Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting information

Efficient hydrogenation of concentrated aqueous furfural solutions in to furfuryl alcohol under ambient conditions in presence of PtCo bimetallic catalyst

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Table S1. Result of ICP –OES analysis of mono and bimetallic catalysts

Catalyst	Pt (wt %)	Co (wt %)
Carbon	-	-
Pt(2)/C	2.09	-
Pt(2)Co(0.25/C	2.07	0.24
Pt(2)Co(1)/C	2.11	1.10
Pt(2)Co(5)/C	2.14	5.08
Pt(0.5)Co(3)/C	0.54	3.11
Pt(1)Co(3)/C	1.15	3.13
Pt(2)Co(3)/C	1.94	3.08
Pt(3)Co(3)/C	3.10	3.12
Pt(3)/C	2.98	-
Co(3)/C	-	3.15

Table S2. BET surface area, pore volume and pore radius of catalyst

Catalyst	Surface area (m^2/g)	Pore volume (cc/g)	Pore radius (Å)
Carbon	753	0.42	16
Pt(2)/C	704	0.39	15
Pt(2)Co(0.25/C	705	0.44	18
Pt(2)Co(1)/C	685	0.45	15
Pt(2)Co(5)/C	582	0.41	17
Pt(0.5)Co(3)/C	710	0.52	16
Pt(1)Co(3)/C	720	0.52	16
Pt(2)Co(3)/C	640	0.47	15
Pt(3)Co(3)/C	630	0.39	15
Pt(3)/C	662	0.41	15
Co(3)/C	712	0.44	17

Table S3. Adsorption study of FAL and FOL on carbon

Substrate	Adsorption on carbon (%)
FAL	4
FOL	3

Study was carried out at room temperature, FAL, FOL, 0.35 g; carbon, 0.078 g; iso-propyl alcohol, 35 mL; 600 rpm stirring; 1 h; (FAL: Furfural, FOL: Furfuryl alcohol).

Table S4. Polarity index, Hansen solubility parameters (HSP) and solubility of FAL, FOL in different solvents

Solvent	Polarity index	Hansen solubility parameter HSP (δ/Mpa)	FAL Solubility (%)[a]	FOL Solubility (%)[a]
Methanol	5.1	29.7	97	100
Ethanol	4.3	26	98	93
1-Propanol	4	24.3	100	98
2-Propanol	3.9	23.5	91	91
1-Butanol	3.9	23.1	100	100
2-Butanol	4	22.1	95	92
Toluene	2.4	18.2	88	88
Water	10.2	47.9	98	95
Water[a]	10.2	47.9	8	98
Furfural	-	22.9	-	-
Furfuryl Alcohol	-	25.6	-	-

Solubility was determined at room temperature, 35 mL solvent, 0.35 g FAL and FOL, (a) 14 g (40 *wt%*) FAL and 14 g (40 *wt%*) FOL (FAL: Furfural, FOL: Furfuryl alcohol).

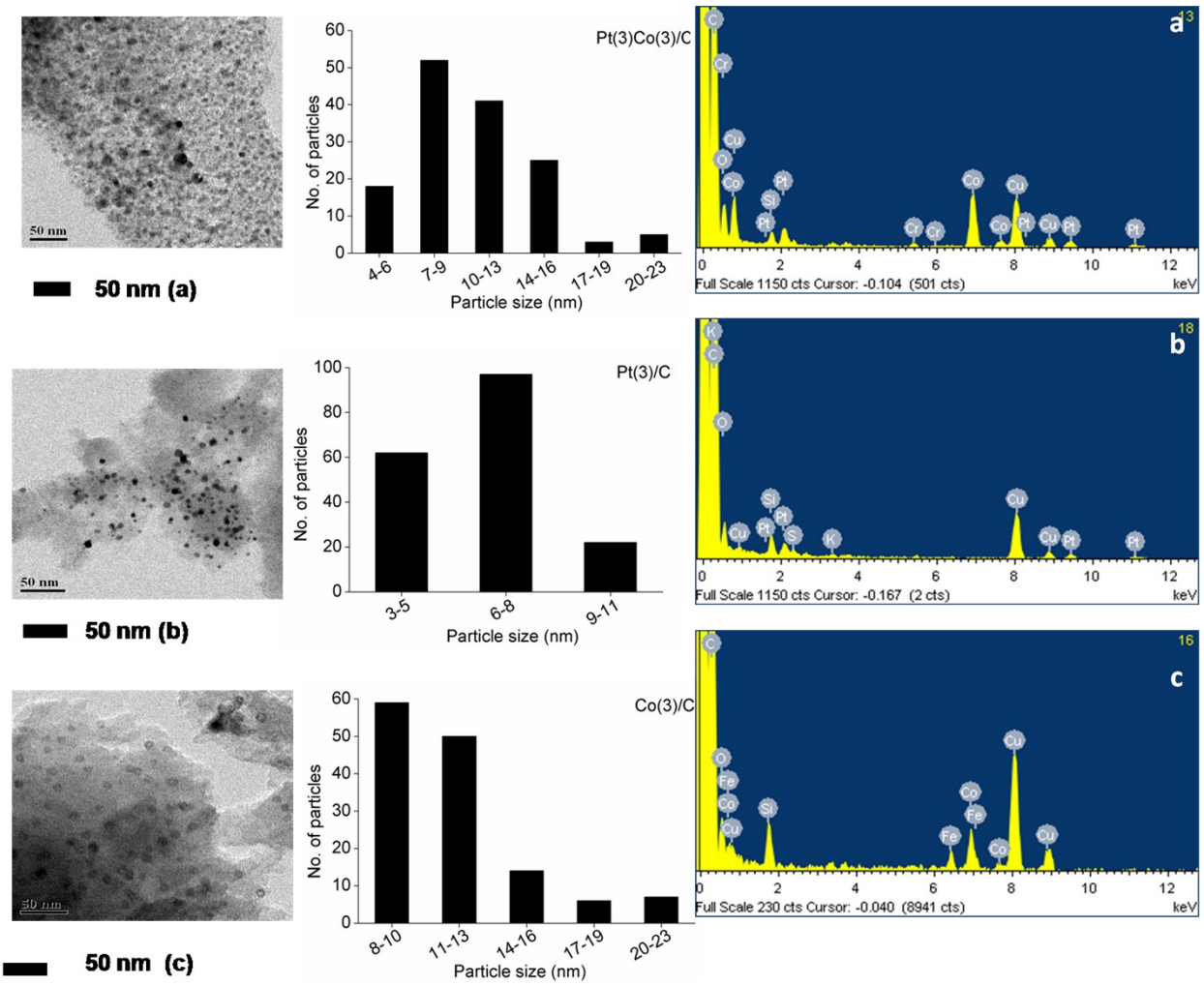
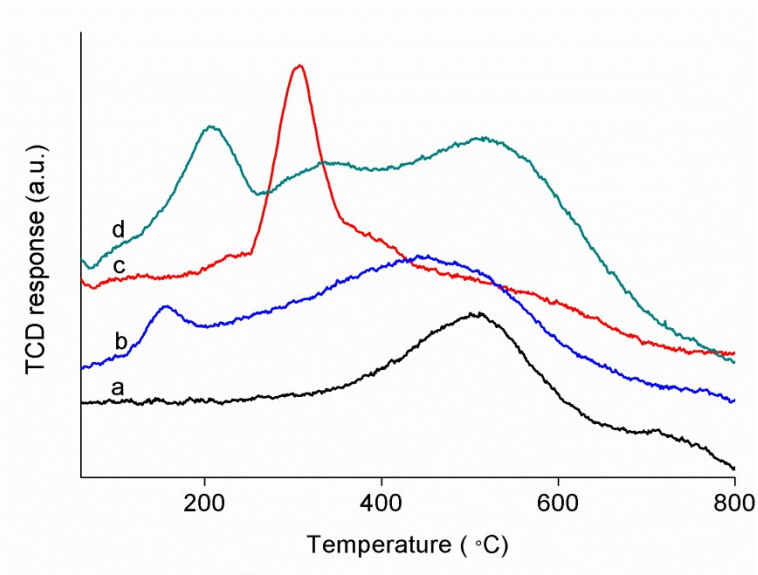


Figure S1. TEM images, particle size distribution and EDX spectra of (a) Pt(3)Co(3)/C, (b) Pt(3)/C, (c) Co(3)/C catalyst.



FigureS2. TPR profile of the mono and bimetallic catalyst supported on Carbon; (a) Carbon (b) Pt(3)/C, (c) Co(3)/C, (d) Pt(3)Co(3)/C, catalyst.

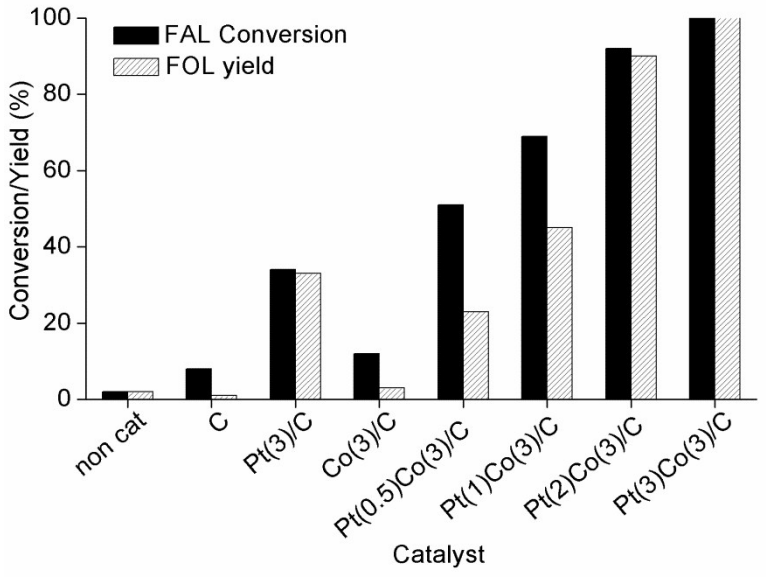


Figure S3. Effect of varying Pt loading with Co(3)/C on hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g; catalyst, 0.078 g; iso-propyl alcohol, 35 mL; 100 °C; 5 h; H_2, 1 MPa at room temperature; 900 rpm (FAL: Furfural, FOL: Furfuryl alcohol).

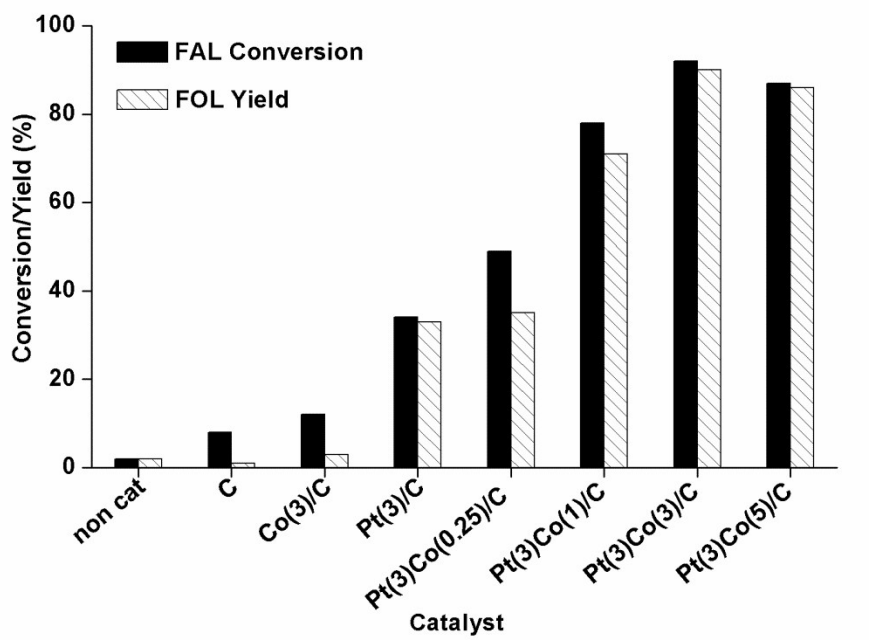


Figure S4. Effect of varying Co loading with Pt(3)/C on hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g; catalyst, 0.078 g; iso-propyl alcohol, 35 mL; 100 °C; 5 h; H_2, 1 MPa at room temperature; 900 rpm (FAL: Furfural, FOL: Furfuryl alcohol)

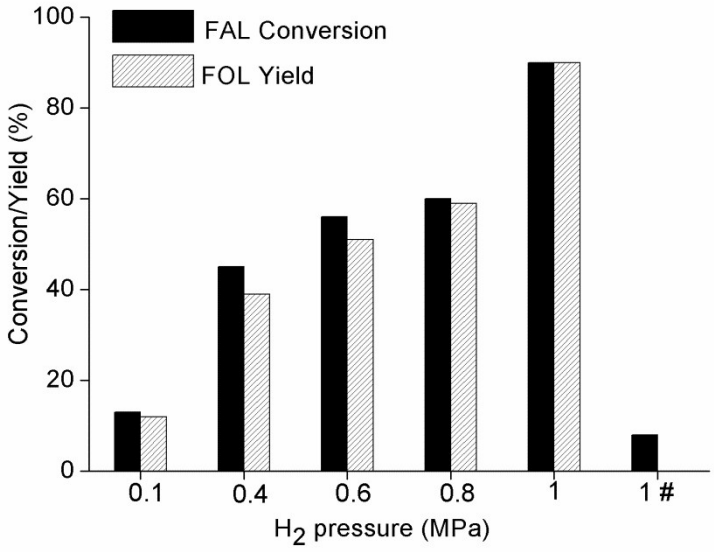


Figure S5. Effect of H_2 pressure on the hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g; Pt(3)Co(3)/C, 0.078 g; iso-propyl alcohol, 35 mL; 50 °C; 10 h; 900 rpm (FAL- Furfural, FOL – Furfuryl alcohol, # - N_2 pressure)

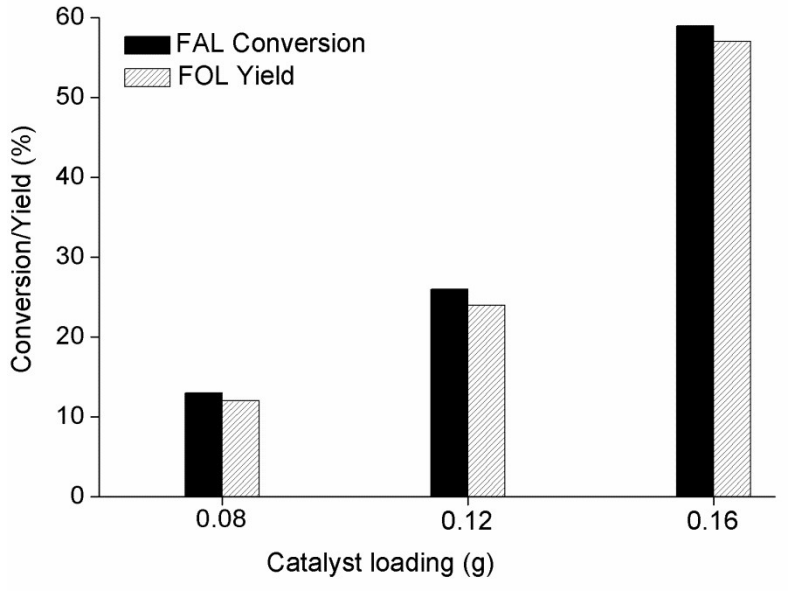


Figure S6. Effect of catalyst loading at 0.1 MPa H_2 pressure on hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g; Pt(3)Co(3)/C; iso-propyl alcohol, 35 mL; 50 °C; 10 h; H_2, 0.1 MPa at room temperature; 900 rpm (FAL: Furfural, FOL: Furfuryl alcohol)

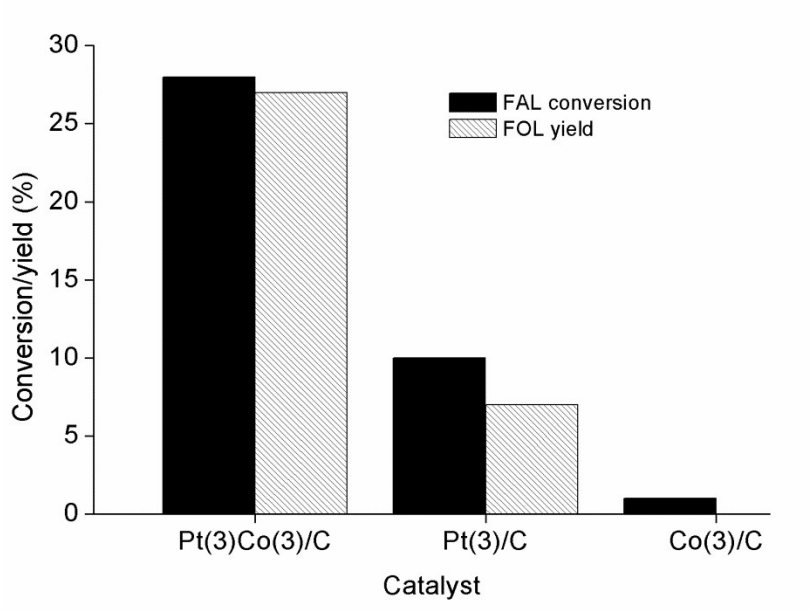


Figure S7. Effect of mono and bimetallic catalyst in water on hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g; Pt(3)Co(3)/C; water, 35 mL; 35 °C; 10 min; H_2, 1 MPa at room temperature; 900 rpm (FAL: Furfural, FOL: Furfuryl alcohol)

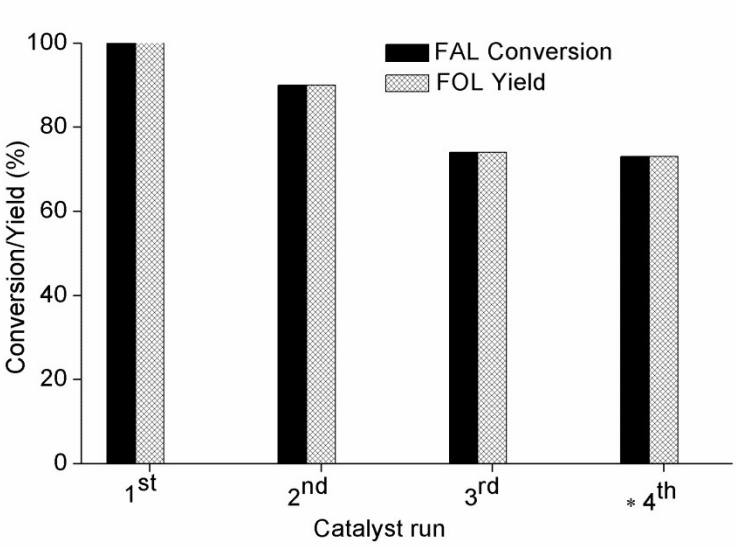


Figure S8. Recycle study of Pt(3)Co(3)/C catalyst in hydrogenation of FAL to FOL. Reaction condition: FAL, 0.35 g, water, 35 mL, Pt(3)Co(3)/C catalyst, 0.078 g, H_2, 1 MPa at room temperature, 35 °C, 10 h, 900 rpm (*4th catalytic run: Catalyst recovered from 3rd catalytic run was reduced at 400 °C, 2 h under H_2 flow. 0.050 g catalyst was recovered from 3rd run. FAL: Furfural, FOL: Furfuryl alcohol.

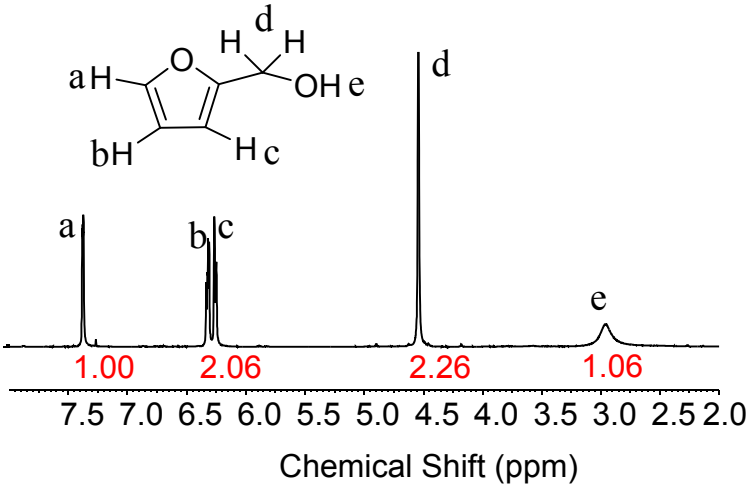


Figure S9. ^{1}H NMR spectra of Furfuryl alcohol (extracted product).

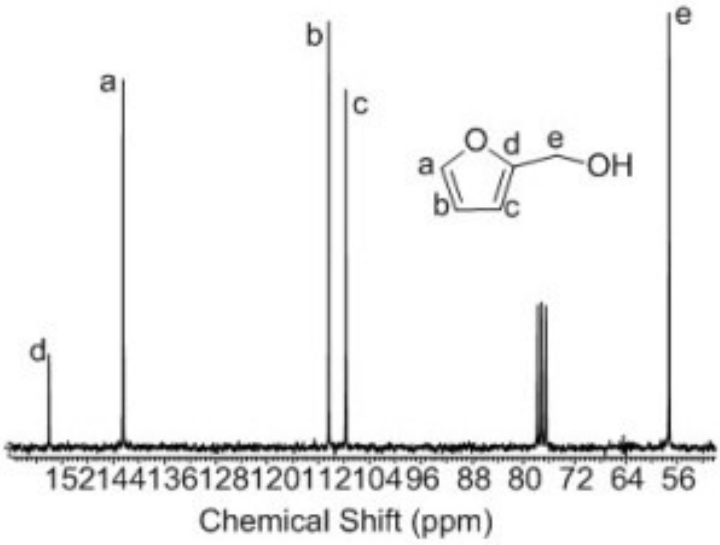


Figure S10. ^{13}C NMR spectra of Furfuryl alcohol (extracted product).

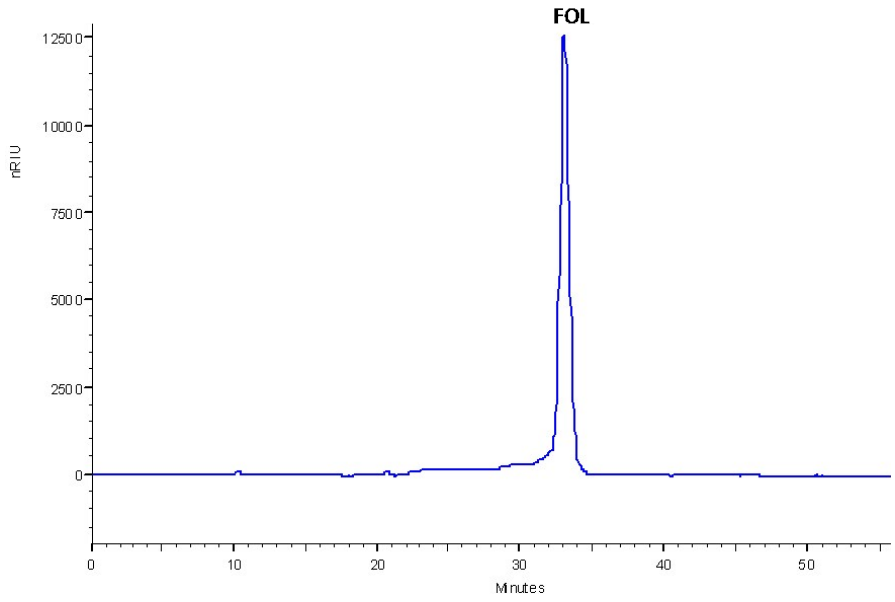


Figure S11. HPLC profile of reaction mixture after completion of reaction (Reaction condition; FAL, 0.35 g; water, Pt(3)Co(3)/C, 0.078 g; water, 35 mL; 35 °C; 10 h; H_2, 0.1MPa at room temperature) (FAL: Furfural, FOL: Furfuryl alcohol)

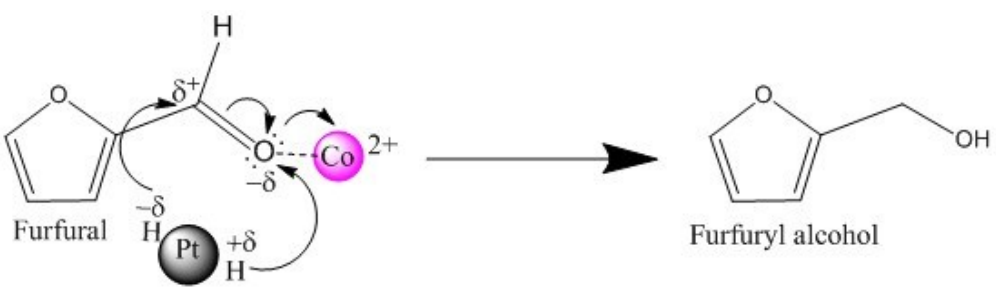


Figure S12. Proposed reaction mechanism for conversion of furfural to furfuryl alcohol

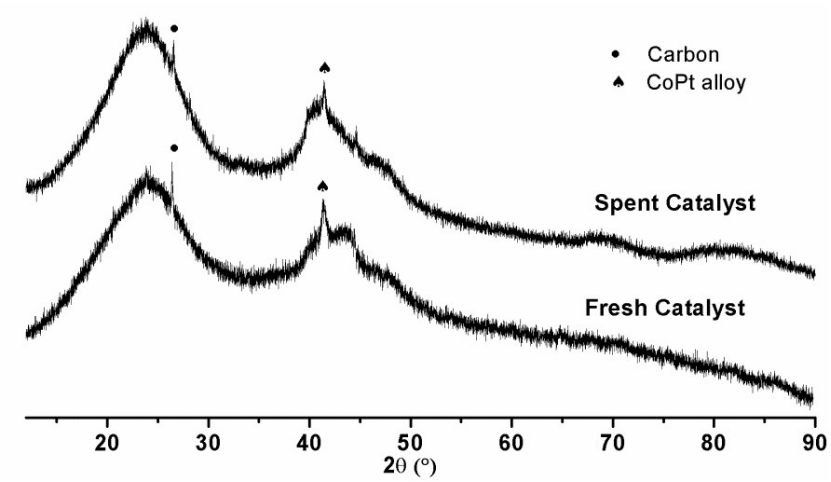


Figure S13. XRD patterns of fresh and spent Pt(3)Co(3)/C catalyst.

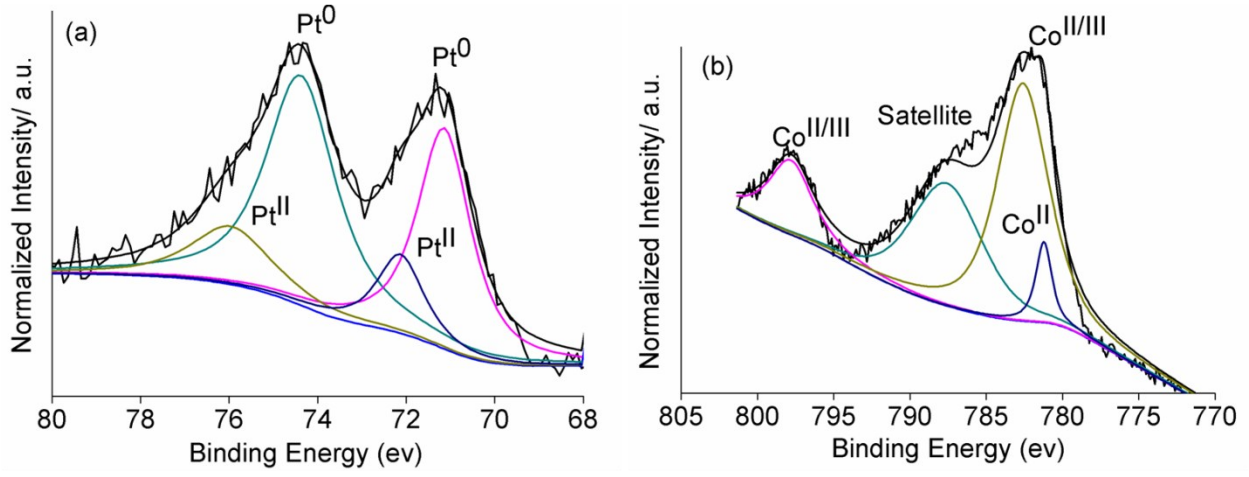


Figure S14. XPS spectra of spent Pt(3)Co(3)/C catalyst (a) deconvoluted XPS spectrum for Pt 4f level, (b) deconvoluted XPS spectrum Co 2p level.

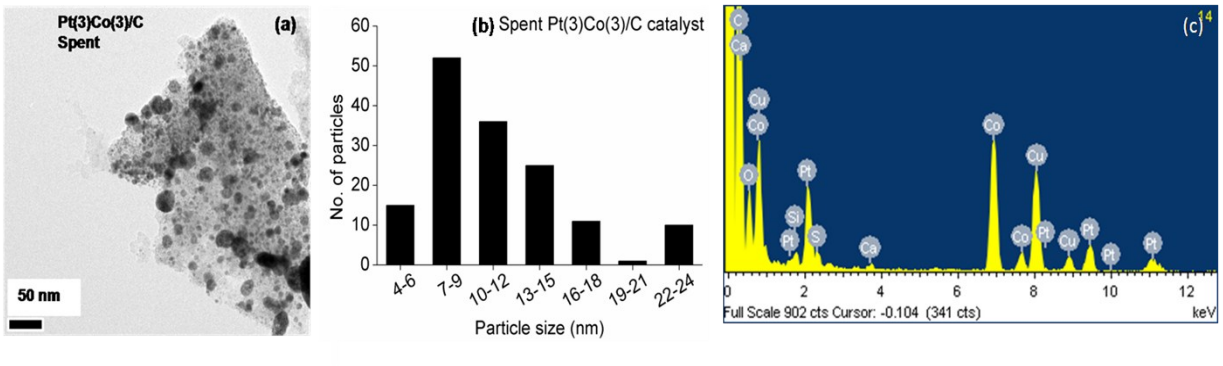


Figure S15. (a) TEM image of Pt(3)Co(3)/C spent catalyst, (b) Particle size distribution of Pt(3)Co(3)/C spent catalyst, (c) EDX spectra of spent catalyst