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

Improved hydrogenation function (Pt@SOD) incorporated inside sulfided (NiMo) hydrocracking catalyst

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Supplementary information

Table S1: Selectivity of various hydrocarbons over NiMo-Pt@SOD@ZSM-5 catalyst (at ≥ 99% jatropha oil conversion).

Temp	H_2/HC	<C_8	C_9-C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{18+}
380	500	3.11	1.59	8.16	10.97	35.35	34.95	3.18
400	500	5.3	2.35	2.78	9.39	39.35	34.95	5.82
420	500	0.37	3.51	9.02	10.77	37.3	35.94	3.12
380	1000	7.81	11.77	7.97	12.44	23.25	30.38	6.3
400	1000	3.68	3.79	5.76	12.79	28.2	42.83	2.8
420	1000	7.33	10.22	7.15	12.83	22.96	32.25	7.22
450	1000	19.07	26.8	6.47	12.34	10.86	18.18	6.31
380	1500	3.74	7.09	5.21	15.29	16.16	47.29	5.23
420	1500	11.88	17.4	7.21	13.37	15.51	25.28	8.5
450	1500	27.69	29.4	7.27	10.74	10.03	12.43	1.22
380	2000	3.65	5.81	4.61	15.21	15.8	49.36	5.5
400	2000	7.38	13.96	5.94	15.38	13.42	36.5	7.48
420	2000	10.19	18.89	4.79	10.69	8.03	19.51	7.89
450	2000	21.58	25.36	5.88	13.63	11.04	19.64	2.85
380	250	1.67	3.8	6	11.8	31.1	43.8	1.68

Table S2: Composition of effluent gas

H_2	CH_4	CH_3-CH_3	CH_2=CH_2	$CH_3CH_2CH_3$	CO_2	CO
88.57[a]	0.69	0.28	0.006	1.23	6.74	2.45
93.7[b]	0.79	0.32	0.003	1.05	2.46	1.192

a: H_2/HC, 250, T: 380^0C, Lhsv:1, P:80, b: H_2/HC, 1000, T: 420 ^{0}C, Lhsv:1, P:80.

Figure: S1: Geometrically optimized H_2 (a), SOD (b), Pt (c, 0.4 nm), Pt (d, 0.57 nm), and hydrogen adsorbed SOD (e, f)

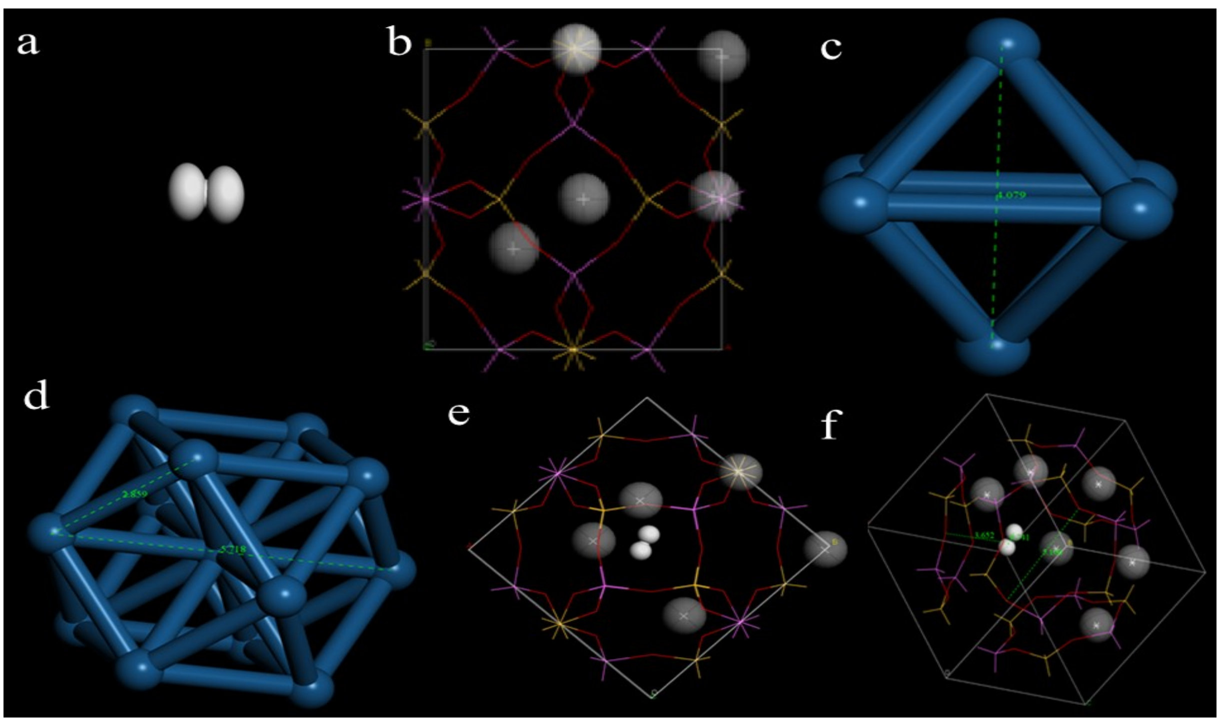


Figure:S2: Geometrically optimized Pt-SOD-H_2. (a,b) Small platinum nanoparticle (0.4 nm); and (c,d) bigger platinum nanoparticle (0.57 nm).

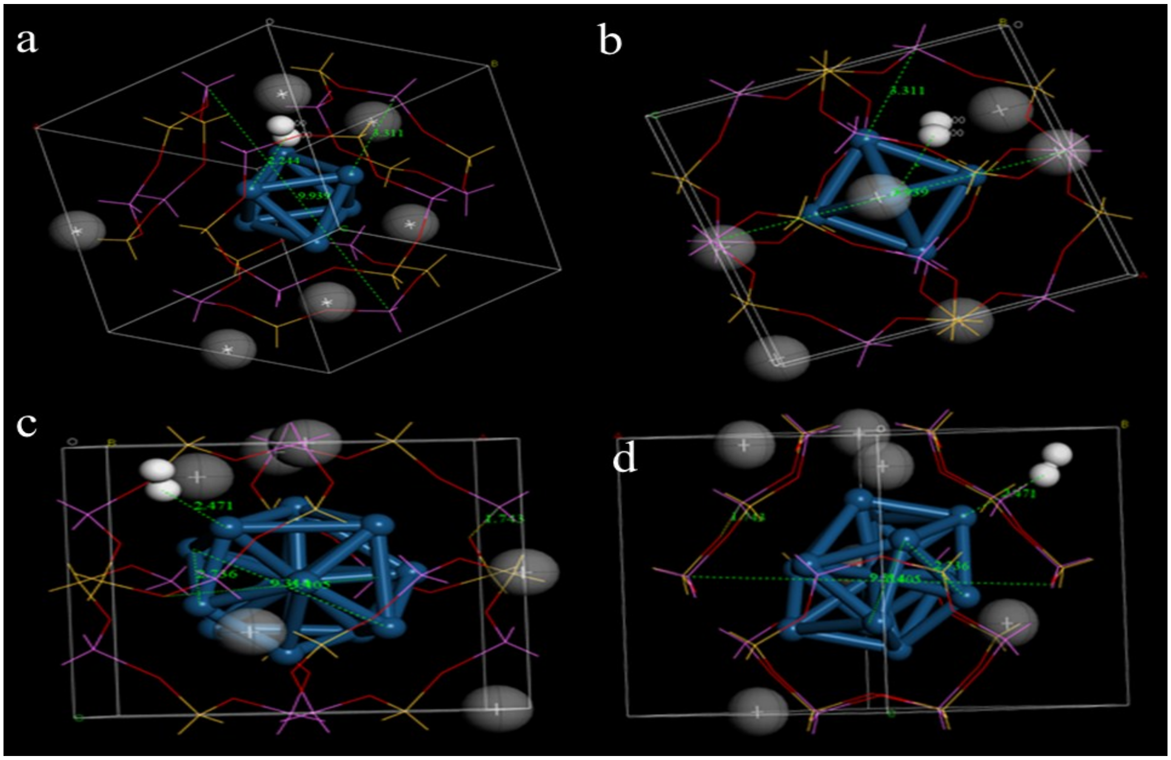


Figure: S3: Geometry optimization of Pt@SOD

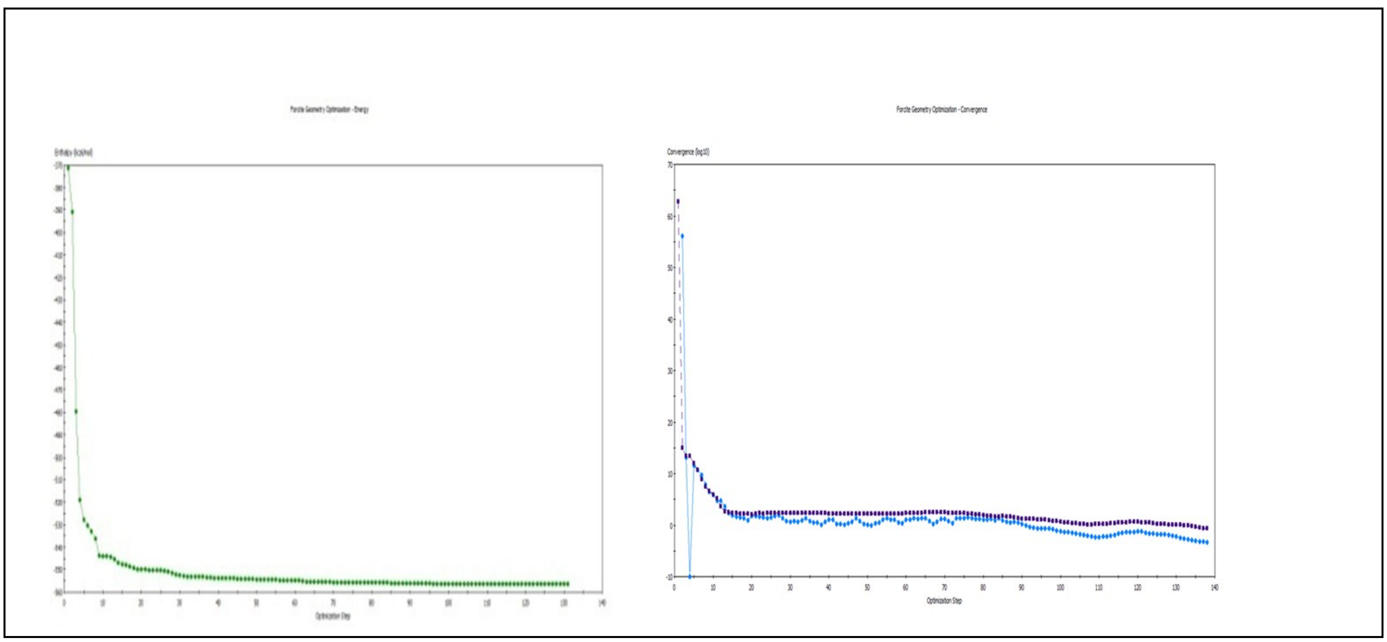
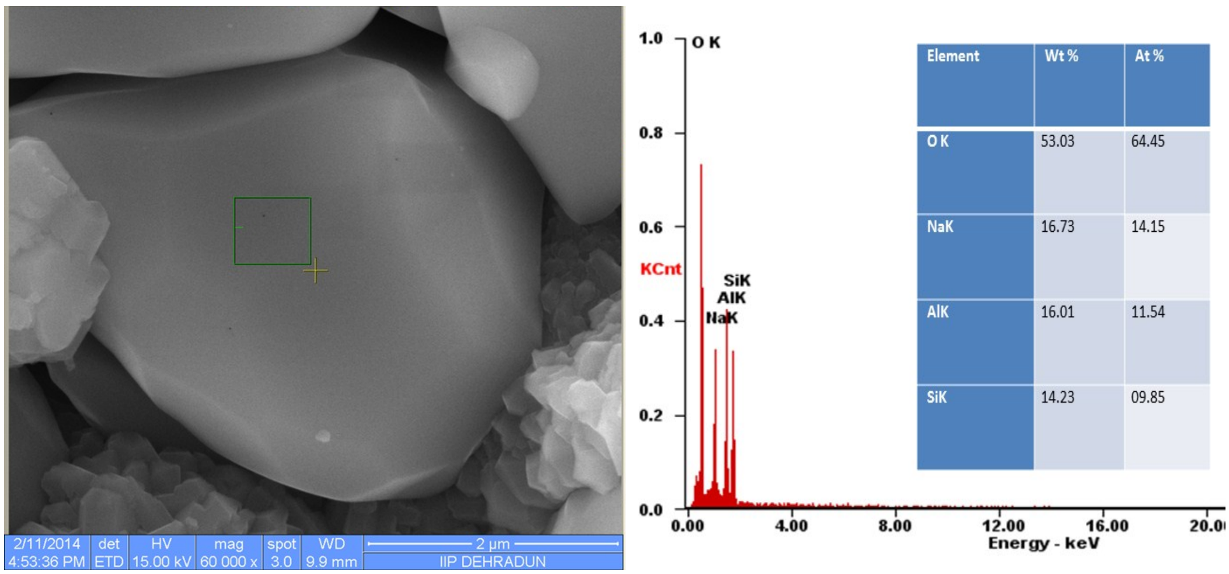


Figure S4: EDX analysis of Pt@SOD



Element	Wt %	At %
O K	53.03	64.45
NaK	16.73	14.15
AlK	16.01	11.54
SiK	14.23	09.85

Figure S5: Influence of reaction temperature on yield of various products (H_2/HC ratio 500, P 80, GL: Gasoline,KR: Kerosene, DL:Diesel).

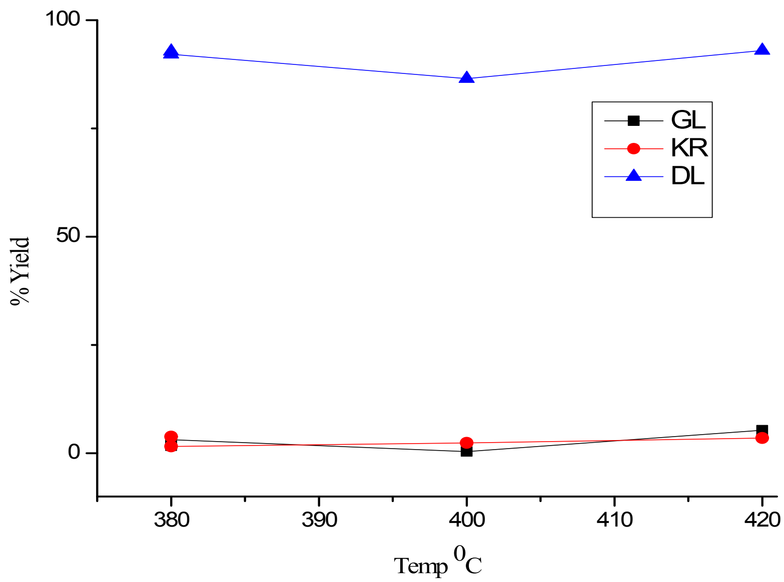


Figure S6: Influence of reaction temperature on yield of various products (H_2/HC ratio 1000, P 80, GL: Gasoline,KR: Kerosene, DL:Diesel, HVY: Oligomers).

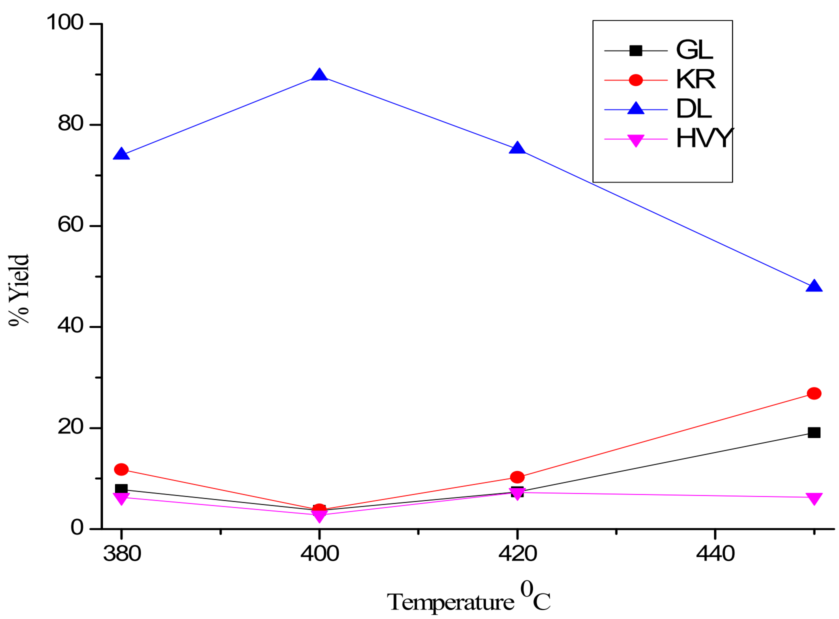
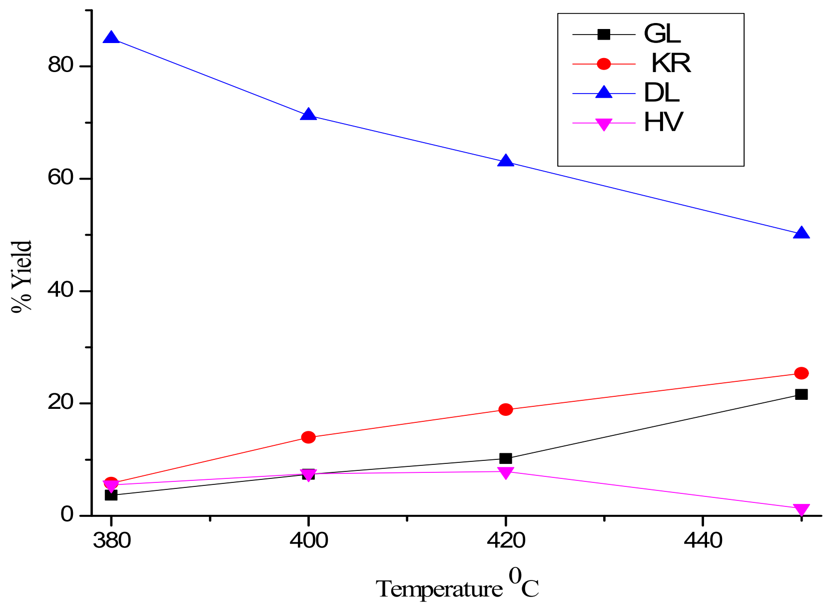


Figure S7: Influence of reaction temperature on yield of various products (H_2/HC ratio 1500, P 80 bar, GL: Gasoline, KR: Kerosene, DL:Diesel, HV: Oligomers).



GL
KR
DL
HV
80
60
40
20
0
% Yield
380
400
420
440
Temperature 0C