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) TiO₂ and 8W/TiO₂.
Fig. S3 XRD patterns of 8W/SBA-15 prepared in different calcination temperatures (400, 550 and 700 °C).

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

Fig. S5 Raman spectra of 8W/SBA-15 prepared in different calcination temperatures (400, 550, and 700 °C).
**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$_2$O-pretreated 15W/SBA-15 catalysts.

**Fig. S11** H$_2$-TPR profiles of fresh 15W/SBA-15 and calcined spent H$_2$O-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 °C, 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-buene 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 W⁵⁺ 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 (m² g⁻¹)ᵃ | Pore volume (cm³ g⁻¹)ᵇ | Pore size (nm)ᵇ | Surface density (W nm⁻²) | Acidity (μmol g⁻¹) | Brønsted acid | Lewis acid |  |
|--------------|------------------------|------------------------|----------------|--------------------------|-------------------|----------------|------------|---|
| SiO₂         | 287                    | 1.05                   | 13.0           | N/A                      | N/A               | N/A           | N/A        |   |
| 8W/SiO₂      | 247                    | 0.87                   | 11.8           | 0.91                     | 1.1               | 7.3            | 3.6        |   |
| SBA-15       | 719                    | 1.09                   | 6.1            | N/A                      | 0.0               | 12.0          | 3.6        |   |
| 8W/SBA-15    | 551                    | 0.83                   | 5.9            | 0.41                     | 2.4               | 12.0          | 3.6        |   |
| γ-Al₂O₃      | 209                    | 0.42                   | 8.1            | N/A                      | N/A               | N/A           | N/A        |   |
| 8W/γ-Al₂O₃   | 185                    | 0.38                   | 6.3            | 1.23                     | 0.0               | 47.1          |           |   |
| TiO₂         | 13                     | 0.06                   | 18.9           | N/A                      | N/A               | N/A           | N/A        |   |
| 8W/TiO₂      | 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 WO₃ and 8 wt% W-containing catalysts with different support material.

| Catalyst           | Conversion (%)ᵃ | Selectivity (%) | Specific activity (mmol C₄⁺ g<sub>cat</sub>⁻¹ h⁻¹) |
|--------------------|-----------------|----------------|-----------------------------------------------|
|                    |                 | Propene C₅⁺ | trans-2-butene | cis-2-butene | iso-butene |                      |
| 8W/SiO₂            | 79.5            | 47.4         | 6.0         | 26.5         | 20.1       | 0.1               | 12.8               |
| 8W/γ-Al₂O₃         | 77.1            | 13.6         | 2.3         | 42.7         | 31.4       | 10.5              | 12.4               |
| 8W/TiO₂            | 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               |
| WO₃                | 14.5            | 0.9          | 1.2         | 62.9         | 35.4       | 0.2               | 2.3                |

ᵃ Reaction conditions: T = 450 °C, 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 (°C) | Conversion (%)ᵃ | Selectivity (%) | Specific activity (mmol C₄⁺ g<sub>cat</sub>⁻¹ h⁻¹) |
|--------|-----------------|----------------|-----------------------------------------------|
|        |                 | Propene C₅⁺ | 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 °C, 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 (mmol C$_4$ eq g$_{cat}$$^{-1}$ h$^{-1}$) |
|-------------------|----------------|-----------------|----------------------------------------------------------|
|                   |                | Propene | C$_5$  | trans-2-butene | cis-2-butene | iso-butene |                                      |
| 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: $T = 450$ °C, $P = 0.1$ MPa, catalyst weight = 0.5 g, WHSV (E+B) = 1.8 h$^{-1}$, $n$ (E) / $n$ (B) = 2.