Supporting information

1. Catalyst Characterization methodology

Catalysts were fully characterized by following techniques.

1.1. X-ray Diffraction (XRD)

Powder X-ray diffraction of the catalysts was recorded using a Philips X'Pert-Pro diffractometer using a Cu K_α irradiation. Diffractograms were recorded from 5 to 80° with a step size of 0.0334°.

1.2. Ammonia temperature programmed desorption

Ammonia TPD was carried out to measure the total acidity of catalysts on Micromeritics (Autochem-II chemisorptions analyzer) instrument with TCD detector.

1.3. Fourier transform infrared spectroscopy (FTIR)

Functional groups of catalyst were detected by FTIR spectra on Perkin Elmer Spectrum 100 in the range of 400-4000 cm^{-1} with a resolution of 4 cm^{-1} by using KBr pellets.

1.4. Scanning electron microscopy (SEM)

External surface morphology was analyzed by using the scanning electron microscope on a JEOL – JSM 6380 LA instrument

1.5. High Resolution Transmission electron microscopy (HRTEM)

The structure of prepared catalysts was further examined by high resolution transmission electron microscopy micrographs of FeDTP@ZIF-8 were obtained on Tecnai G2, F30 microscope at 300 kV.

1.6. Surface area analysis

The surface properties like pore size, pore volume and surface area of catalysts were measured by nitrogen adsorption-desorption process at 77K temperature on ASAP 2010 instrument, Micromeritics, USA. The samples were degassed under high vacuum at 300 °C for 6 h prior to measurement.

1.7. Thermal Gravimetric analysis (TGA)

Thermogravimetric analysis was carried out by taking 20 mg of the sample on TGA instrument (NETZSCH). The temperature was varied from 30 °C to 700°C with a scan rate of 30°C/min under nitrogen atmosphere.

1.8. DRIFTS

The DRIFT spectra of the catalysts (~50 mg) were recorded using a Collector II accessory housed in a Bruker Tensor 27 spectrometer. The spectra were recorded at room temperature after being heated to 200 °C under Ar (50 ml min^{-1} flow rate) to remove adsorbed water. The background spectrum for all catalysts was KBr and all spectra were recorded with 128 scans at a resolution of 4 cm^{-1}.

1.9 XPS

The XPS was acquired using AXIS SUPRA having a PHI 5000 Versa Probe II equipped with a mono-chromatic Al Kα (1486.6 eV) X-ray source and a hemispherical analyzer. Electrical compensation was applied during analysis.

2. Effect of speed of agitation

In the glass reactor the speed of agitation was studied between 600-900 rpm (Fig. S1). It was observed that with the increase in speed of agitation from 600 rpm to 800 rpm the conversion of furfuryl alcohol increased remaining almost the same between 800 and 900 rpm. The increased agitation speed beyond 800 rpm did not reveal any significant effect on the conversion of furfuryl alcohol and all further experiments were conducted at 800 rpm where there was no external mass transfer limitation.

In our earlier reports we have provided the proof of absence of external mass transfer resistance and intra-particle resistance for DTP encapsulated ZIF-8[18]. The calculations given reveals that the reaction is kinetically controlled and free from intra particle diffusion resistance.

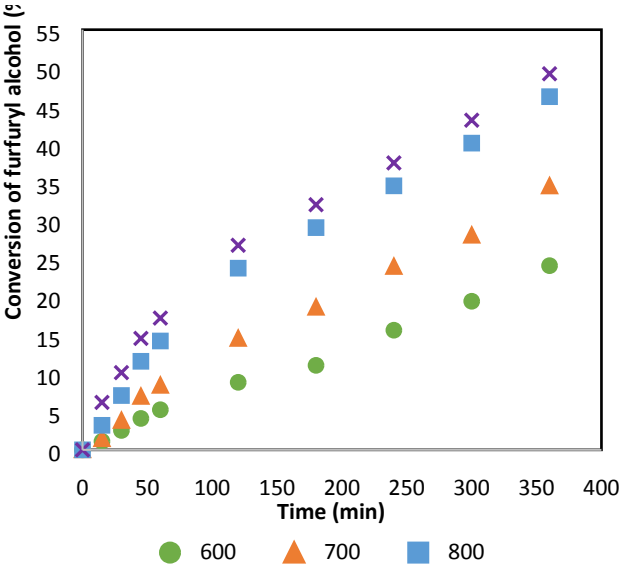

Fig. S1 Effect of speed of agitation Catalyst FeDTP@ZIF-8, Furfuryl alcohol 0.053 mol, acetic acid 0.271 mol, temperature 90 °C, catalyst loading 0.005 g/cm^3, total volume 21 ml, time 6 h.

Proof of absence of external mass transfer resistance

For better understanding of solid-liquid or heterogeneous catalytic reactions, different controlling mechanism are available. The liquid phase diffusivity of furfuryl alcohol (A) at 100 °C was estimated using Wilke-Chang equation as 1.1633*10^{-4} cm^2/s. Considering the limiting value of Sherwood number ($Sh_A = k_{SL\text{-}A} * d_P / D_{AB}$) as 2, mass transfer coefficient was evaluated as 2.326 cm/s. The particle surface per liquid volume was calculated as,

$$a_p = \frac{6w}{\rho_p d_p} = 1601.70 \quad \text{Cm}^2/\text{cm}^3 \qquad (1)$$

The observed initial rates for furfuryl alcohol was calculated as, 3.16*10^{-5} mol.cm^{-3}.s^{-1}, while the mass transfer rate for furfuryl alcohol was evaluated as 0.004954*10^4 mol.cm-3.s-1

As,

i.e. 3.15*10^4 >> 0.0049*10^4

Thus the comparison of relevant resistances shows that

$$\frac{1}{r_{obs}} >>>> \frac{1}{k_{SLA} - a_p(A_0)}$$

Hence it gets prove that there is no external mass transfer resistance in the reaction. The only resistance could be because of intra-particle diffusion, surface reaction, chemisorption or desorption.

Proof of absence of intra-particle resistance

Considering the average particle size of FeDTP@ZIF-8 as 1 µm, a theoretical calculations were carried out to compute Weisz-Prater criterion (C_{wp}). It is observed to be $5.5*10^{-7}$ which is far less that unity confirming that there is absence of intra particle diffusion resistance. Hence the reaction is kinetically controlled which is further confirmed from the calculated activation energy in section 3.7.6.

Fig. S2 XPS analysis of Zn 2p, O 1s, N 1s, C 1s, W 4f and Fe 2p for Fe-DTP@ZIF-8