Supplementary Materials

Hydrogenation of Dodecanoic Acid over Iridium-Based Catalysts

Heny Puspita Dewi[1] and Shun Nishimura[1,2,*]

[1]Graduate School of Advanced Science and Technology, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan

[2]Research Center for Carbon Neutral, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan

*Correspondence: s_nishim@jaist.ac.jp

Table S1 Element screening of various metals supported AlOOH for the hydrogenation of dodecanoic acid to dodecanol[a]

Element	Precursor (Purity; Supplier)	Conversion (%)	Yield (%) Dodecanol
Ir	$H_2IrCl_6•nH_2O$ (36.0-44.0% Ir; Sigma-Aldrich)	72.5	52.2
Pt	$H_2PtCl_6•6H_2O$ (98.5%; Fujifilm-Wako)	56.0	27.1
Ru	$RuCl_3•nH_2O$ (38.0%-42.0% Ru; Sigma-Aldrich)	36.6	5.0
Cu	$Cu(CO_2CH_3)_2•nH_2O$ (99.99%; Sigma-Aldrich)	28.3	3.0
Ni	$Ni(OCOCH_3)_2•4H_2O$ (99.99%; Sigma-Aldrich)	25.0	0
Pd	$Pd(NO_3)_2•nH_2O$ (99.99%; Sigma-Aldrich)	22.0	0
In	$In(NO_3)_3•3H_2O$ (97.0%; Fujifilm-Wako)	22.0	0
Au	$HAuCl_4•4H_2O$ (99.0%; Fujifilm-Wako)	17.0	0
Mo	$(NH_4)_6Mo_7O_{24}•4H_2O$ (99.0%; Kanto)	14.0	0

[a]Reaction conditions: dodecanoic acid (0.1 g), catalyst (0.1 g), 1,4-dioxane (10 mL), H_2 (8.0 MPa), 200°C, 17 h.

Table S2. Hydrogenation of dodecanoic acid over Ir-based catalyst with various oxide supports

Entry	Support	Conversion (%)	Yield (%)	
			Dodecanol	Dodecane
1[a]	MoO_3	100	9.3	90.7
2[b]		22.2	16.5	5.7
3[a]	Ta_2O_5	100	39.5	60.5
4[a]	Nb_2O_5	100	82.2	17.8
5[b]		100	89.1	10.9
6[a]	AlOOH	72.5	52.2	N.A.
7[a]	TiO_2	50.0	48.7	1.3
8[a]	ZrO_2	6.2	1.8	0
9[a]	SiO_2	5.0	1.1	0
10[a]	WO_3	4.3	1.2	0

[a]Reaction conditions: dodecanoic acid (0.1 g), 1,4-dioxane (10 mL), H_2 (8.0 MPa), 200°C, 17 h.
[b]Reaction conditions: dodecanoic acid (0.1 g), 1,4-dioxane (10 mL), H_2 (4.0 MPa), 170°C, 17 h.

Table S3. Time-dependent reaction profile of the Hydrogenation of dodecanoic acid over Ir/Nb_2O_5 and Ir/MoO_3

Catalyst	Temp (°C)	H_2 (MPa)	Time	Conversion (%)	Yield (%)	
					Dodecanol	Dodecane
Ir/Nb_2O_5	200	8.0	8	55.3	54.4	0.9
			17	100	82.2	17.8
			24	100	86.2	13.8
			40	100	58.9	41.1
	170	4.0	8	100	80.2	19.8
			17	100	89.1	10.9
			24	99.1	65.7	33.4
			40	100	60.0	40.0
Ir/MoO_3	200	8.0	8	100	3.4	91.3
	200	4.0	8	20.7	12.6	8.1
			17	73.0	47.0	26.0
			24	97.4	40.0	57.4
			40	100	14.7	85.3

Common reaction conditions: dodecanoic acid (0.1 g), 1,4-dioxane (10 mL).

Table S4. Large scale hydrogenation[a]

Entry	Catalyst	Time (h)	Conversion (%)	Yield (%)		
				Dodecanol	Dodecane	unknown
1	Ir/Nb_2O_5	40	99.8	68.2	30.5	1.1
2	Ir/MoO_3	24	100	7.4	91.7	0.9

[a]Reaction conditions: dodecanoic acid (1.0 g), catalyst (0.1 g), 1,4-dioxane (10 mL), H_2 (8.0 MPa), 200°C.

Table S5. Recycling test of Ir/Nb_2O_5 catalyst[a]

Reuse	Conversion (%)	Yield (%)	
		Dodecanol	Dodecane
Fresh	100	89.1	10.9
1st	100	72.6	27.4
2nd	100	77.2	22.8
3rd	100	82.5	17.5
4th	100	68.6	31.4
5th	97.0	72.0	25.0

[a]Reaction conditions: dodecanoic acid (1.0 g), catalyst (0.1 g), 1,4-dioxane (10 mL), H_2 (4.0 MPa), 170°C, 17 h.

Table S6. Results of hydrogenation of various fatty acid over Ir/Nb_2O_5 catalyst[a]

Entry	Substrate	Conversion (%)	Yield (%)		
			Main product	Alcohol form	Alkane form
1	Hexadecanoic acid (Palmitic acid)	100	Hexadecanol	80.8	19.2
2	Tetradecanoic acid (Myristic acid)	100	Tetradecanol	52.0	48.0
3	Oleic acid	100	Oleyl alcohol	78.0	22.0

[a]Reaction Conditions: dodecanoic acid (0.1 g), catalyst (0.1 g), 1,4-dioxane (10 mL), H_2 (8.0 MPa), 200°C, 17 h.

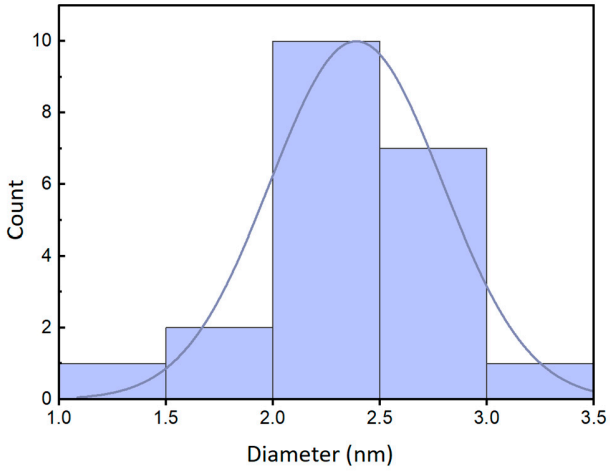

Figure S1. Particle distribution of Ir/Nb_2O_5 before use (after reduction treatment)

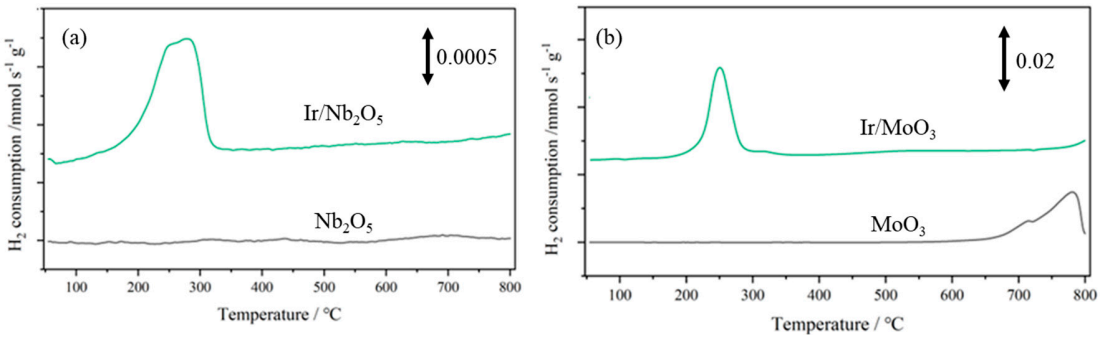

Figure S2. H_2-TPR profile of (a) Ir/Nb_2O_5 and Nb_2O_5, and (b) Ir/MoO_3 and MoO_3

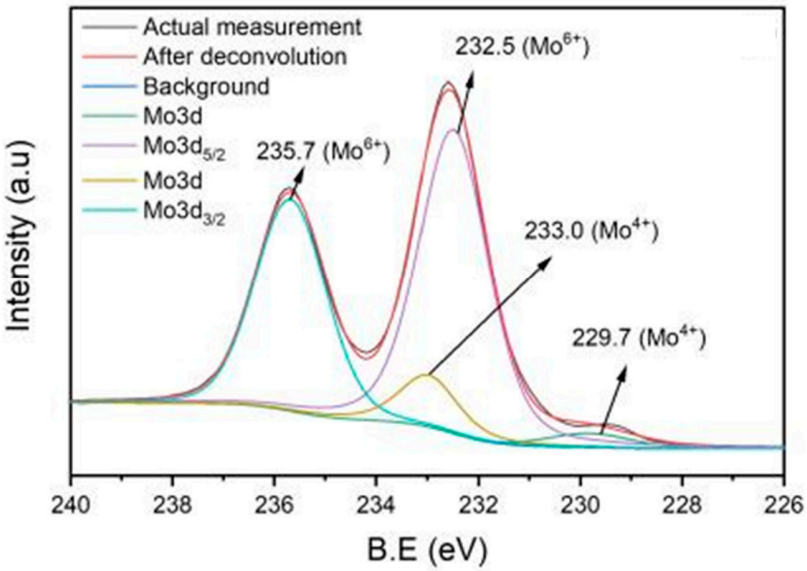

Figure S3. Deconvoluted XPS spectra of Ir-based catalysts of Ir/MoO_3 after the reaction at the Mo 3d region

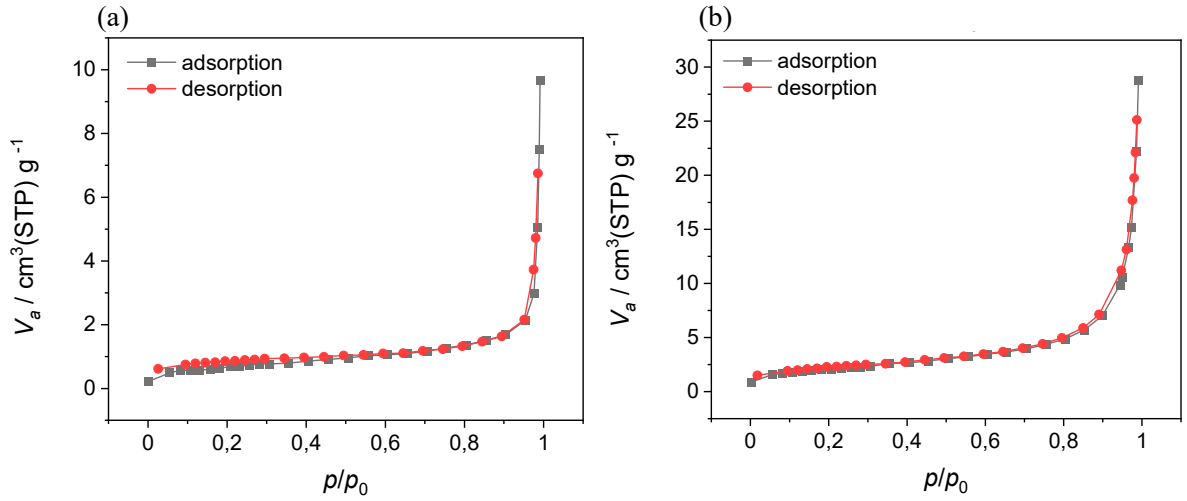

Figure S4. N_2 adsorption-desorption isotherm of (a) Ir/Nb_2O_5 and (b) Ir/MoO_3