Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Lignin-first depolymerization of native corn stover with unsupported MoS2 catalyst

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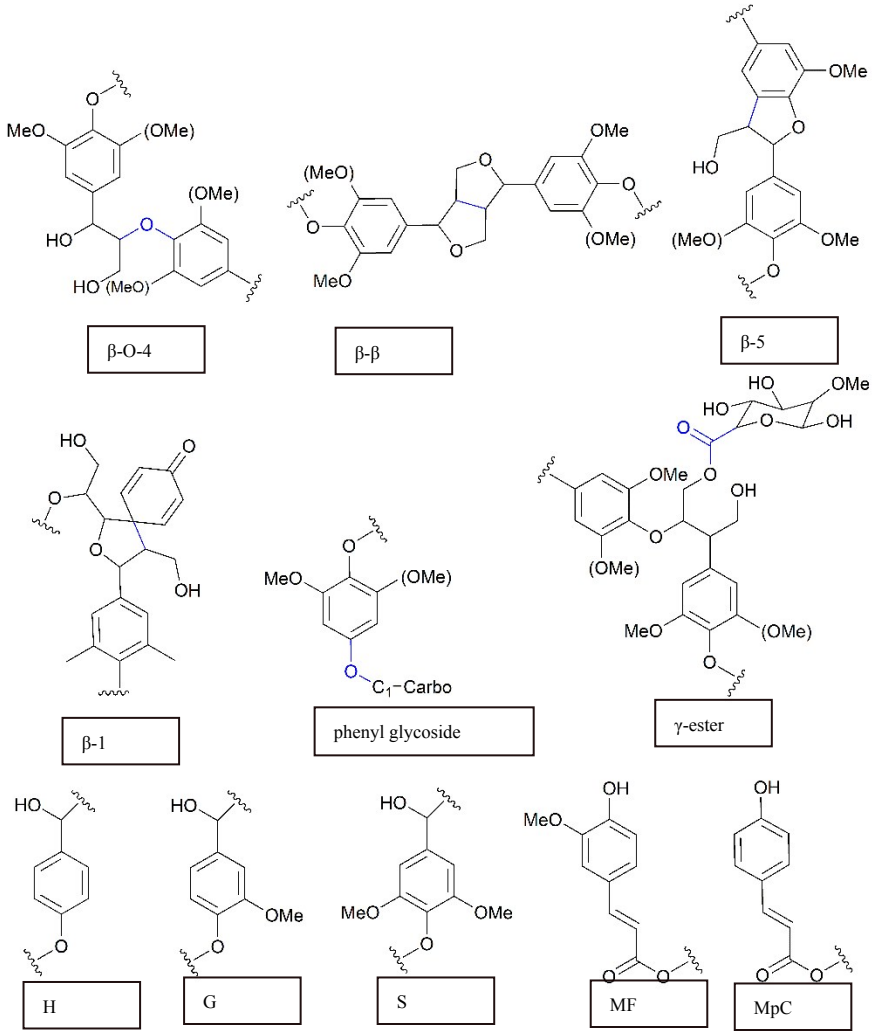

Fig. S1 Key structural details of lignin and carbohydrates and typical lignin composing units

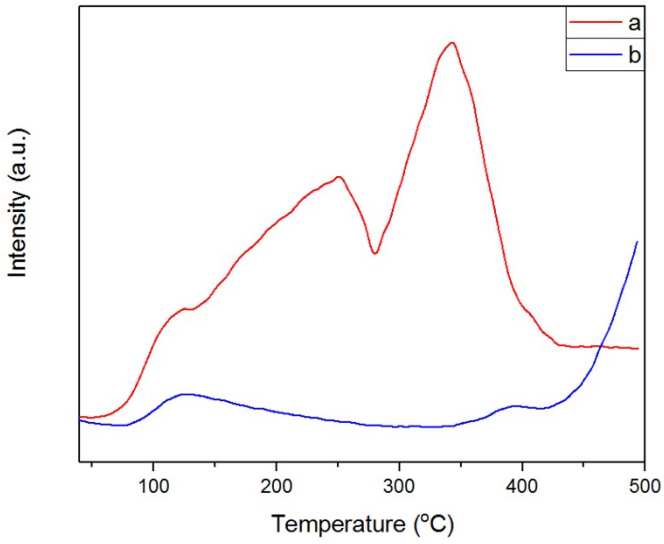

Figure S2 The NH_3-TPD pattern of the MoS_2 catalyst (a: fresh catalyst, 4078.4 μmol/g, b: used after five times, 215.16 μmol/g)

Table S1 Main components of corn stover

Component		Content (%)
Cellulose	Glucan	31.73
Hemicellulose	Xylan	20.31
	Araban	1.00
Lignin	Acid-solluble lignin	2.95
	Acid-insoluble lignin	18.15
Moisture		1.62
Extractives		4.75
Ashes		5.02
Other components		14.47

Table S2 The phenolic monomer yield at different catalyst circulation cycles [a]

Run	Yield of phenolic monomer (%)													
number	1[b]	2[c]	3[d]	4[e]	5[f]	6[g]	7[h]	8[i]	9[j]	10[k]	SumG	SumS	SumH	Sum
1	2.63	0.61	1.30	3.75	1.55	1.45	0.64	3.01	2.02	1.51	8.11	3.65	6.10	18.47
2	2.64	0.51	0.43	2.53	1.52	0.81	0.29	2.08	2.74	2.44	6.91	2.37	6.19	15.97
3	2.01	0.53	0.36	2.20	1.39	0.54	0.21	2.11	2.22	2.29	6.24	2.31	4.77	13.86
4	1.95	0.75	0.39	1.99	1.25	0.63	0.15	1.95	2.92	2.55	6.18	2.11	5.49	14.52
5	1.87	0.80	0.39	2.07	1.17	0.63	0.26	1.84	2.65	2.61	6.24	2.10	5.15	14.30

[a] Condition: 2.0 g corn stover, 40 ml methanol, 0.3 g MoS_2, 250 °C, 3MPa H_2, 2 h. [b]1: 4-ethylphenol. [c]2:2, 3-dihydrobenzofuran. [d]3: 2-methoxy-4-ethylphenol. [e]4: 2-methoxy-4-propylphenol. [f]5: 2-methoxy-4-propenylphenol. [g]6: methyl 3-(4-hydroxyphenyl) propionate. [h]7: 2, 6-dimethoxy-4-allylphenol. [i]8: 2, 6-dimethoxy-4-propylphenol. [j]9: methyl trans-p-coumarate. [k]10: methyl trans-4-hydroxy-3-methoxycinnamate. [c, g, j] The calibration factor of internal standard method was calculated by Effective Carbon Number (ECN) method explained in supporting information.

Table S3 The ECN increments of different functional groups

Founctional group	ΔECN
Olefinic C[1]	-0.05
Aromatic[2]	0
Ether[2]	-1.0
Phenolic hydroxyl[2]	-1.0
Primary hydroxyl groups[2]	0.4 to 0.6
Carbonyl[3]	-0.79
Ester bond[3]	-1.16

$ECN_{monomer} = TCN + \Delta ECN_i$

$\lambda_{ECN} = MW_{monomer}/MW_{acetophenone} * ECN_{acetophenone} /ECN_{monomer}$

$\lambda = M_{monomer}/M_{acetophenone} * S_{acetophenone} /S_{monomer}$

$M_{monomer} = M_{acetophenone} * S_{monomer} * \lambda(\text{ or } \lambda_{ECN})/ S_{acetophenone}$

TCN: the total carbon number of monomer.

ΔECN_i: the ECN increments of different functional groups

$MW_{monomer}$: the molecular weight of monomer

$MW_{acetophenone}$: the molecular weight of acetophenone

$S_{acetophenone}$: the peak area of acetophenone

$S_{monomer}$: the peak area of monomer

References

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