Supporting information:

UV-vis spectroscopy

UV-vis spectra of the fresh Ti-SSZ-70 are shown in Figure S1 with a band between 200 nm and 300 nm and a maximum at 209 nm. The spent material shows a maximum at 218 nm and one shoulder at 241 nm. The spent/calcined catalyst shows one a little bit broader band than represented by the fresh catalyst, with a maximum at 221 nm. The maximum at 209 nm presents isolated $Ti(OSi)_4$ or $Ti(OSi)_3OH$ framework sites.[22] We interpret the shoulder at 241 nm as representing higher coordinated (6-coordination number) Ti sites, and it may also indicate titanium sites that are not fully condensed to the framework, i.e. containing a titanol, but still present isolated Ti sites represented by the maximum at 218 nm.[23] The spent/calcined Ti-SSZ-70, however, is not showing the same Ti sites as the fresh one, but because framework sites have been previously attributed to be in the range of 206 nm – 220 nm, we infer that the this material comprise isolated Ti sites in the framework, but with a shift towards titanols (Ti-OH).[22] These results show, that Ti-SSZ-70 is not fully recyclable.

The UV-vis spectrum of fresh Ti-UCB-4 is shown in Figure S1 and indicates one major band spanning from 200 nm to 328 nm, with a maximum at 209 nm. The spent material shows two maxima, one at 211 nm and one less intense at 247 nm. After calcining, the second maximum disappears and the resulting catalyst shows a maximum at 211 nm, similar to the starting wavelength. Based on this, we infer that Ti-UCB-4 comprises isolated Ti framework sites. The shoulder around 247 nm indicates presence of titanium sites in non-framework positions, such as those grafted on external-surface isolated silanols.[24] After calcination, the material shows the same absorbance (211 nm) as before the usage, which shows that Ti-UCB-4 is recyclable, consistent to previously reported data.[1]

Figure S1 shows UV-Vis data for Ti-SSZ-70-DEL-HIGHPH. The maximum band for the fresh material is at 220 nm and a weak shoulder around 260 nm. The spent catalyst shows two nearly equal maxima at 216 nm and 233 nm and a broad band up to high wavelengths to 400 nm. After calcination, the maximum of the band is at 220 nm. The fresh Ti-SSZ-70-DEL-HIGHPH indicates primarily isolated framework Ti(IV)-sites ($Ti(OSi)_4$ or $Ti(OSi)_3(OH)$ units) with a small amount of Ti oxide oligomers on the surface. During catalysis, the material builds up organic compounds, as discussed previously, shown by absorbance at higher wavelength. The maxima at 217 nm and 234 nm demonstrate the presence of two Ti-sites species: four-fold coordinated Ti-sites in the framework and tripodal titanols. After calcination, there is no significant difference visible in the absorbance between the fresh catalyst and the spent catalyst. Thus, based on these data, the material can be fully regenerated.

The UV-vis data for the mix of Ti-SiO_2 and Ti-UCB-4 are shown in Figure S1. The absorbance for the fresh material shows a plateau from 213 nm to 223 nm and a shoulder at 267 nm. This region is between the reported isolated framework sites consisting of $Ti(OSi)_4$ or $Ti(OSi)_3(OH)$ units and the shoulder indicates non-framework Ti sites. After catalysis, the maximum is at 214 nm and a huge shoulder at around 245 nm and a small shoulder at 290 nm. This shows three different Ti sites with the major being non framework sites but also isolated framework sites at lower wavelength and organic residue at high wavelength > 300 nm. After calcination, the maximum appears at 234 nm. This is between $Ti(OH)(OSi)_3$ (~230 nm) and $Ti(OH)(H_2O)(OSi)_3$ (~260 nm).[22]

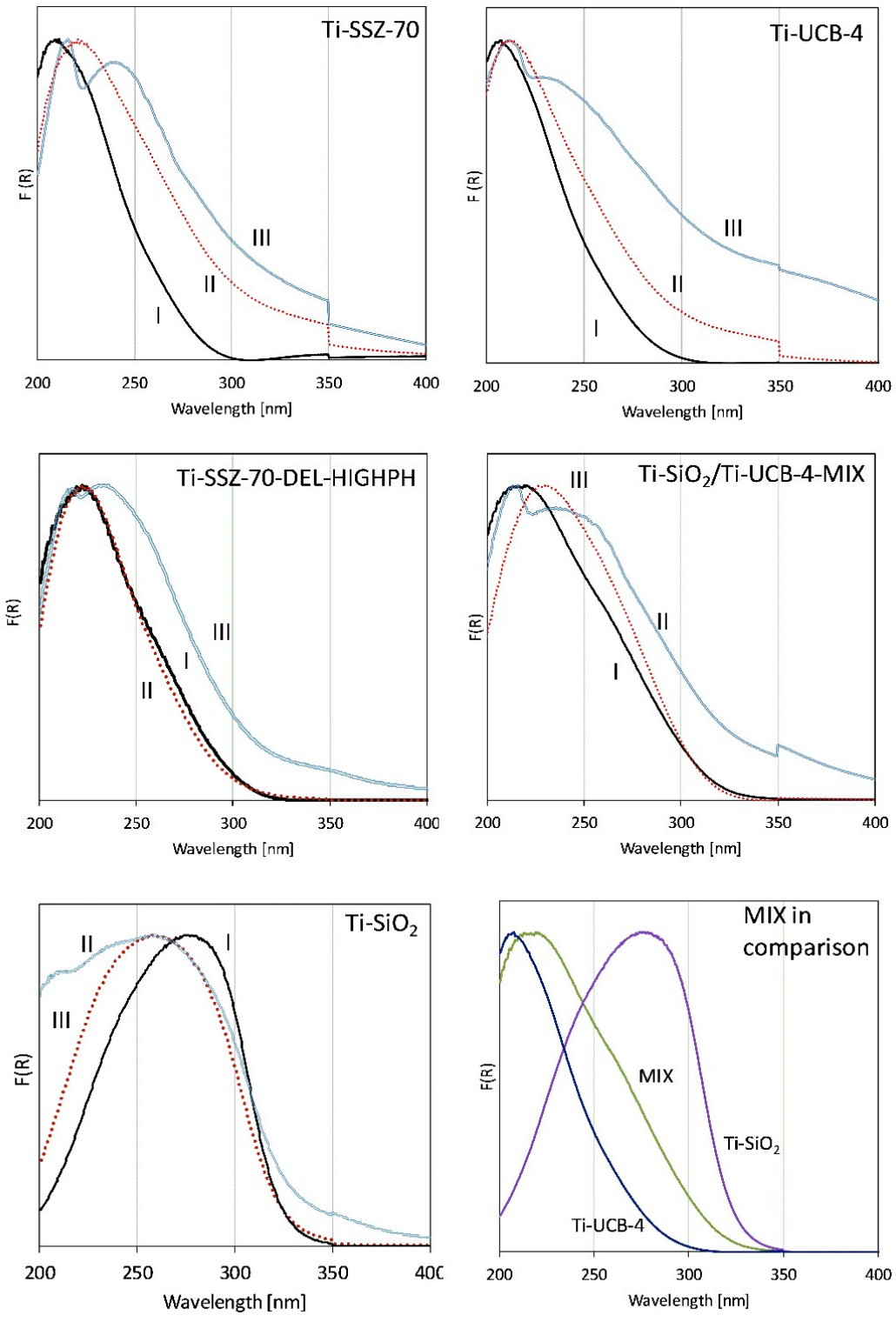

Figure 7: UV-vis spectra of A) Ti-SSZ-70, B) Ti-UCB-4, and C) Ti-SSZ-70-DEL-HIGHPH, fresh calcined (black), spent (blue) and spent/calcined (red).

Calculation for reaction rate constant k', based on catalyst mass:

$$k' = \frac{-\ln\left(1 - X_{EBHP}\right) \cdot \dot{v}}{m_{cat}}$$

Calculation for reaction rate constant k, based on Ti-content:

$$k = \frac{-\ln\left(1 - X_{EBHP}\right) \cdot \dot{v}}{m_{Ti}}$$

X_{EBHP} = average EBHP conversion 89 hours – 100 hours time on stream

$\dot{v}$ = flow rate = 1.0 mL/h

m_{cat} = mass of the catalyst; 0.025 g Ti-UCB-4, Ti-SSZ-70, Ti-SiO_2/Ti-UCB-4; 0.040 g for Ti-SSZ-70-HIGHPH; 0.018 g for Ti-SiO_2.