Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting information

Hydrogenation of 5-hydroxymethylfurfural to liquid fuel 2, 5 dimethylfuran over nickel supported tungsten oxide nanostructured catalyst †

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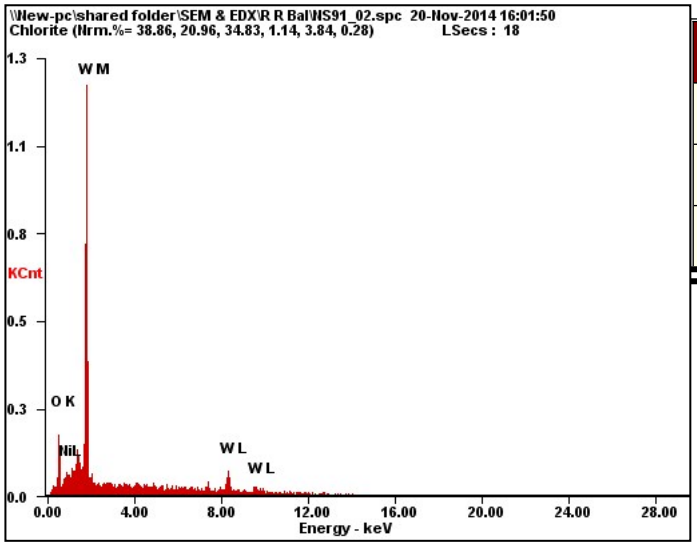

Element	Wt %	At %
O K	27.53	77.59
NiL	08.85	06.80
W L	63.62	15.61

Fig-S1 EDX pattern of catalyst

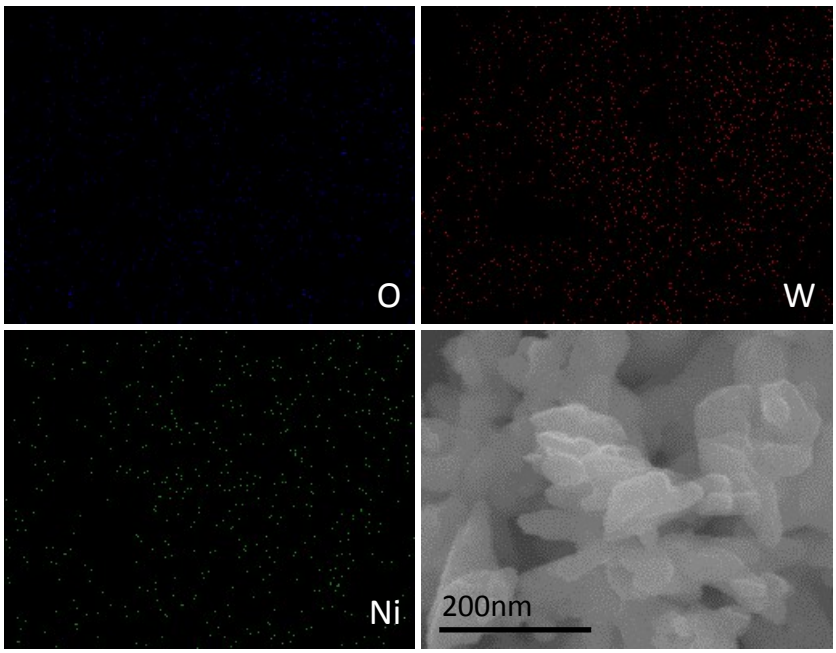

Fig-S2 SEM elemental mapping of Ni/WO_3

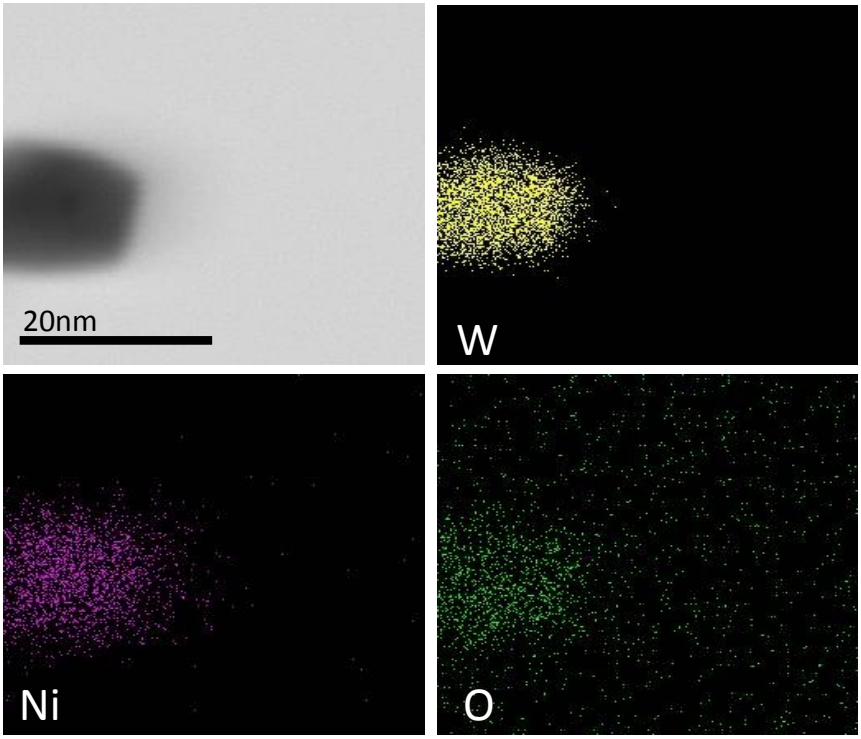

Fig-S 3 TEM elemental mapping of Ni/WO_3

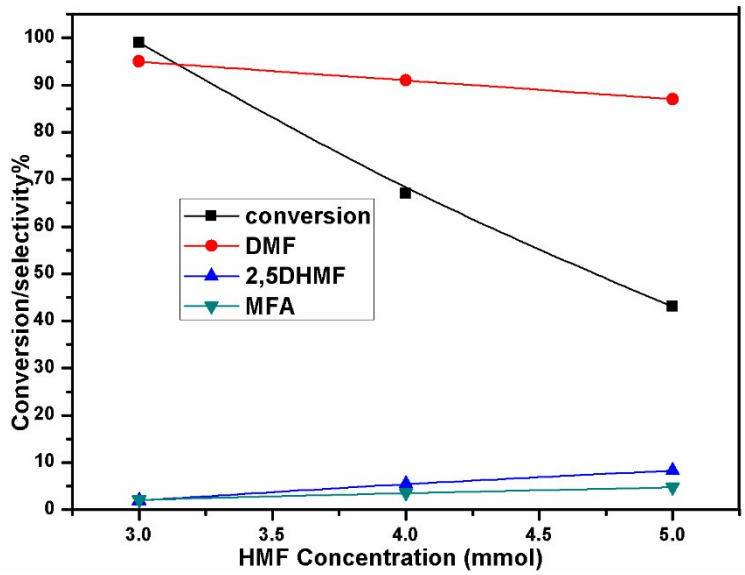

Fig-S 4 Effect of HMF concentration

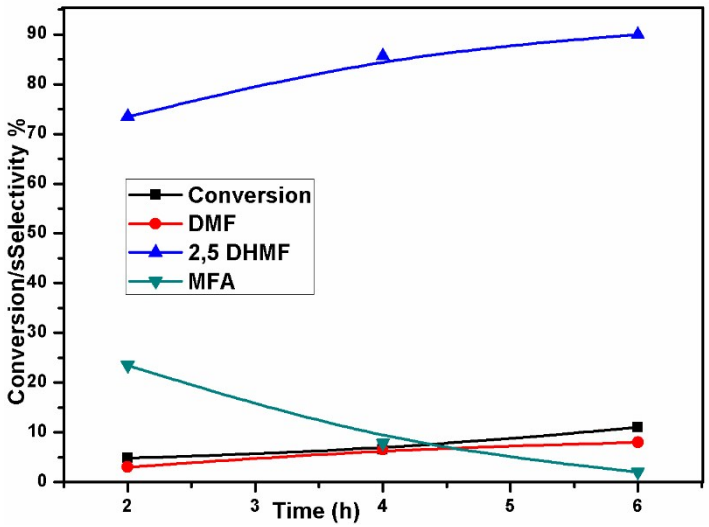

Fig-S 5 Effect of Time at 100^0C

Detail kinetic calculation given below

$t_{1/2} = 0.03r^2/Dp$ (I)

$t_{1/2} = 0.23r\delta/Df \times (C_0/Ce)$ (II)

Where
r = Radius of adsorbent in cm
δ = Thickness of water film adhered to the adsorbent in cm (assume = 0.001cm)
Dp = Pore diffusion coefficient in cm2/s
Df = Film diffusion coefficient in cm2/s
C_0 = Concentration of metals on adsorbent in mg/gm
Ce = Concentration of metals in solution at equilibrium in mg/l
$t_{1/2}$ = time required to bring down the metals concentration to half of initial concentration in seconds.
$t_{1/2}$ has been calculated from equation no. (III)

$t_{1/2} = -[(0.5)]/K_1$ (III)

To find out the rate limiting step of the overall adsorption the value of first order rate constant

(K_1) obtained from the slopes of the straight lines of first order model.[1]
$\ln(qe - qt) = \ln(qe) - K_1 t$

$qt = (C_i - Ct)V/m$

q_e = (Ci-Ce)V/m

Where Ci and Ce are the initial and equilibrium concentration of HMF, respectively (mg/l), V is the volume of the solution (l), and W is the weight of the catalyst used (g). qe and qt are the amount of HMF adsorbed per gram metal (mg/g) at equilibrium and time t,

K_1 is the slope of graph

Initial concentration of HMF =0.05g
Density of HMF = 1.29 gm/ml
Water = 20ml
Total volume= 20ml water + 0.4 ml
So, The HMF concentration= (1000*1000)/20.4
Ci = 49019.6 mg/l

Table: 1 kinetic calculation parameters

t (s)	Conv.	ct	qt	ln(qe-qt)
7200	29.8	34411.7592	5843.13632	9.515515324
10800	37.2	30784.3088	7294.11648	9.402417812
14400	63.3	17990.1932	12411.76272	8.853665039

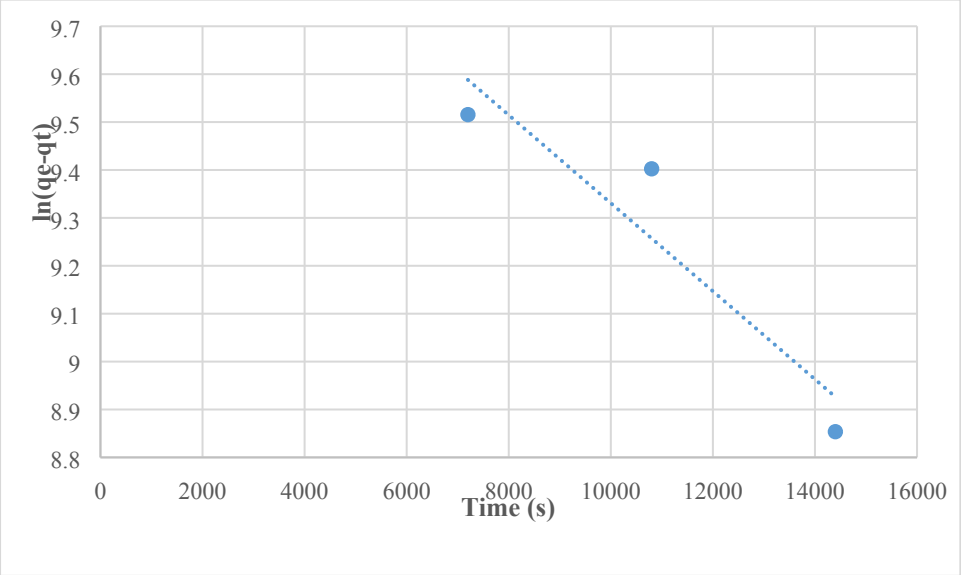

Fig-S 6 plot of ln (qe-qt) vs Time.

Slop = $-9x10^{-5}$

$K_1 = 9x10^{-5}$

$t_{1/2} = -[ln(0.5)]/ 9x10^{-5}$

=7701

r = 11 Nm

$=11x10^{-7}$cm

$t_{1/2} = 0.03r^2/Dp$

$Dp = 0.03x (11x10^{-7}cm)^2 /7701$

$Dp = 4.7x10^{-20}$

$t_{1/2} = 0.23r\delta/Df\ x(C_0/Ce)$

Co =Concentration of metals on adsorbent in mg/gm

Ce = Concentration of metals in solution at equilibrium in mg/l

Ce = 17990.19

Co = (49019.6-17990.19)*(0.0204/0.05)

= 31029.5mg/gm

$Df = 0.23x11x10^{-7}x0.001x31029.5/(3465x77990.1)$

$= 1.4x10^{-13}\ Cm^2/s$

Here we concluded that Df value is very small so this reaction is not a control reaction.

Table: 1 Comparison with reported literature

S.No	Catalysts	Solvent	Pressure (bar)	Time (h)	Temp.(^{0}C)	DMF Selectivity%	Ref.
1	$CuCrO_4$	1-Butanol	-	10	220	61	[2]
2	CuRu/C	1-Butanol	-	10	220	71	[2]
3	Ru/C	THF	20	2	180	80.6	[3]
4	PtCo@HCS	1-	10	2	180	98	[4]

		Butanol					
5	Pd/C	CO_2/H_2O	10barH_2/4MPaCO_2	2	80	100	[5]
6	Ni-W_2C/AC	THF	40	3	180	80.1	[6]
7	PdAu/C	THF	H_2 Balloon	6	60	96	[7]
8	Ru/Co_3O_4	THF	7	24	130	93.4	[8]
9	Ru/C	IPA	-	6	190	81	[9]
10	Pd/Fe_2O_3	IPA	-	6	180	72	[10]
11	NiSi-PS	1,4 Dioxane	15	3	130	72.9	[11]
12	Ni/HT	1,4 Dioxane	12	4h	180	91.1	[12]
13	Ru/NaY	THF	15	1	220	78	[13]
14	Ni/CNx	H_2O	30	6	200	98.7	[14]
15	**Ni/WO_3**	**H_2O**	**10**	**6**	**180**	**>95**	**This Work**

ICP Result Expressed in: percent (%)

S.No	Sample	Element %	
		W	Ni
1	Fresh 5% Ni/WO_3	35.64	1.62
2	2nd recycle spent catalyst	35.64	1.61
3	5th recycle spent catalyst	35.63	1.60

References

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