Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary material

Investigation of converting 1-butene and ethylene into propene via metathesis reaction over W-based catalysts

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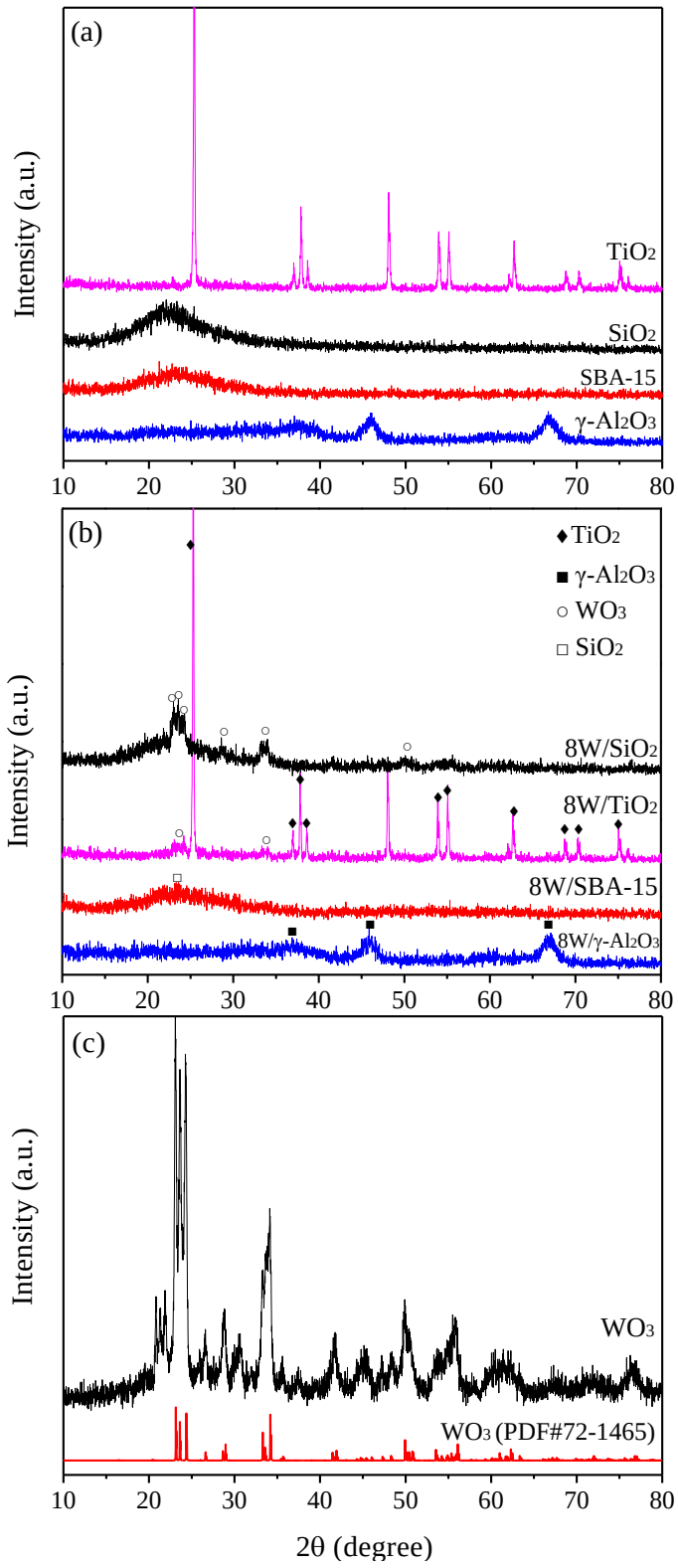


Fig. S1 XRD patterns of (a) various support materials, (b) their 8 wt% corresponding W-containing catalysts, and (c) unsupported WO_3 as a reference.

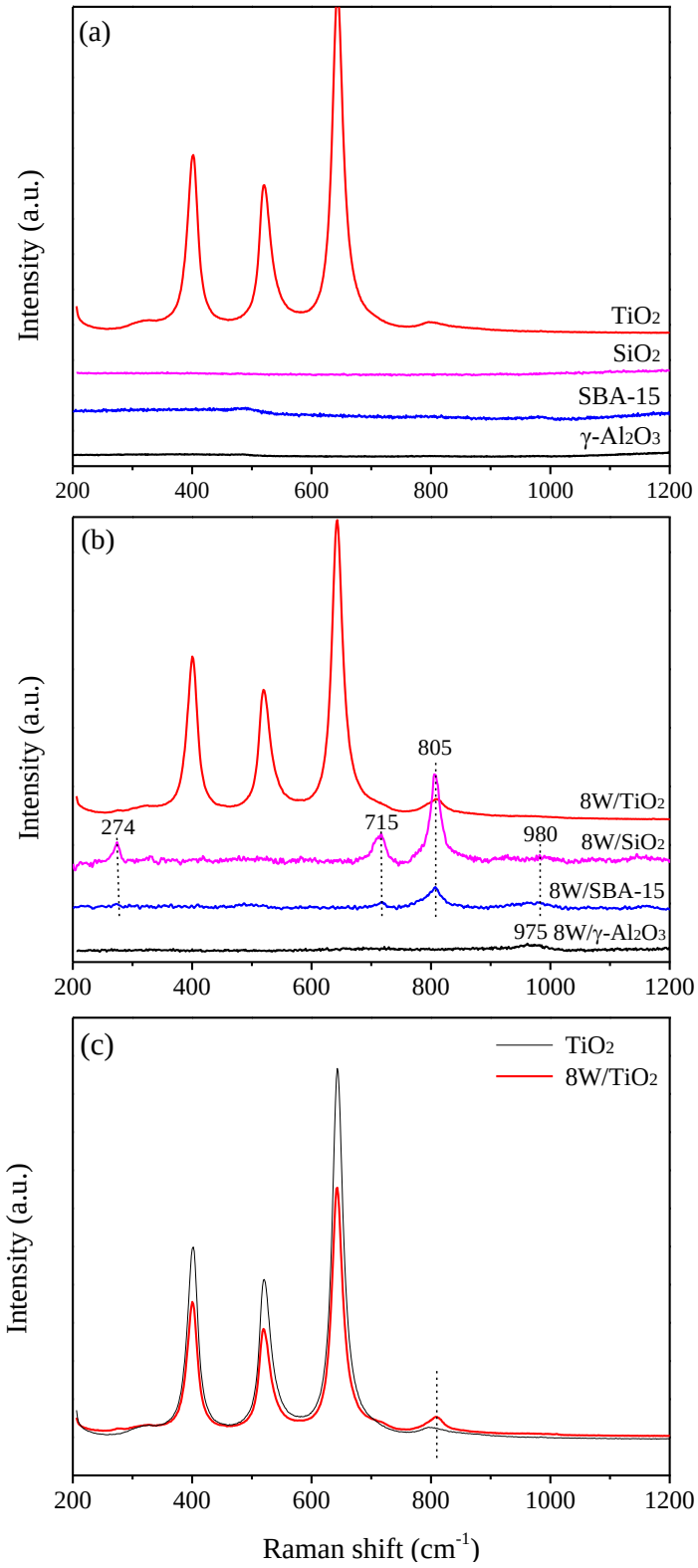


Fig. S2 Raman spectra of (a) various support materials, (b) their corresponding 8 wt% W-containing catalysts, and (c) TiO_2 and $8W/TiO_2$.

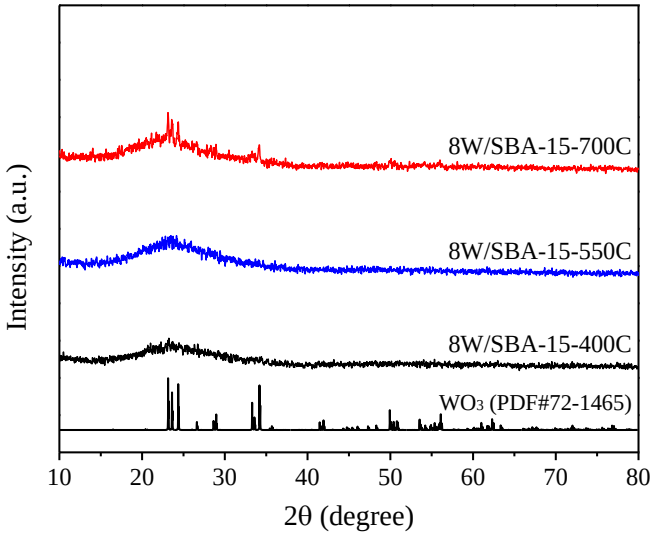


Fig. S3 XRD patterns of 8W/SBA-15 prepared in different calcination temperatures (400, 550 and 700 ℃).

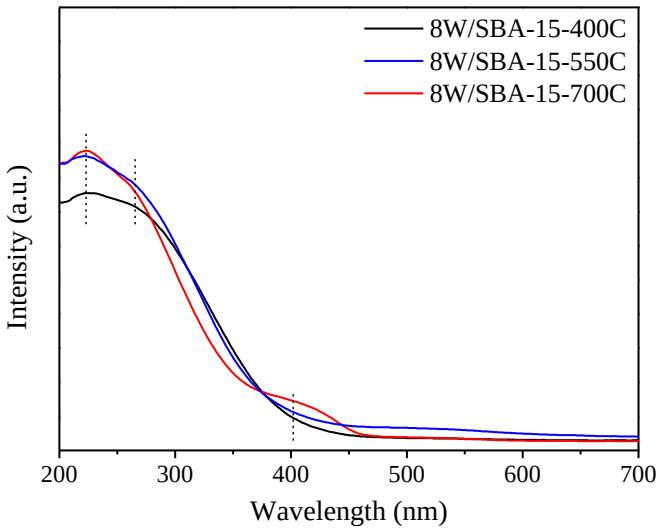


Fig. S4 UV-vis DRS spectra of 8W/SBA-15 prepared in different calcination temperatures (400, 550, and 700 ℃).

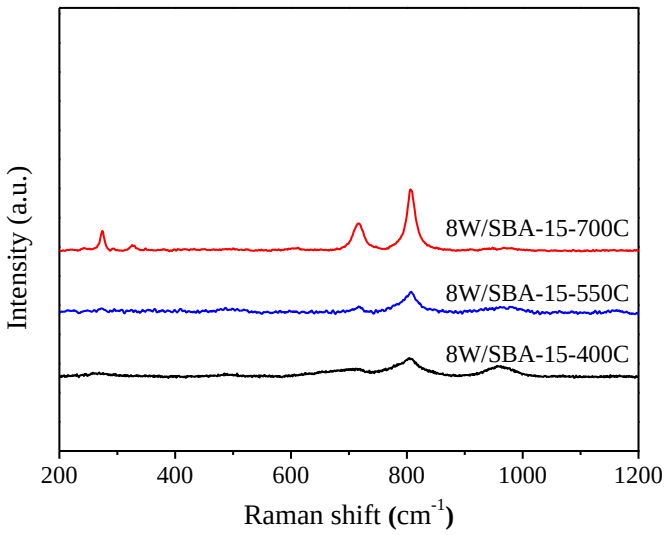


Fig. S5 Raman spectra of 8W/SBA-15 prepared in different calcination temperatures (400, 550, and 700 ℃).

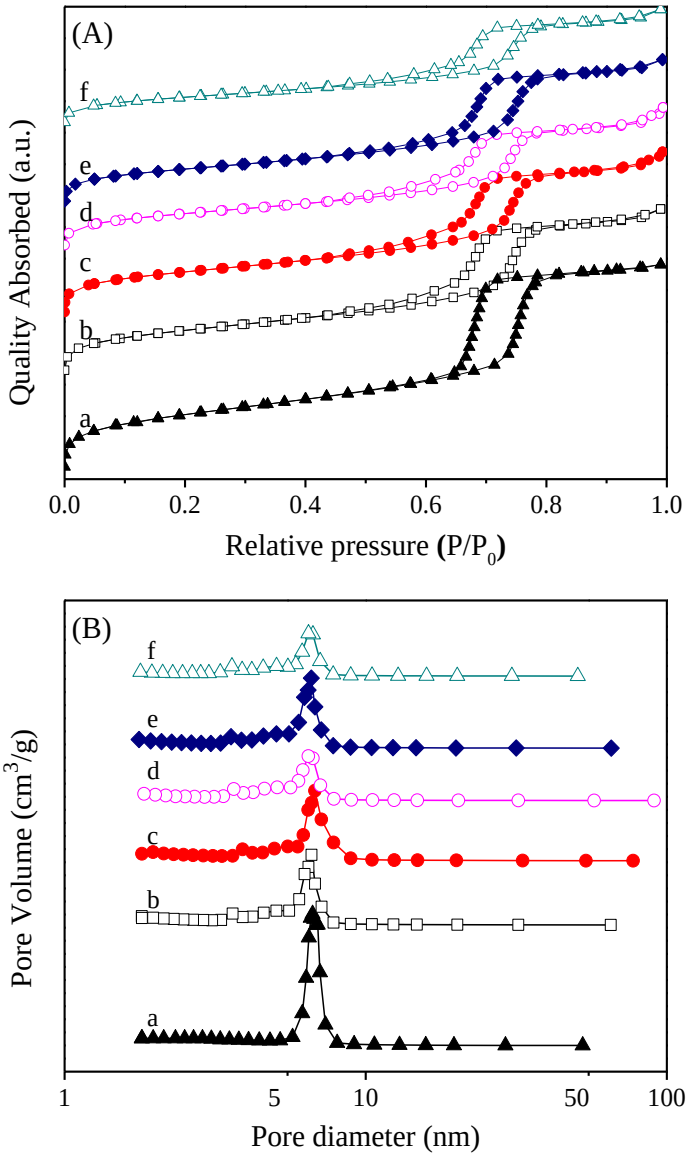


Fig. S6 (A) Nitrogen adsorption-desorption isotherms and (B) corresponding pore size distribution curves of (a) SBA-15, (b) 4W/SBA-15, (c) 8W/SBA-15, (d) 15W/SBA-15, (e) 20W/SBA-15, and (f) 30W/SBA-15 catalysts.

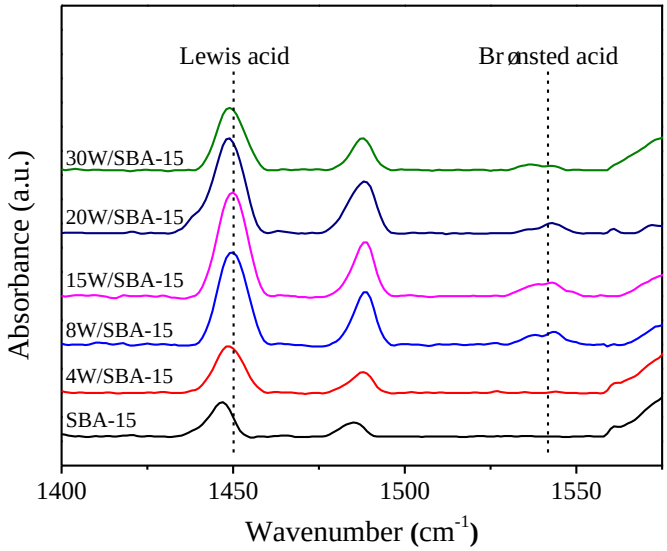


Fig. S7 FT-IR spectra of pyridine adsorbed SBA-15 and W/SBA-15 catalysts with different W loadings.

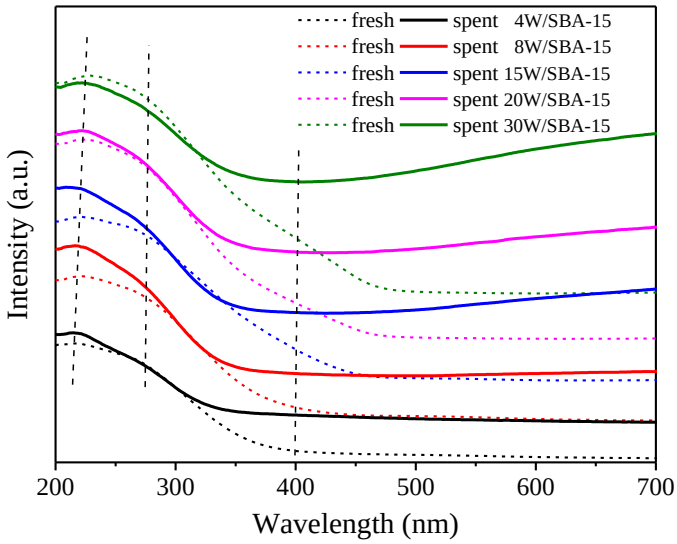


Fig. S8 UV-vis DRS spectra of fresh W/SBA-15 catalysts with different W loadings and their corresponding spent catalysts.

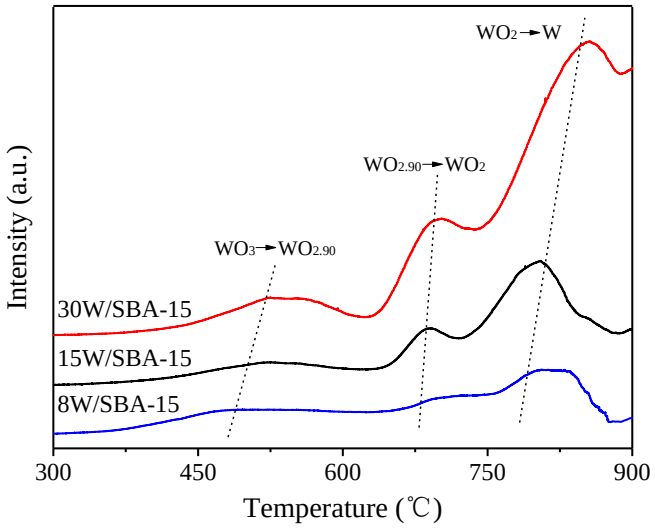


Fig. S9 H_2-TPR profiles of fresh 8W/SBA-15, 15W/ SBA-15, and 30W/SBA-15 catalysts.

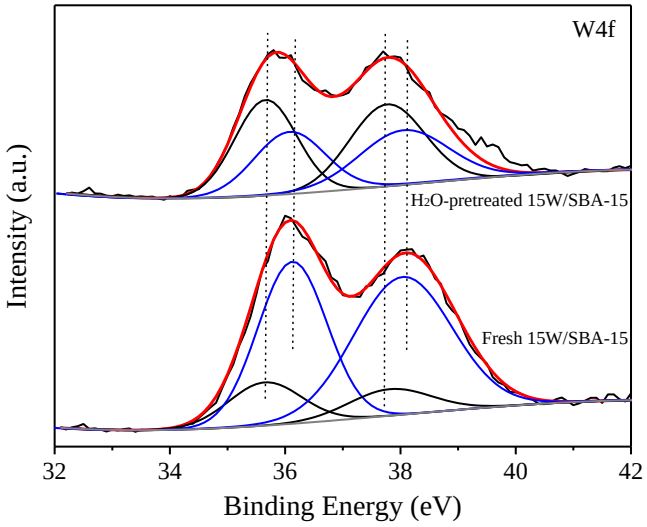


Fig. S10 XPS spectra of fresh 15W/SBA-15 and H_2O-pretreated 15W/SBA-15 catalysts.

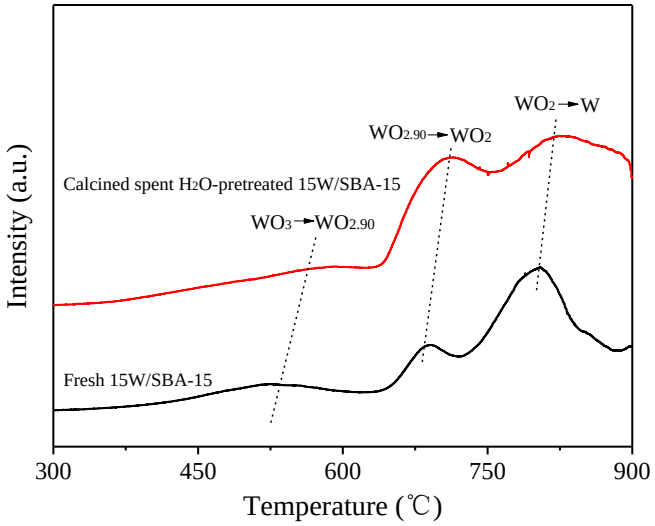


Fig. S11 H_2-TPR profiles of fresh 15W/SBA-15 and calcined spent H_2O-pretreated 15W/SBA-15 catalysts.

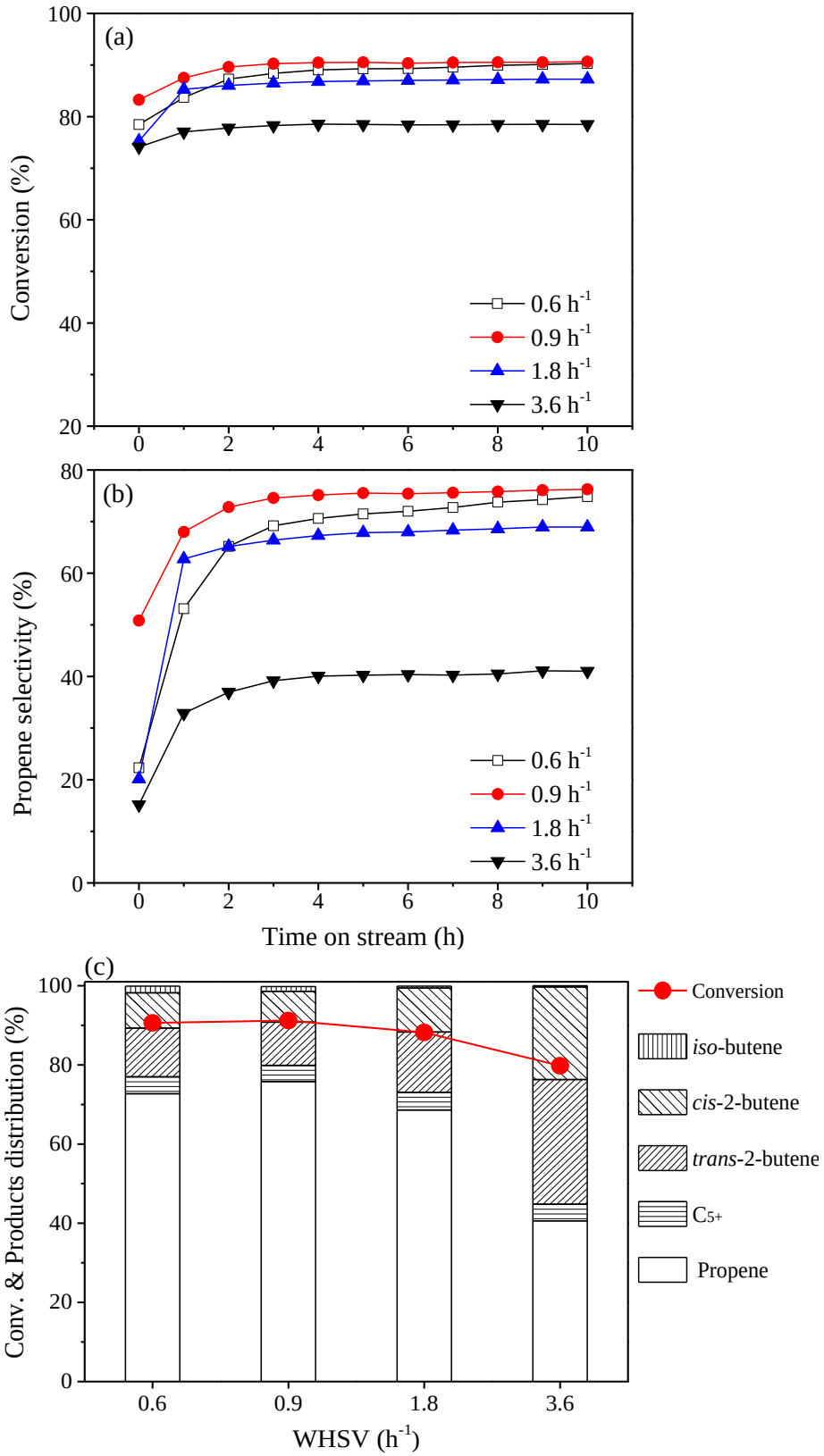


Fig. S12 Time-dependence of 1-buene conversion (a), propene selectivity (b), and products distribution (c) obtained over 15W/SBA-15 catalyst with different WHSV at the reaction conditions of 450 ℃, 0.1 MPa, 1.5, 1.0, 0.5, and 0.25 g of catalyst weight, and an ethylene/1-butene molar ratio of 2.

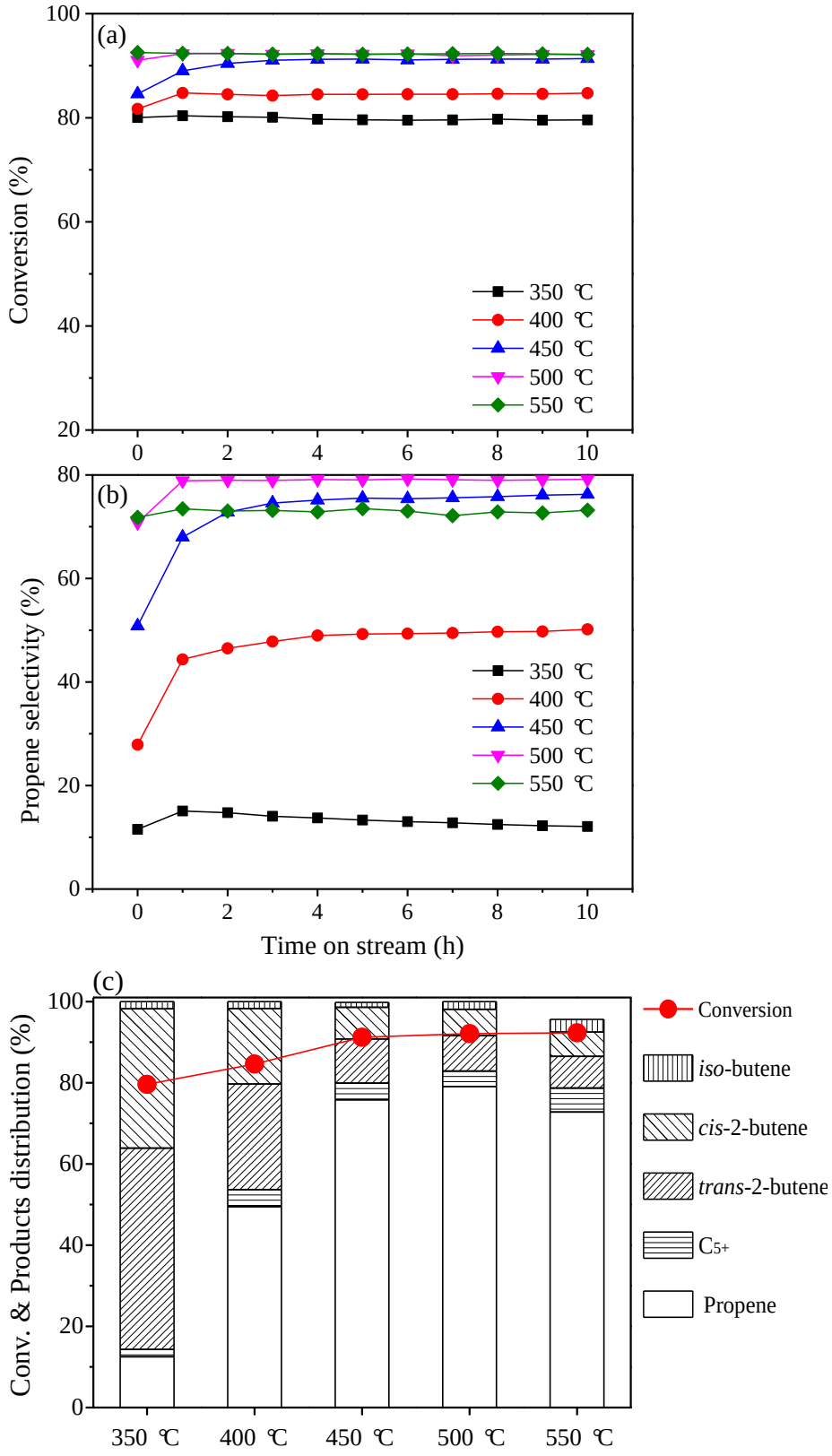
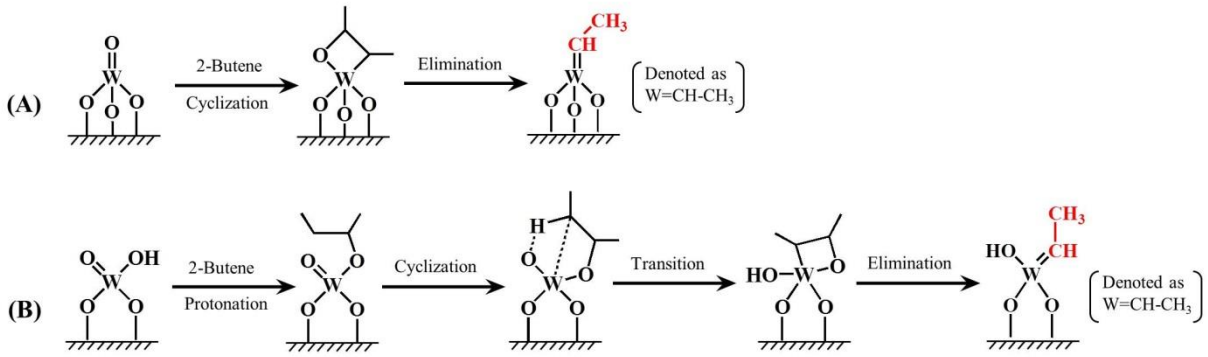
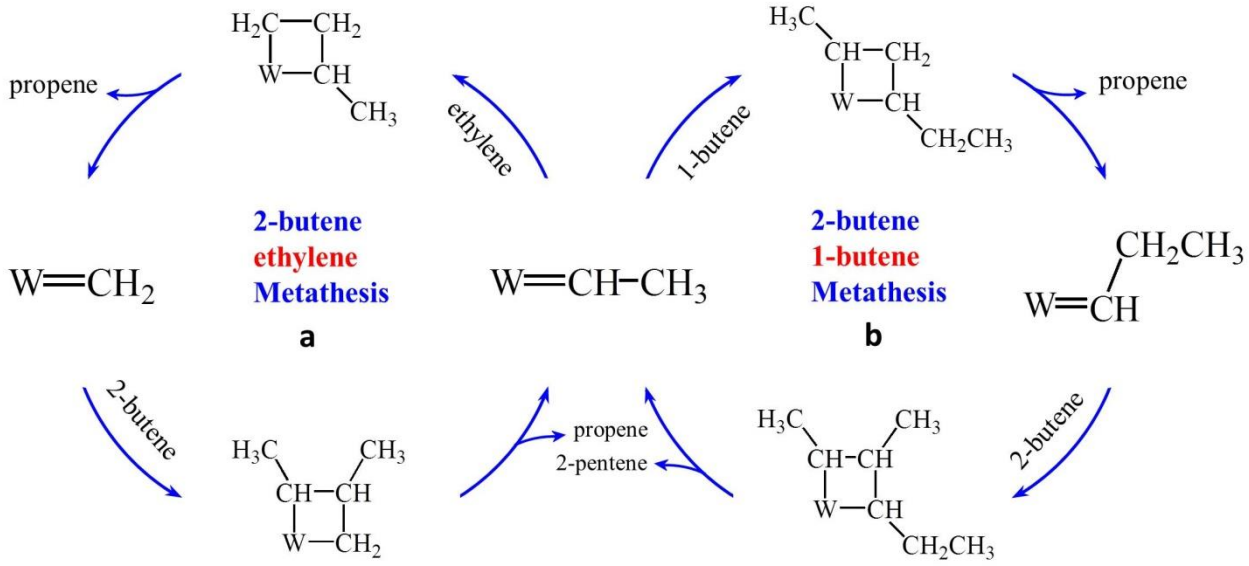


Fig. S13 Time-dependence of 1-buene conversion (a), propene selectivity (b), and products distribution (c) obtained over 15W/SBA-15 catalyst with different reaction temperatures at the reaction conditions of 0.1 MPa, 1.0 g of catalyst weight, 0.9 h^{-1} of WHSV, and an ethylene/1-butene molar ratio of 2.



Scheme S1 Formation pathway of active sites denoted as W-carbene from the terminal W=O (A), and W-OH (B) of isolated tetrahedral W^{5+} species.



Scheme S2 Reaction mechanism of the metathesis of 2-butene and ethylene (a), and 2-butene and 1-butene (b) over SBA-15 supported W catalysts.

Table S1 Physicochemical properties of SBA-15 and W/SBA-15 catalysts with different W loadings.

Sample	Surface area (m^2 g^{-1})[a]	Pore volume (cm^3 g^{-1})[b]	Pore size (nm)[b]	Surface density (W nm^{-2})	Acidity (μmol g^{-1})	
					Brønsted acid[c]	Lewis acid[c]
SiO_2	287	1.05	13.0	N/A	N/A	N/A
8W/SiO_2	247	0.87	11.8	0.91	1.1	7.3
SBA-15	719	1.09	6.1	N/A	0.0	3.6
8W/SBA-15	551	0.83	5.9	0.41	2.4	12.0
γ-Al_2O_3	209	0.42	8.1	N/A	N/A	N/A
8W/γ-Al_2O_3	185	0.38	6.3	1.23	0.0	47.1
TiO_2	13	0.06	18.9	N/A	N/A	N/A
8W/TiO_2	8	0.03	17.7	28.3	0.0	1.9

[a] Determined by BET method.

[b] Evaluated by the BJH method.

[c] Determined by pyridine-IR spectra.

Table S2 Catalytic performance of unsupported WO_3 and 8 wt% W-containing catalysts with different support material.

Catalyst	Conversion (%)[a]	Selectivity (%)					Specific activity (mmol $C_4^=$ g_{cat}^{-1} h^{-1})
		Propene	C_{5+}	*trans*-2-butene	*cis*-2-butene	*iso*-butene	
8W/SiO_2	79.5	47.4	6.0	26.5	20.1	0.1	12.8
8W/γ-Al_2O_3	77.1	13.6	2.3	42.7	31.4	10.5	12.4
8W/TiO_2	62.6	1.5	0.8	56.4	41.1	0.2	10.1
8W/SBA-15	83.3	54.6	3.6	23.8	17.5	0.5	13.4
WO_3	14.5	0.9	1.2	62.9	35.4	0.2	2.3

[a] Reaction conditions: T = 450 ℃, P = 0.1 MPa, catalyst weight = 0.5 g, WHSV (E+B) = 1.8 h^{-1}, *n* (E) / *n* (B) = 2.

Table S3 Catalytic performance of 8W/SBA-15 catalyst prepared at different calcination temperatures.

T (℃)	Conversion (%)[a]	Selectivity (%)					Specific activity (mmol $C_4^=$ g_{cat}^{-1} h^{-1})
		Propene	C_{5+}	*trans*-2-butene	*cis*-2-butene	*iso*-butene	
400	84.1	54.2	4.0	23.3	17.1	1.4	13.5
550	83.3	54.6	3.6	23.8	17.5	0.5	13.4
700	83.1	55.2	4.4	23.3	16.9	0.2	13.4

[a] Reaction conditions: T = 450 ℃, P = 0.1 MPa, catalyst weight = 0.5 g, WHSV (E+B) = 1.8 h^{-1}, *n* (E) / *n* (B) = 2.

Table S4 Catalytic performance of SBA-15, WO_3, and W-containing catalysts with different loadings.

Catalyst	Conversion	Selectivity (%)					Specific activity
	(%)[a]	Propene	C_{5+}	*trans*-2-butene	*cis*-2-butene	*iso*-butene	(mmol $C_4^=$ g_{cat}^{-1} h^{-1})
SBA-15	72.3	2.9	0.3	55.4	40.8	0.6	11.6
4W/SBA-15	78.9	37.4	2.4	34.7	25.3	0.4	12.7
8W/SBA-15	83.3	54.6	3.6	23.8	17.5	0.5	13.4
15W/SBA-15	88.2	68.6	4.5	15.2	11.1	0.5	14.2
20W/SBA-15	86.7	63.7	4.4	18.0	13.2	0.7	13.9
30W/SBA-15	85.9	61.5	4.3	19.5	14.1	0.7	13.8
WO_3	14.5	0.9	1.2	62.9	35.4	0.2	2.3

[a] Reaction conditions: T = 450 ℃, P = 0.1 MPa, catalyst weight = 0.5 g, WHSV (E+B) = 1.8 h^{-1}, *n* (E) / *n* (B) = 2.