Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

High yield conversion of cellulosic biomass into 5-Hydroxymethylfurfural and a study of reaction kinetics of cellulose-to-HMF in a biphasic system

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Table S1 Furan yield calculation from biomass feedstock

mass of feed stock = 7.5 g

	Untreated		Alkali-organocat treated	
		Sugarcane bagasse		
	%	g	%	g
cellulose	41.5	3.11	84.4	6.33
xylan	24.1	1.81	6.56	0.49
		Rice husk		
	%	g	%	g
cellulose	35.2	2.64	82.0	6.15
xylan	18.7	1.40	5.47	0.41

$$mole\ of\ glucose = \frac{mass\ of\ cellulose}{162.14}$$

$$mole\ of\ xylose = \frac{mass\ of\ xylan}{132.12}$$

$$total\ moles = mole\ of\ glucose + mole\ of\ xylose$$

$$HMF\ yield = \frac{moles\ of\ HMF\ produced}{total\ moles}$$

$$furfural\ yield = \frac{moles\ of\ furfural\ produced}{total\ moles}$$

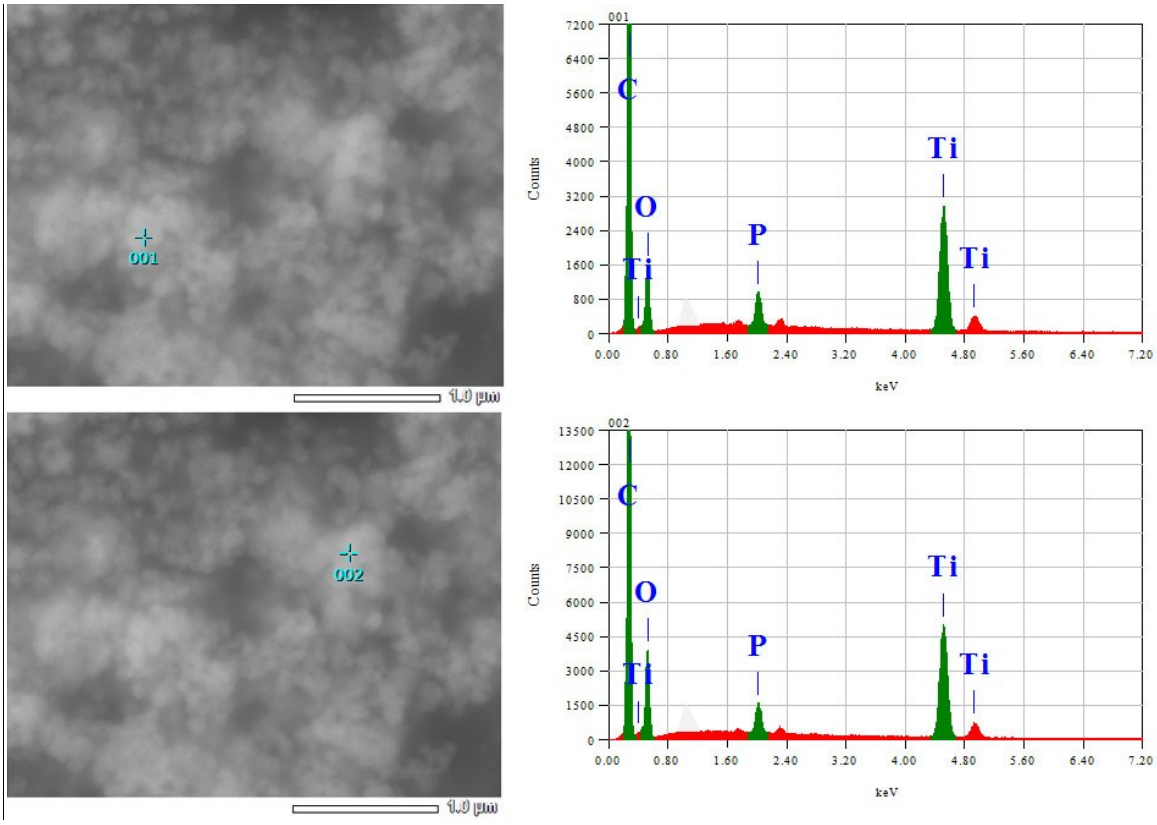


Fig. S1 EDS analysis of phosphated-TiO_2 nanoparticle.

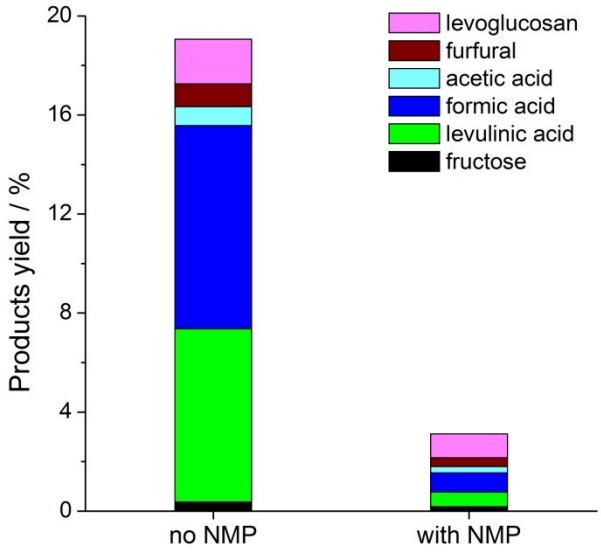


Fig. S2 Product distribution of glucose conversion on phosphated-TiO_2 catalyst. Reaction conditions: 10 g glucose, 1.25 g catalyst, 448 K, 80 min, 100 mL solvent volume (water–organic solvent 3:7 v/v). MeTHF:NMP 6:1 v/v for the modified reaction system.

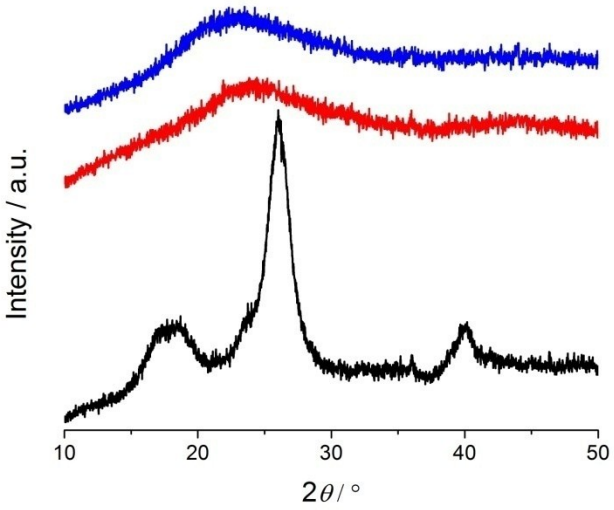
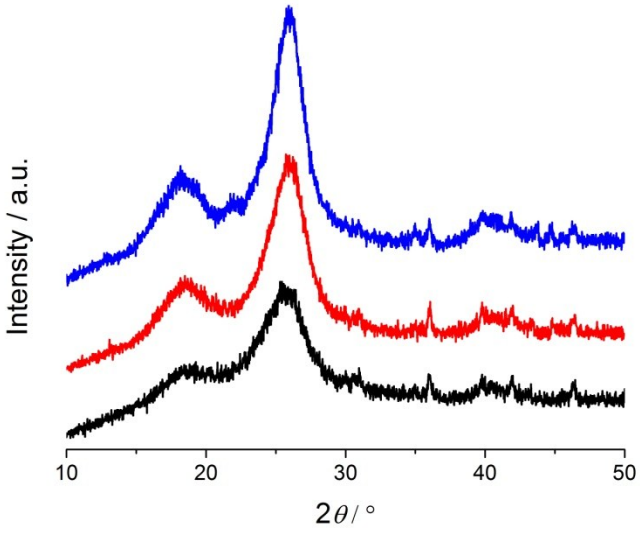
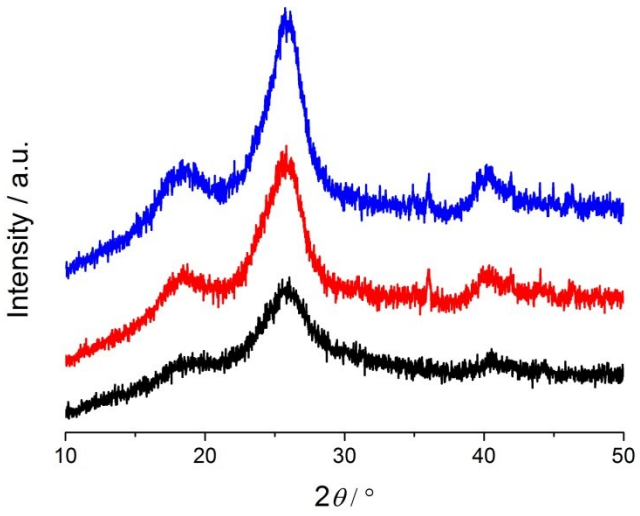


Fig. S3 XRD pattern of microcrystalline cellulose (black), ball-milled cellulose (red), mechanocatalytically depolymerized cellulose (blue)



a) sugarcane bagasse



b) rice husk

Fig. S4 XRD pattern of biomass substrates: a) sugarcane bagasse and b) rice husk. untreated (black), alkali-treated (red), organocat-alkali treated (blue).

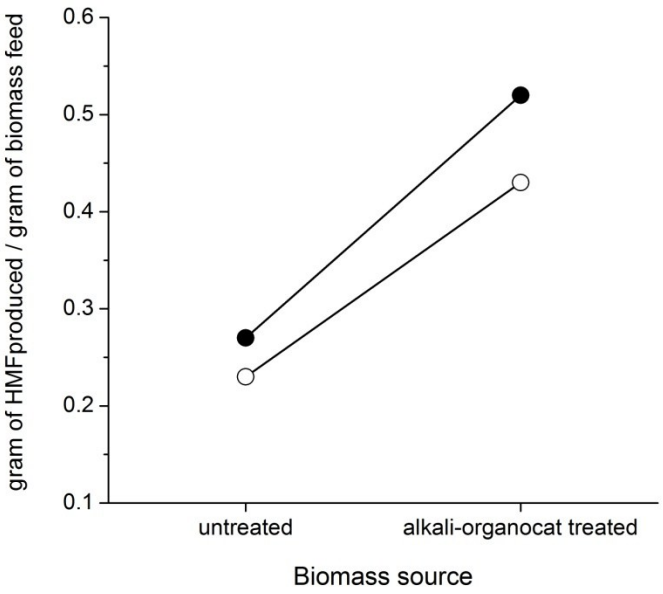


Fig. S5 HMF production per quantity of biomass source.

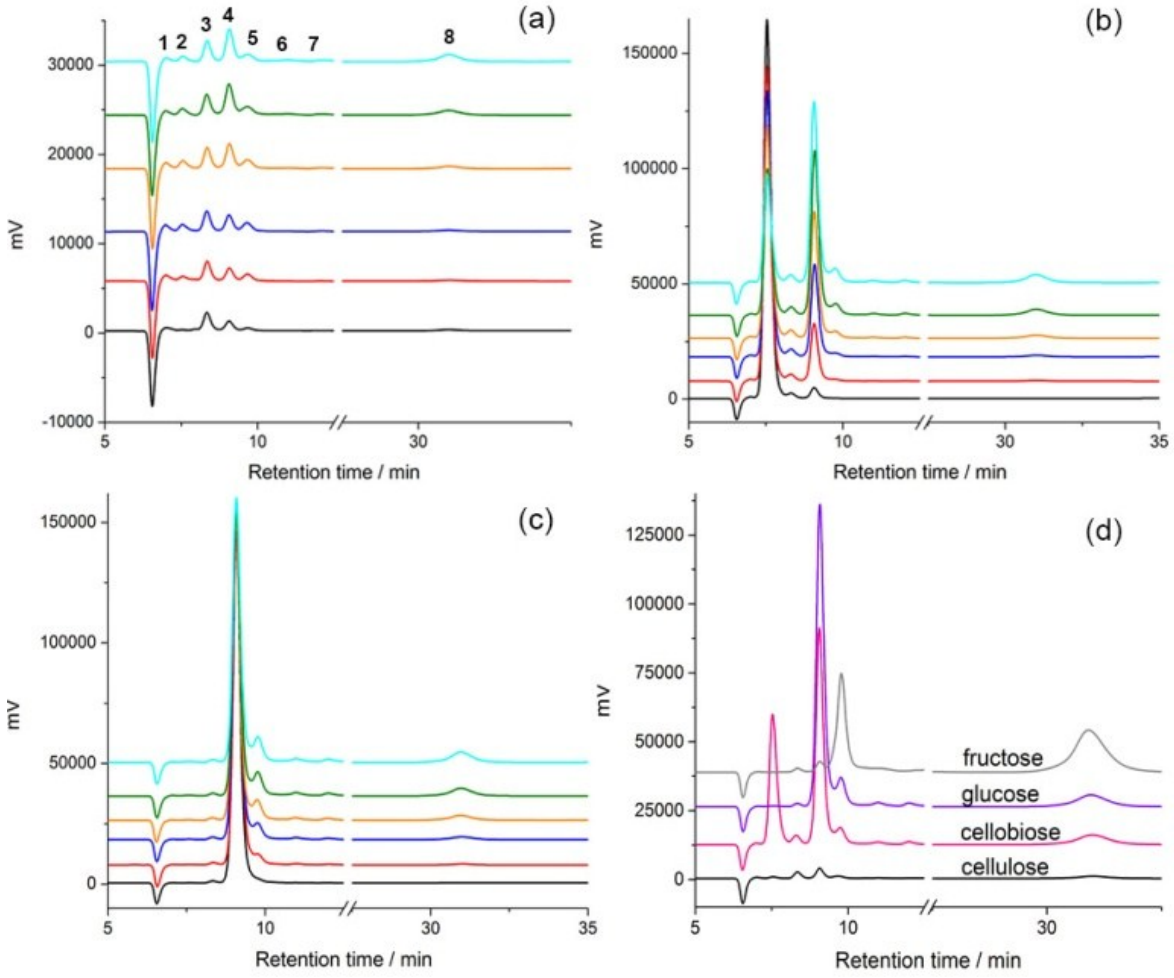


Fig. S6 HPLC analytical profile of carbohydrates conversion measured using RID detector. a) cellulose, b) cellobiose, c) glucose.[a] Reaction conditions: 1 g substrate, 0.4 g cat. wt. (0.2 g)[a], 453 K (433 K)[a], 100 mL water. d) comparison of carbohydrates conversion at 60 min reaction time. Reaction time: 0 min (black), 10 min (red), 20 min (blue), 30 min (orange), 45 min (green) and 60 min (cyan). Products: cellobiose – 2, glucose – 4, fructose – 5, HMF – 8, unknowns – 1, 3, 6 and 7.

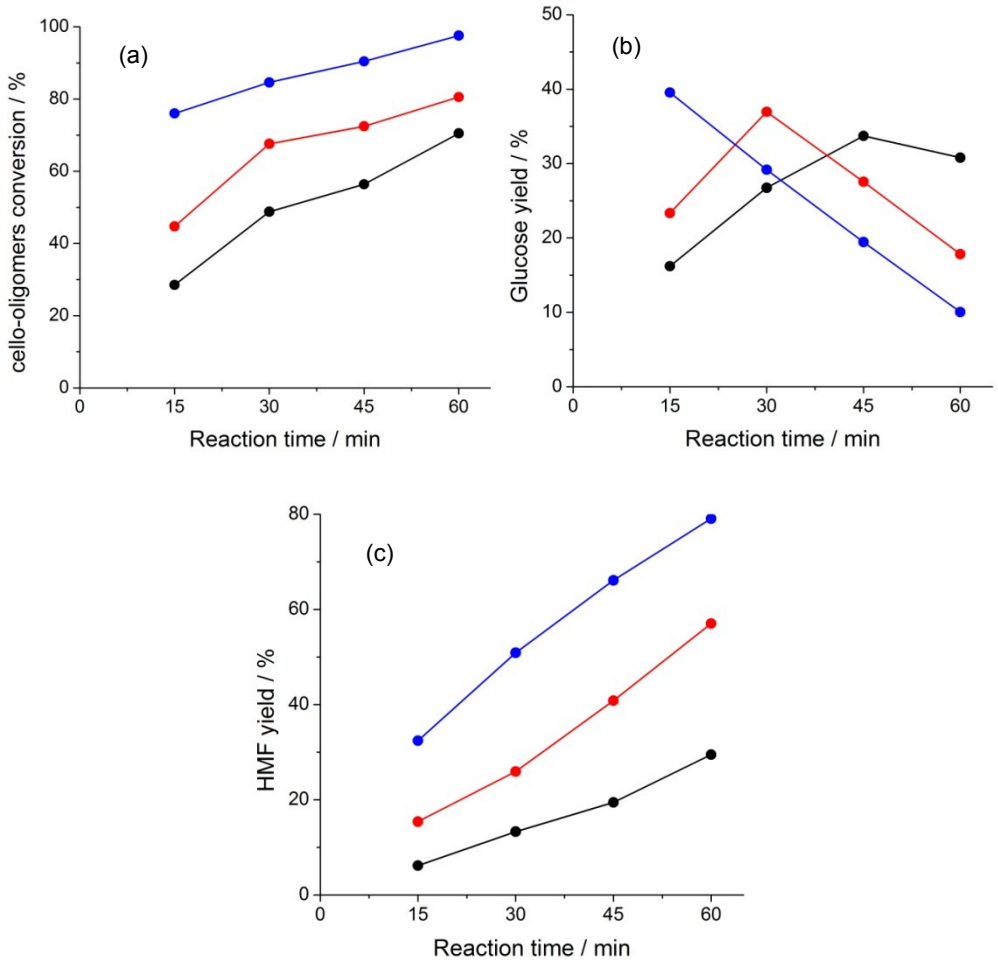


Fig. S7 Experimental rate data as a function of reaction temperature and time for: a) cello-oligomers conversion and yields of b) glucose and c) HMF. Reaction conditions: 10 g substrate, 1.25 g catalyst, 100 mL solvent volume (water–MeTHF/NMP 3:7 v/v). Reaction temperature: 428 K (black), 438 K (red) and 448 K (blue); reaction time: 15–60 min.