Electronic Supplementary Material

Catalytic hydrogenation of insoluble organic matter of CS_2/Acetone from coal over mesoporous HZSM-5 supported Ni and Ru

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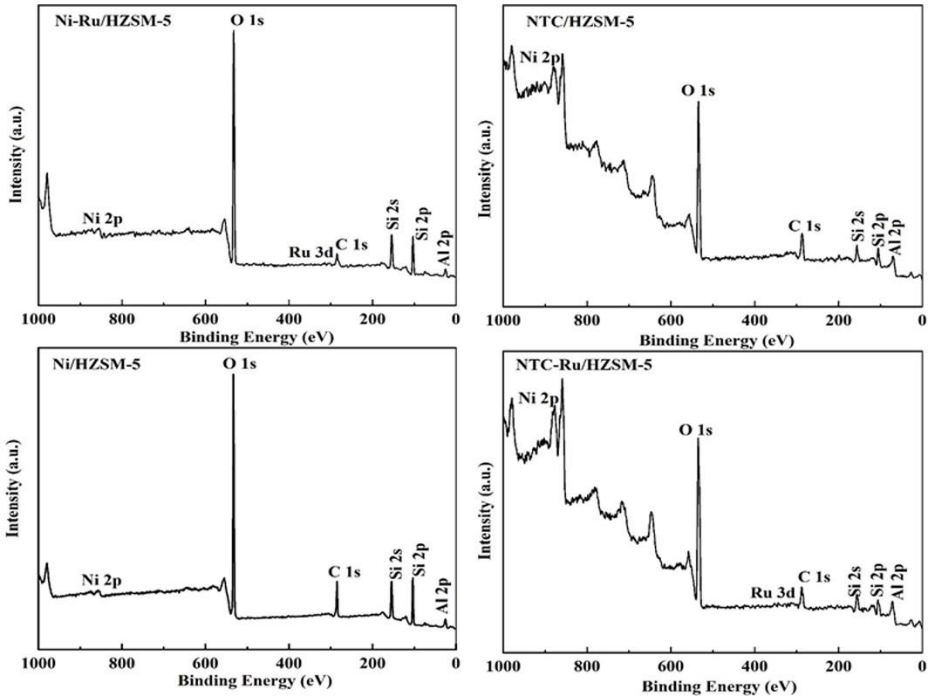

Fig. S1 X-ray photoelectron spectrum of Ni/HZSM-5, NTC/HZSM-5, Ni-Ru/HZSM-5 and NTC-Ru/HZSM-5

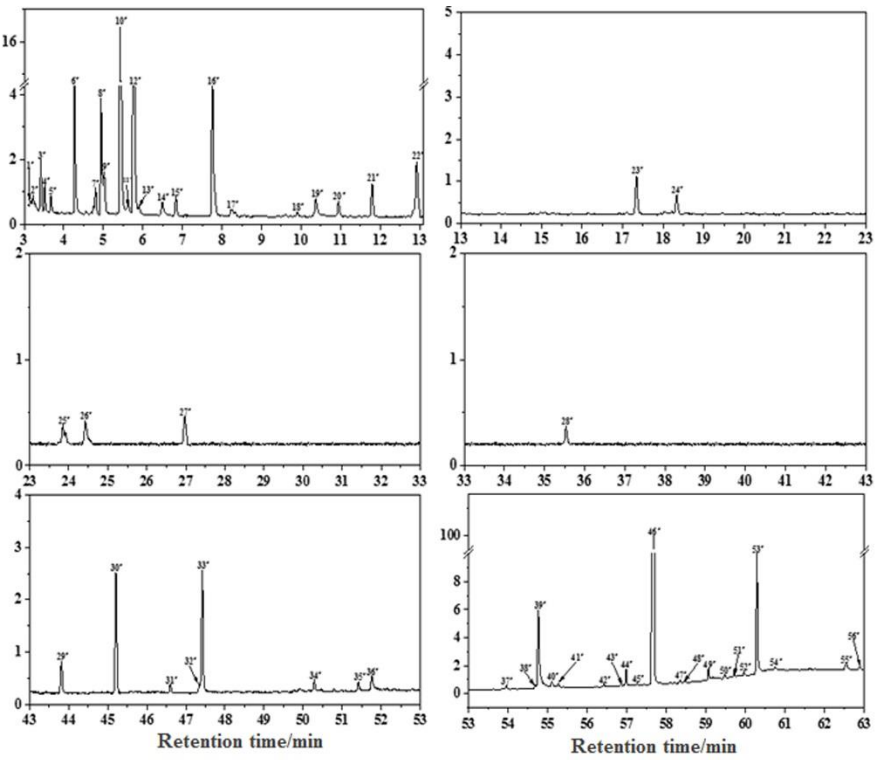

Fig. S2 Total ion chromatogram of soluble portions from ROM_{NCHC}

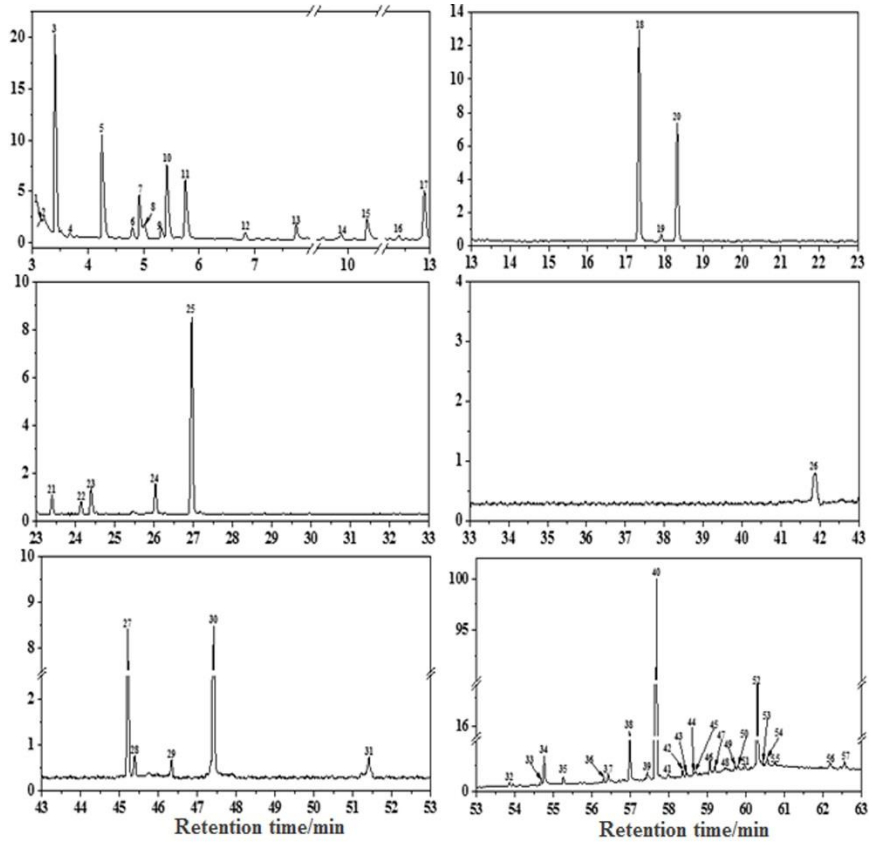

Fig. S3 Total ion chromatogram of soluble portions from ROM_{CHC}

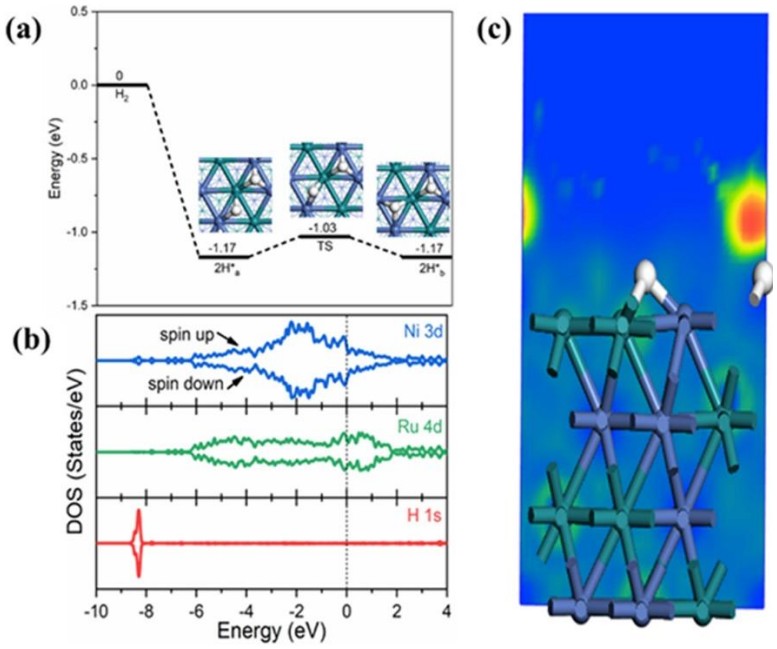

Fig. S4 (a) Potential energy changes of H_2 adsorption and dissociation process on Ni-Ru(111) crystal surface, (b) Electron-added fractional density of states of Ni-Ru(111) surface after adsorption of hydrogen molecules, and (c) Electron localization function diagram of Ni-Ru(111) surface after adsorption of hydrogen molecules.

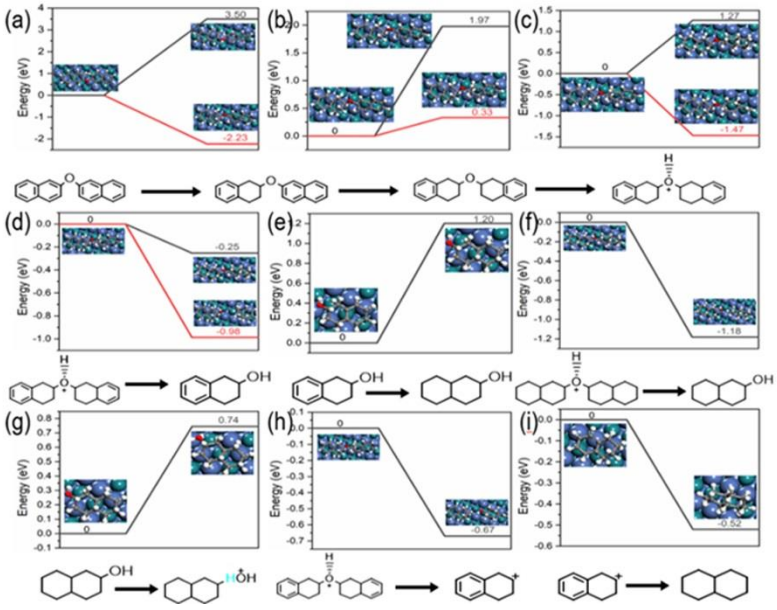

Fig. S5 Potential energy change during hydrogenation of 2,2'-Dinaphthyl ether.

Table S1 Soluble components in R_{CHC} and R_{NCHC} detected by GC/MS

Peak number	chemical compound	R_{CHC}	R_{NCHC}
1/1	Methyl cycloheptane	√	√
2/2	1-(vinyloxy)-hexane	√	√
3	3,4-dimethyl-(E)-2-pentene	√	
3	4-Methyl-3-heptene-2-one		√
4	1,1-dimethoxy-propane	√	
4	2-Methyl-2-heptyl mercaptan		√
5	Butyl acetate	√	
5/6	4-hydroxy-4-methyl-2-pentanone	√	√
6	1,3-Dimethyl benzene		√
7′	ethylbenzene	√	
7/8	1-(acetoxy)-2-Acetone	√	√
8/9	O-xylene	√	√
9	6-Methyl heptyl vinyl ether		√
10/10	Cyclohexanol	√	√
11	(z)-4-Hexene-1-alcohol	√	
11/12	cyclohexanone	√	√
13	3-methyl-1,2-Cyclopentanediol	√	
14	2,4-dimethyl-3-hexanol	√	
12/15	(1-methylethyl)-benzene	√	√
13/16	2,2-diethyloxy-propane	√	√
14	5-Ethyl-2-heptanol		√
15	3-Methyl-2-butanol acetate		√
16	N-butyl benzene		√
17	Benzaldehyde	√	
18	Decane	√	
19	4-SEC butoxy-2-butanone	√	
20	Thiazolidinic acid	√	
21	Cyclohexyl acetate	√	
17/22′	Acetophenone	√	√
18/23	1,2,3,4-tetrahydro-naphthalene	√	√
19	Ethyl benzoate		√
20/24	naphthalene	√	√
21	1-Methylnaphthalene		√

Peak number	chemical compound	R_{CHC}	R_{NCHC}
22	2-Methylnaphthalene		√
25	1,1 &apos-bicyclohexane	√	
23/26	Phthalic anhydride	√	√
24	1,2,3,4-Tetrahydro-1-naphthol		√
25/27	3,4-dihydrogen-1(2H)-naphthone	√	√
26	2-Tert butyl-4-(dimethylbenzyl) phenol		√
27	1,2-Bis (2-methylpropyl) phthalate		√
28	Dibutyl glutarate	√	
28	Tetrahydroxy tetramethyl dihydrobenzo [1,2-b] furan-3-one		√
29	Pyrido [4,3-b] quinoline-4-carbon	√	
29	Dibutyl phthalate		√
30	1,2-Benzoic acid	√	
30	1,2-Butyl 2-methylpropyl phthalate		√
31	Methyl hexadecanoate	√	
31	Octadecanoic acid		√
32	N-hexadecanoic acid	√	
33	1,2-Butyl 2-methylpropyl phthalate	√	
34	oleic acid	√	
44/35	Estradiol-1,3,5 (10)-triene-17β-alcohol	√	√
36	4-Cyclohexyl butylamine	√	
32/37	3-Nitro-1-methylindole	√	√
33/38	10-Octadecyl aldehyde	√	√
34/39	(z)-9-Octadecylamide	√	√
40	Octadecylamide	√	
35/41	2,6,10-trimethyl-tetradecane	√	√
36	Tert hexadecyl mercaptan		√
37/42	6-methyl-octadecane	√	√
43	pterin-6-carboxylic acid	√	
38/44	Mono (2-ethylhexyl) phthalate	√	√
39	4-Methyl hydroxyoctadecanoate		√
45	1-Naphthalene propanol, α-ethyl	√	
40/46	2,2 &apos-naphthalene ether	√	√

Peak number	chemical compound	R_{CHC}	R_{NCHC}
41	Z-5-methyl-6-undecylene-11-one		√
42/47	2-(octadecanoxy)-ethanol	√	√
43/48	(+)-coconut acid	√	√
45	E-8-methyl-9-tetradecene-1-ol acetate		√
46/49	Trans-13-docosamide	√	√
47	Eicosane		√
48	12-Methyl-e, e-2,13-octadecene-1-ol		√
50	12-Methyl-e, e-2,13-octadecene-1	√	
49/51	gibberellin	√	√
50	Cholesteric-4-ene-3,6-dione		√
51	Secondary oleic acid-5,7,10 (19)-triene-3,24,25-triol		√
52	9,10-Dichloroethylene-5,7,10 (19)-trichloroethylene	√	
52	Androsterol-4-ene-3,6,17-trione		√
53	Retinoic acid	√	
53	prednisone		√
54	Ethyl isocholate		√
55/54	Isohumulone	√	√
55	Ergosterol-5,22-diene-3-ol, acetate,	√	
56	3-hydroxy-stud-8-ene-11-one	√	
56	Dimethyl amyl hexahydro dimethyl 6h dibenzopyran diol		√
57	(3β,22e)-ergosterol-5,22-diene-3-ol acetate		√