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Catalytic Oppenauer oxidation of secondary alcohols over post-synthesized Sn-Beta

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Experimental

Materials

HBeta zeolite (SiO_2/Al_2O_3 = 25) was purchased from Nankai University Catalyst Co. (China). $SnCl_4{\cdot}5H_2O$ (≥99%), naphthalene (AR) and acetone (≥99%) were obtained from Tianjin Kermel Reagent Co. (China). MOP (≥99.5%), MOA (≥99%), pyridine (≥99%), deuterated acetonitrile (≥99.8%), 1-ethoxy-2-propanol (≥99%), 1-methoxy-2-butanol (>93%), cyclopentanol (≥99%), cyclohexanol (≥98.5%), 2-butanol (≥99.5%), 2-pentanol (≥98%), 1-phenylethyl alcohol (≥98%), lactic acid (≥98%) and methyl lactate (>98%) were purchased from Aladdin Chemical Reagent Corporation (China). All reactants were used without further purification.

Calculation the average TORs of different Sn species

Three Sn species (open framework Sn, closed framework Sn, and extraframework Sn species) can be discriminated by the FTIR spectra of adsorbed pyridine and CD_3CN. The TOR (μmol g_{cat}^{-1} h^{-1}) calculated based on the conversion lower than 15% according to the following equation:

$$TOR = \frac{initial\ moles\ of\ MOP\ \times\ conversion\ of\ MOP}{mass\ of\ catalyst \times reaction\ time}$$

According to the respective fractions of FTIR spectra adsorbed CD_3CN (Figure 3), the TOR of different Sn species, can be calculated with the following equation:

$$TOR_{1Sn-Beta} = TOR_{Sn\ open} \times LAC_{Sn\ open}\% + TOR_{Sn\ closed} \times LAC_{Sn\ closed}\% + TOR_{Sn\ extra} \times LAC_{Sn\ extra}\%$$

$$TOR_{2Sn-Beta} = TOR_{Sn\ open} \times LAC_{Sn\ open}\% + TOR_{Sn\ closed} \times LAC_{Sn\ closed}\% + TOR_{Sn\ extra} \times LAC_{Sn\ extra}\%$$

$$TOR_{3Sn-Beta} = TOR_{Sn\ open} \times LAC_{Sn\ open}\% + TOR_{Sn\ closed} \times LAC_{Sn\ closed}\% + TOR_{Sn\ extra} \times LAC_{Sn\ extra}\%$$

The average activity of different active Sn species, denoted as $TOR_{Sn\ open}$, $TOR_{Sn\ closed}$ and $TOR_{Sn\ extra}$.

→

$$1600 = TOR_{Sn\ open} \times 31\% + TOR_{Sn\ closed} \times 48\% + TOR_{Sn\ extra} \times 21\%$$

$$3026 = TOR_{Sn\ open} \times 46\% + TOR_{Sn\ closed} \times 41\% + TOR_{Sn\ extra} \times 13\%$$

$$4006 = TOR_{Sn\ open} \times 52\% + TOR_{Sn\ closed} \times 27\% + TOR_{Sn\ extra} \times 21\%$$

→

$$TOR_{Sn\ open} = 8642$$

$$TOR_{Sn\ closed} = -2758$$

$$TOR_{Sn\ extra} = 1195$$

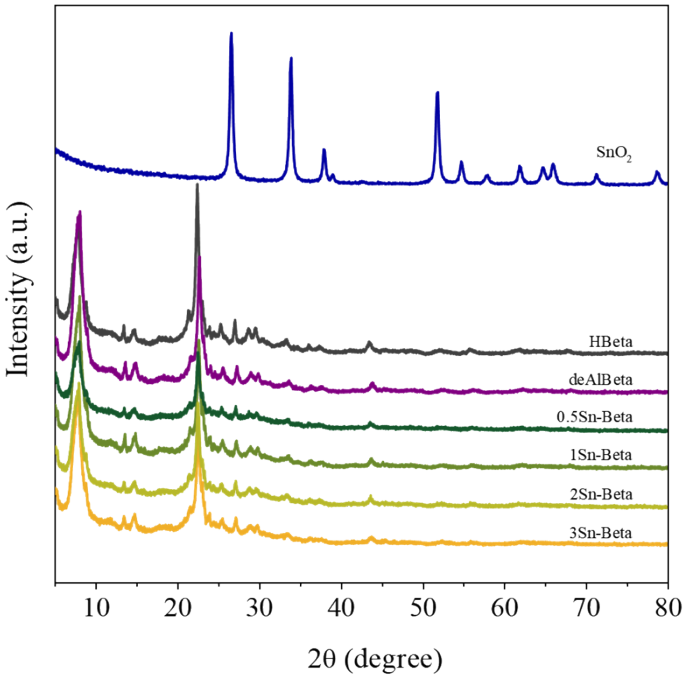

Figure S1. XRD patterns of the samples.

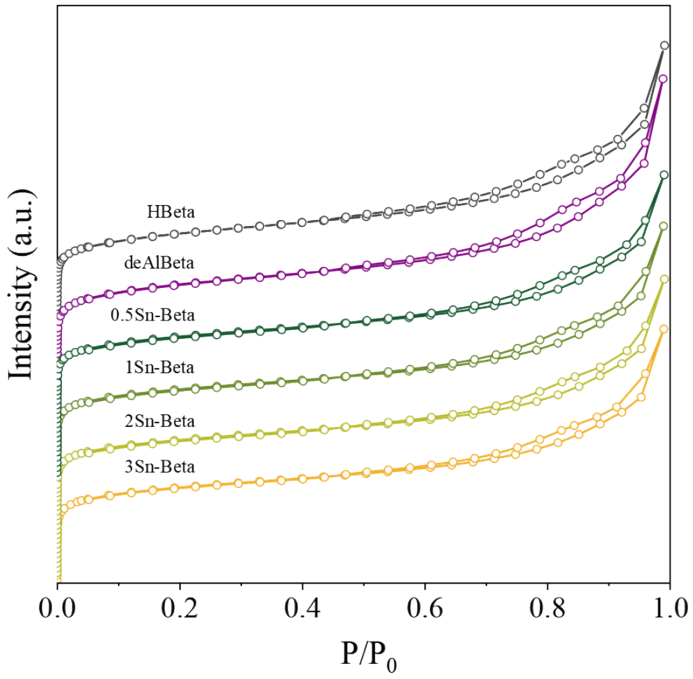

Figure S2. N_2 adsorption-desorption isotherms of HBeta, deAlBeta and *x*Sn-Beta.

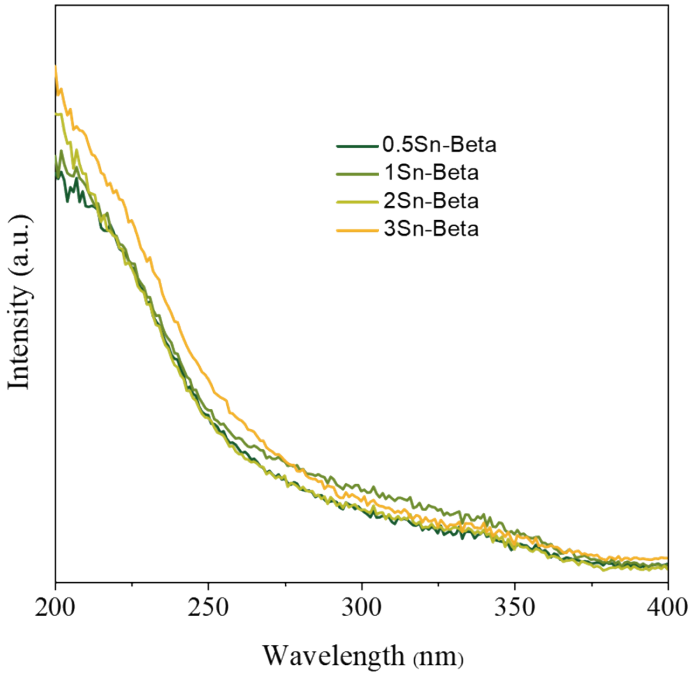

Figure S3. UV-vis spectra of *x*Sn-Beta.

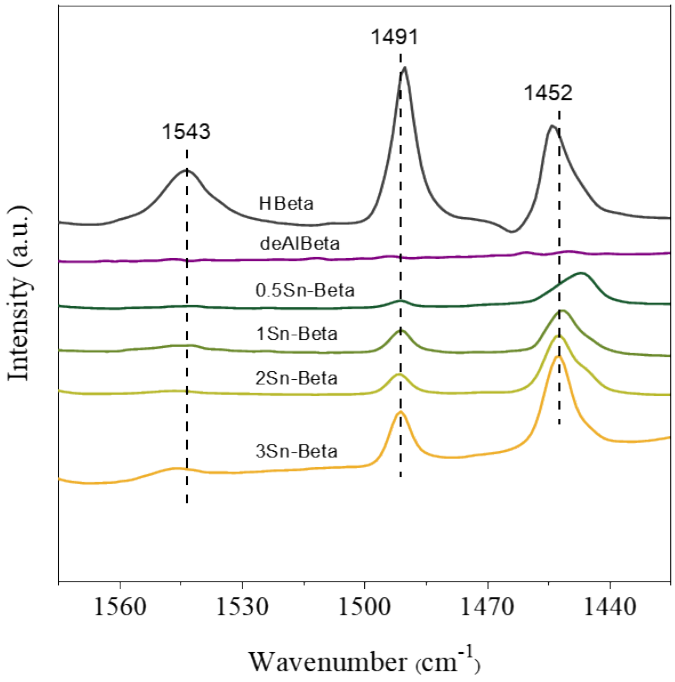

Figure S4. FTIR spectra of pyridine adsorbed on the samples. These spectra were collected after evacuation at 150 °C for 30 min