Electronic Supporting Information

Heteropolytungstic Acids Incorporated in Ordered Mesoporous Zirconia Framework as Efficient Oxidation Catalysts

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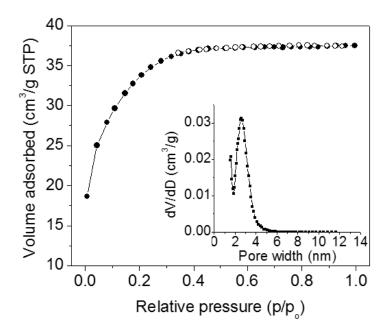


Fig. S1 Nitrogen adsorption and desorption isotherms at 77K of mesoporous zirconia (*meso*-ZrO₂). Analysis of the adsorption data with the BET method gives surface area of 118 m²g⁻¹ and pore volume of 0.06 cm³g⁻¹. Inset: the NLDFT pore size distribution calculated from the adsorption branch, indicating mesopore diameter of 2.5 nm.

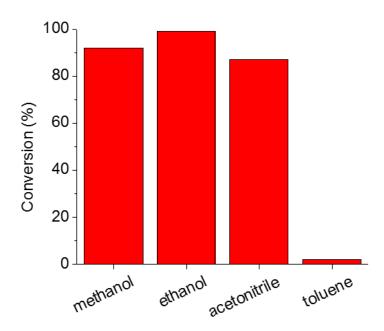


Fig. S2 Oxidation of 1,1-diphenyl-2-methylpropene over ZrSTA(5) catalyst in different media. *Experimental conditions*: 0.1 mmol substrate, 0.5 mmol catalyst (containing 2 mol% STA), 3 equiv. H₂O₂ (30% in water), 3 mL ethanol, 50 °C, 1 h.

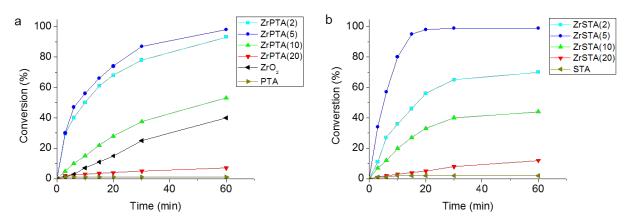


Figure S3. Time evolution of 1,1-diphenyl-2-methylpropene oxidation catalyzed by hydrogen peroxide using mesoporous zirconia (meso-ZrO₂), ZrPTA(w) and ZrSTA(w) materials and PTA ($H_3PW_{12}O_{40}$) and STA ($H_4SiW_{12}O_{40}$) compounds as catalysts.

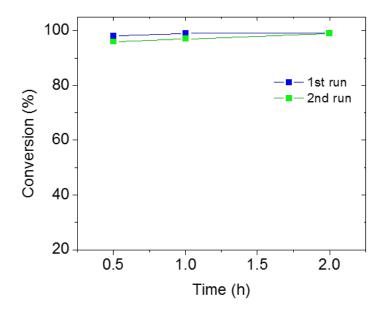


Figure S4. Recycling study of the mesoporous ZrSTA(5) catalyst (*experimental conditions*: 0.1 mmol of 1,1-diphenyl-2-methylpropene, 0.5 mmol of catalyst (containing 2 mol% STA), 3 equivalent of H_2O_2 (30% in water), 3 mL of ethanol, 50 °C).

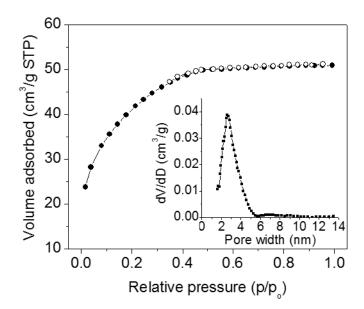


Figure S5. N_2 adsorption and desorption isotherms at 77K of reused ZrSTA(5) catalyst. Analysis of the adsorption data with the BET method gives surface area of 149 m²g⁻¹ and total pore volume of 0.08 cm³g⁻¹. Inset: the corresponding NLDFT pore size distribution, indicating pore size of ~2.6 nm.

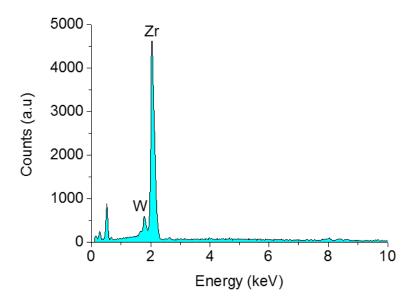


Figure S6. Typical EDS-SEM microanalysis spectrum obtained from the ZrSTA(5) sample after catalytic reactions.

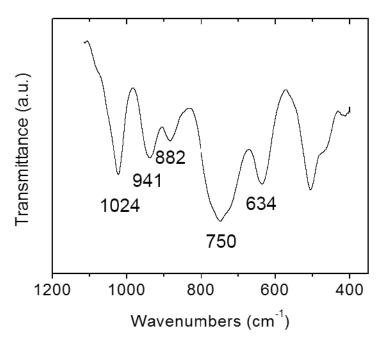


Figure S7. IR spectrum of reused ZrSTA(5) catalyst, showing intense absorption peaks at \sim 1024, \sim 941 and \sim 882 cm⁻¹ that are attributed to the stretching vibrations of Si–O, W=O_d and W-O_b–W bonds in the $[SiW_{12}O_{40}]^{4-}$ Keggin clusters. The strong absorption peaks at \sim 750 and \sim 634 cm⁻¹ are assigned to the stretching vibration bands of Zr–O and Zr–O–Zr of zirconia matrix, respectively