Supporting information

Synergistic catalysis for promoting selective C–C/C–O cleavage in plastic waste: Structure-activity relationship and rational design of heterogeneous catalysts for liquid hydrocarbon production

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Table S1. C-C/C-O cleavage in aromatic plastic for selective arenes and cycloalkanes production

Entry No.	Polymer	Catalyst	Reaction condition	Solvent	Product	Product yield (%)	Ref.
1.	PET, PS, PPO, PC	Ru/Nb_2O_5	3.0 MPa H_2, 280–320 °C, 8–16 h	Water/ Octane	Arenes	75-85	24
2.	PET	Ru/Nb_2O_5	2.0 MPa N2, 220 °C, 20 bar N_2, 12 h	Water	BTX	~90	37
3.	PC	Ru/Nb_2O_5	0.07 MPa H_2, 270 °C, 0.7 bar H_2, 6 h	Hexane/ methanol	Phenolics	80	42
4.	PET	$Cu/Na\text{-}SiO_2$	210 °C, 6 h	Methanol	P-Xylene	100	38
5.	PET	Co/TiO_2	3.0 MPa H2, 340 °C, 4 h	Dodecane	BTX	~72	40
6.							
7.	PET	Ru/TiO_2	3.0 MPa H_2, 230 °C, 12 h	Water	BTX	77	43
8.	PET	CoMo@NC	H_2 balloon, 260 °C, , 10 h	None	PTA	~90	44
9.	PC (Mw- 3.6 $x10^4$)	Pt/C + H-Beta zeolite	Methonolysis: 140- 200 °C, 3.5- 14 h; HDO: 3.0 MPa H2, 100 °C, 1h	Methanol & Cyclohexane	Low-density alkanes (C7-C8) & High-density alkanes (C15)	~91	52
10.	PC (Mw- 3.6 $x10^4$)	Rh/C + USY	3.5 MPa H2, 200 °C, 12 h	Water	Propane-2,2-diyldicycyclohexane	~95	53
11.	PC	Raney Ni + USY	1st step: 190°C, Raney Ni, 1 h	Isopropanol	C6-C15 hydrocarbons	~75	54
12.	PC	1Ru0.5Ni/H-	3.0 MPa H2, 180 °C, 10 h	Decane	Propane-2,2-	97.3	55

		Beta			diyldicyclohexane		
13.	PET	Pt/C-hydrogenation; RuCu/SiO2-HDO	Methanolysis: 140–200 °C, 3.5–14 h; hydrogenation: 5.0 MPa H2, 80–160 °C1–10 h; HDO: 4.0 MPa H2, 350–400 °C, 8–22 h	Methanol	C7-C8 Cycloalkanes and Aromatics	~94	57

Table S2. C-C activation and cleavage in polyolefins for selective liquid hydrocarbon production.

Entry No.	Polymer	Catalyst	Reaction conditions	Product	Product yield			Ref.
					Gas (%)	Liquid (%)	Others (%)	
1.	LDPE (M_n: ~1700 Da, M_w: ~4000 Da)	Ru/ZrO_2 (ZrO_2-800)	6.0 MPa H_2, 240 °C, 2 h.	Gas (C_1-C_4) Liquid(C_5-C_{21}) Other (C_{22}-C_{45})	~11	~84	~4	67
2.	PE, PP, LDPE	Ru/CeO_2	2.5-3.5 MPa H_2, 200–240 °C, H_2, 8–144 h	Gas (C_1-C_4) Liquid(C_5-C_{26}) solid (C_{27}^+)	~10	~25-45	35- 40	69
3.	LDPE (M_n: ~ 1,7000, M_w: ~ 4,000)	Ru/CeO_2	6 MPa H_2, 240 °C, H_2, 5 h	Gas (C_1-C_4) Liquid(C_5-C_{26}) Wax (C_{27}^+)	31	54	15	70
4.	LDPE (M_n: ~ 1,7000, M_w: ~ 4,000)	Ru/CeO_2	2.0 MPa H_2, 240 °C, H_2, 4 h	Gas (C_1-C_4) Liquid(C_5-C_{21}) Solid (C_{22}^+)	29.4	56.8	13.8	71
5.	LDPE (M_n: ~ 1,7000, M_w: ~ 4,000 Da)	Ru/CeO_2-O	3.0 MPa H_2, 240 °C, H_2, 8 h	Gas (C_1-C_4) Liquid(C_5-C_{36})	~5.0	~ 80.0	--	72
6.	LDPE (M_w=76000 Da)	$Ru/WZrO_x$	5.0 MPa H_2, 250		~18	~73	~9	73

			°C, 2h, in hexane					
7.	PE Mw: (M_n: ~1700 Da, M_w: ~4000 Da)	5 % Ru/C	2-3 MPa H_2, 200–225 °C, 2–16 h	Gas (C_1-C_5) Liquid(C_5-C_{32})	~12	~70	-	75
8.	PE (M_n: 8000–158,000 Da) and used plastic bag (M_n: 31,000 Da)	Pt/SrTiO3	1.2 MPa H_2, 300 °C, 96 h	narrowly-ranged lubricants	~13	~85	-	78
9.	HDPE	5 % Ru/C	3.0 MPa H_2, 220 °C, 1h, in hexane	Liquid(C_5-C_{22}) other (C_{20}^+)	-	~75	-	76
10.	HDPE (M_w: 82600 Da)	mSiO_2/Pt/SiO_2	1.7 MPa H_2, 300 °C, 15 h	Gas (C_1-C_4) Liquid(C_5-C_{29}) Waxes (C_{30}^+)	~12.4	~74	~14	81
11.	LDPE	Pt@Si-1 + H-Beta	3.0 MPa H_2, 250 °C,	Gas (C_1-C_4) Liquid(C_5-C_9)	~10 %	~90 %	-	82
12.	PE, M_w: 4000 Da), PP M_w:12000 Da)	5 % Co/ZSM-5	4.0 MPa H_2, 250 °C, 20 h,	C2-C4 hydrocarbon	~88 %	~11 %	-	83
13.	LDPE (M_w ~4000 Da),	Ni/SiO_2	3.0 MPa H_2, 300 °C, 2 h	Gas (C_1-C_4) Liquid(C_5-C_{26}) solid (C_{27}^+)	~14	~65	~22	84

14.	LLDPE	Rh/Nb_2O_5	3.0 MPa H_2, 300 ºC, 6 h	Liquid(C_5-C_{20}), Squalene	-	~85 %	15	122
15.	i-PP (M_w ~ 250 000, average M_n ~ 67 000)	5.9 % Ru/TiO_2	3.0 MPa H_2, 250 °C, 16 h	Lubricant	~28 %	~65 %	6.4	86
16.	LDPE	Pt_3/SZ	H_2 20 mL/min, 250 ºC,	Gas (C_1-C_4) Liquid(C_5-C_{12})	~25 %	~74 %	-	86
17.	LDPE (M_w: 250,000 Da), HDPE, (M_w: 250,000 Da), PS (M_w: 35,000 Da)	$Pt/WO_3/ZrO_2$ + HY	3.0 MPa H_2, 250 °C.	Diesel, jet, and gasoline-range hydrocarbons	~34%	~65 %	-	87
18.	LDPE (M_w ~ 150 000 g/mol)	Pt/H-Beta	0.5-2.0 MPa H_2, 300-330 °C,	Low molecular weight hydrocarbons	~39 %	~60 %	-	88
19.	PE (M_w: 4000 Da)	5 % Ru/FAU	3.0 MPa H_2, 200 °C, 16 h,	Gas (C_1-C_4) Liquid(C_5-C_{12})	~40 %	~60 %	-	89
20.	n-hexadecane (as model substrate) and PE	2.5 % Ru/HZSM-5	4.5 MPa H_2, 375 ºC, for 2 h	C_1-C_4 hydrocarbons	~91 %	-	~10	90
21.	HDPE (M_w:125,000 g/cm^3)	Sulfide Ni/H-SiAl	6.8 MPa H_2, 375 °C, 60 min	Gas products (C1-C4 Hydrocarbons) Oil products (C5-C12 hydroca)	~53%	~40 %	~5	91

22.	HDPE	Meso-beta-silica composite	2.0 MPa H_2, 360-400 °C,	Gas & Liquid fuel	~40 %	~60 %	-	92