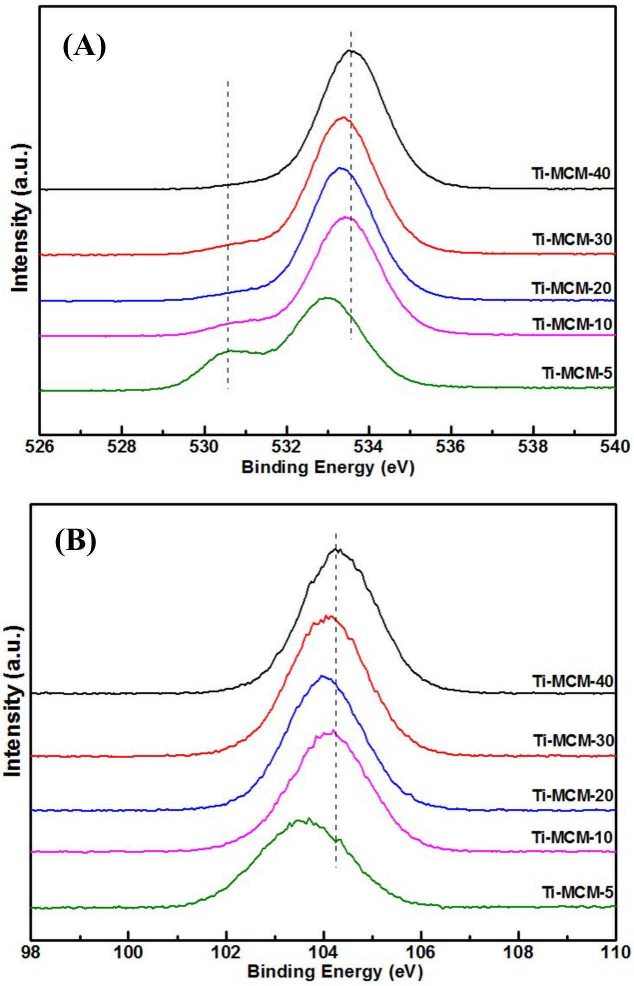


Fig. S5 The high-resolution XPS spectra for the O 1s (A) and Si 2p (B) of Ti-doped MCM-41 mesoporous materials.

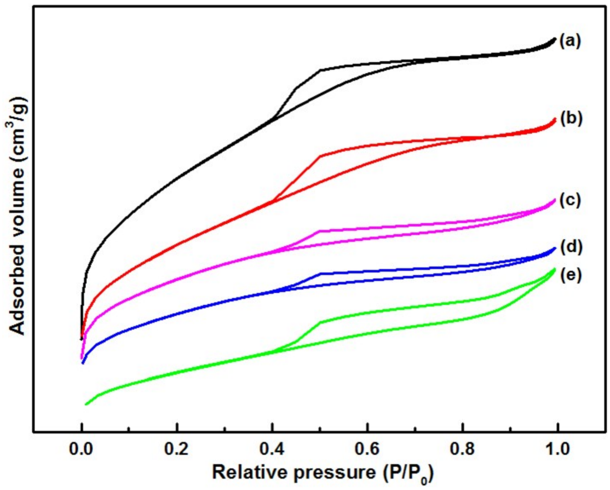


Fig. S6 N_2 adsorption–desorption isotherms of modified catalysts (a) Zn/Ti-MCM-40, (b) Zn/Ti-MCM-30, (c) Zn/Ti-MCM-20, (d) Zn/Ti-MCM-10, (e) Zn/Ti-MCM-5.

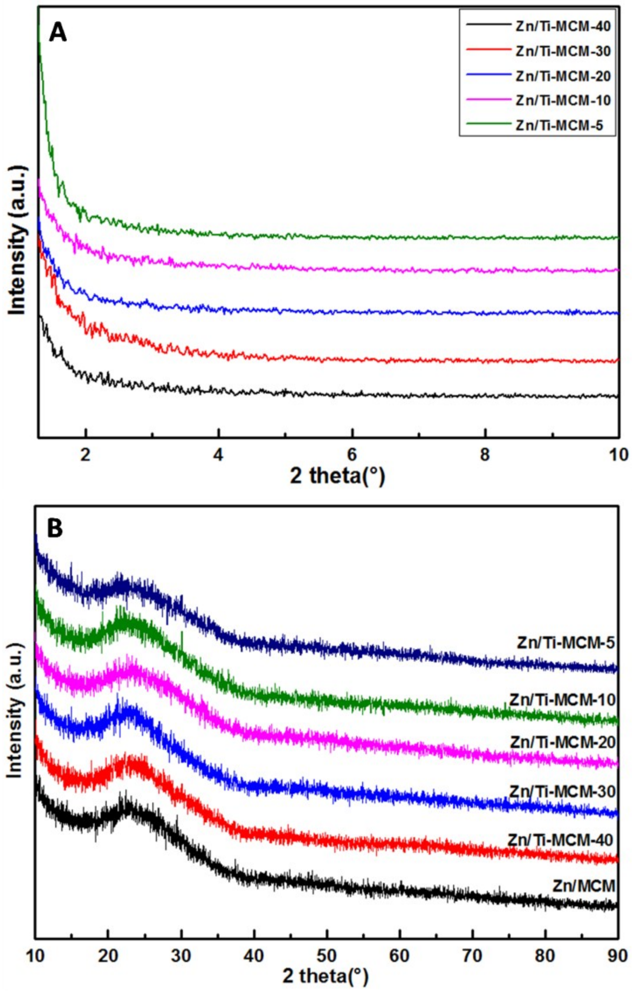


Fig. S7 Small-angel and Wide-angel XRD patterns of fresh Zn/Ti-MCM-*x* catalysts.

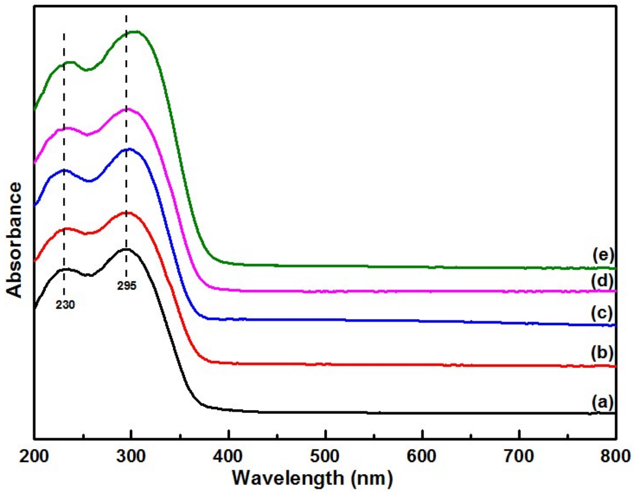


Fig. S8 Solid state UV-vis spectra of modified catalysts (a) Zn/Ti-MCM-40, (b) Zn/Ti-MCM-30, (c) Zn/Ti-MCM-20, (d) Zn/Ti-MCM-10, (e) Zn/Ti-MCM-5.

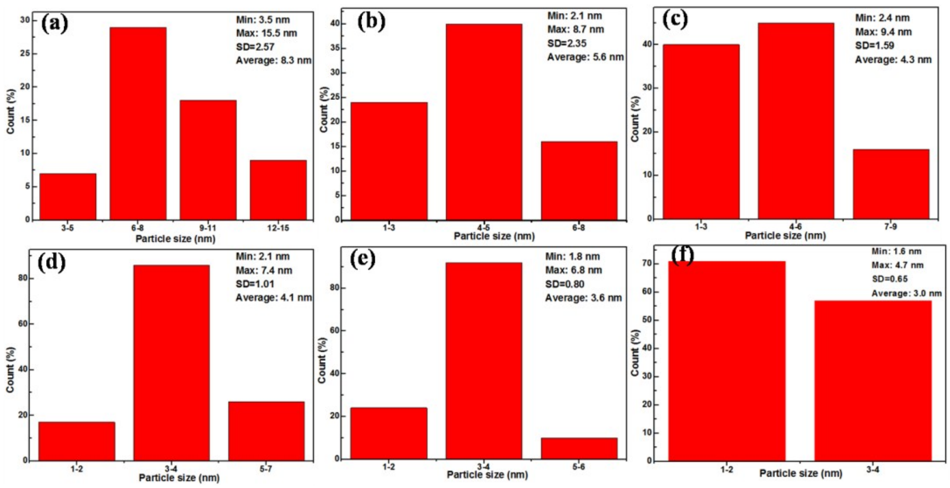
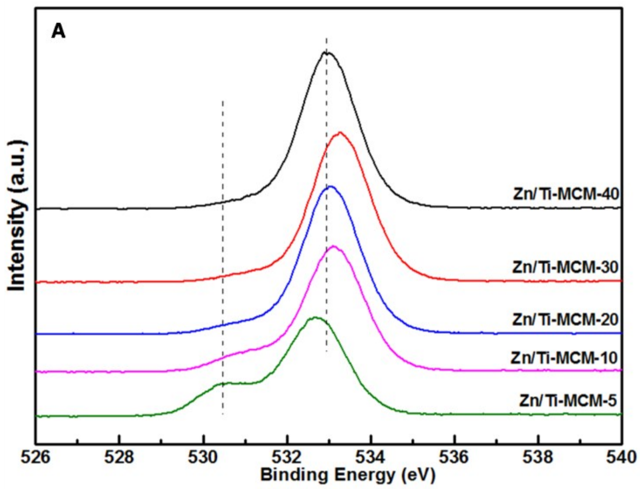


Fig. S9 The particle size distribution of fresh Zn/Ti-MCM-*x* catalysts (a) Zn/MCM, (b) Zn/Ti-MCM-40, (c) Zn/Ti-MCM-30, (d) Zn/Ti-MCM-20, (e) Zn/Ti-MCM-10, (f) Zn/Ti-MCM-5.



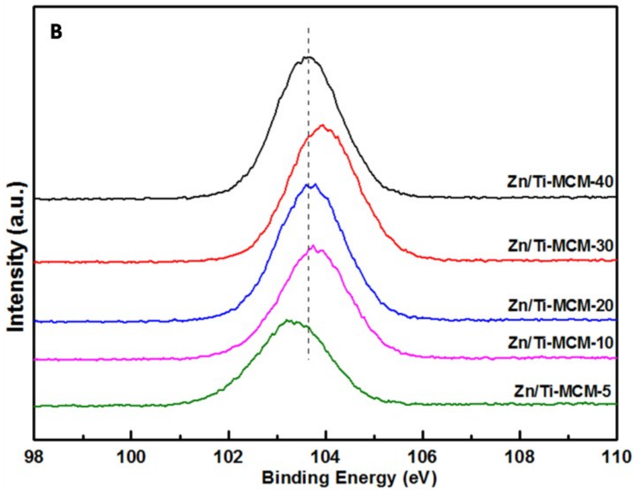


Fig. S10 The high-resolution XPS spectra for the O 1s (A) and Si 2p (B) of fresh Zn/Ti-MCM-*x* catalysts.

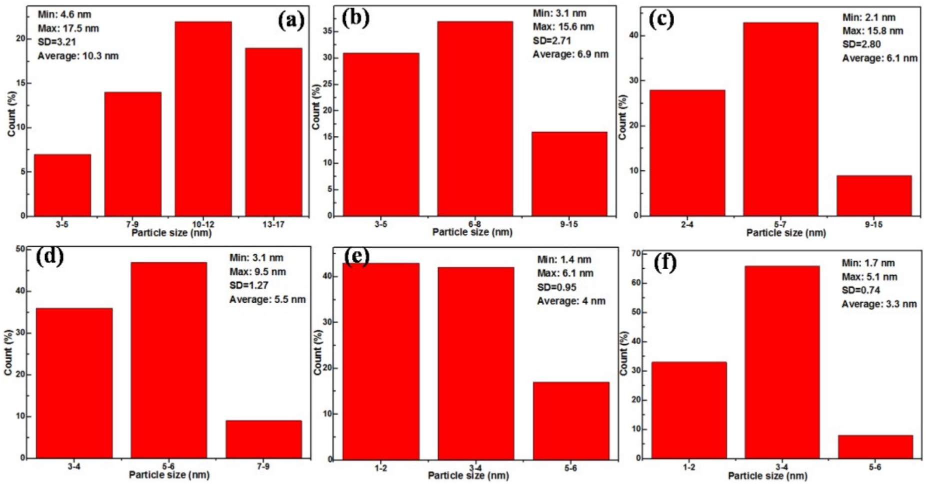
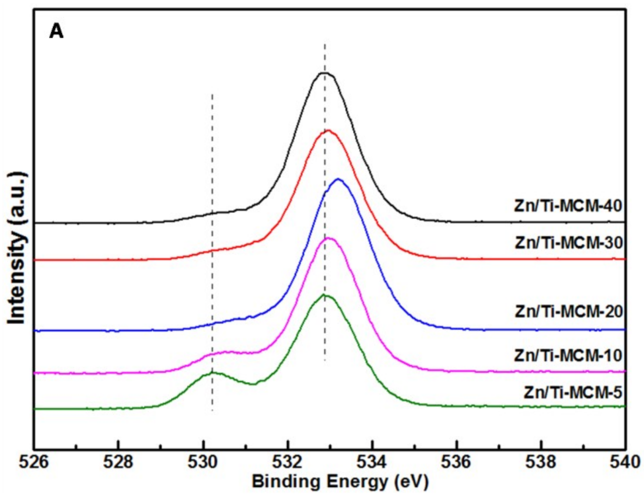


Fig. S11 The particle size distribution of spent Zn/Ti-MCM-*x* catalysts (a) Zn/MCM, (b) Zn/Ti-MCM-40, (c) Zn/Ti-MCM-30, (d) Zn/Ti-MCM-20, (e) Zn/Ti-MCM-10, (f) Zn/Ti-MCM-5.



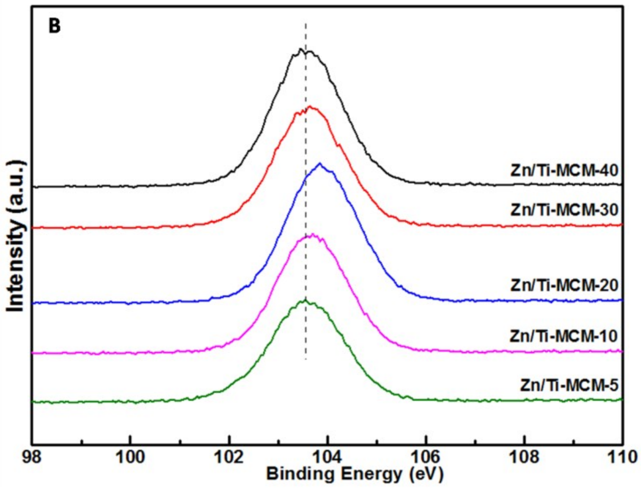


Fig. S12 The high-resolution XPS spectra for the O 1s (A) and Si 2p (B) of the spent Zn/Ti-MCM-*x* catalysts.