Electronic Supplementary Information

A chemical titration method for quantification of carbenes in Mo- or W-containing catalysts for metathesis of ethylene with 2-butenes: verification and application potential

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Tables

Table S1 Specific surface area and absorptive capacity of Siral 10, Siral 40 and Siral 70.

Support	S_{BET}, $m^2 \cdot g^{-1}$	Absorptive capacity, $g_{liq} \cdot g^{-1}$
Siral 10	350	1.2
Siral 40	475	2
Siral 70	337	3.5

Table S2 Specific activity of Mo-Si-Al and W-Si-Al metathesis catalysts in the cross-metathesis of ethylene and 2-butene.

Catalyst	T, °C	A, mmol(C_3H_6)·g(cat)$^{-1}$·h^{-1}	Reference
3Mo/Siral 10	50	193	this work
1.5Mo/Siral 40	50	203	this work
1.5Mo/Siral 70	50	114	this work
10 wt%MoO_3- Al_2O_3-SiO_2	40	32	[1]
10wt%MoO_3-Al_2O_3-SiO_2	40	44.5	[2]
1.09Mo/SBA-15	50	8	[3]
0.85Mo/SBA-15	50	19.6	[3]
5W/Siral 10	50 (150)	6.3 (279)	this work
3W/Siral 40	50 (150)	2.2 (127)	this work
1.5W/Siral 70	50 (150)	1.0 (47)	this work
WH/Al_2O_3	150	142.8	[4]
WO_xSiAl-aer	250	68	[5]
WO_x-impSiAl-aer	250	53	[5]
WOx-imp-SiAl	250	45	[5]
WO_x-imp-Al	250	24	[5]
WO_x-imp-Si	250	2	[5]

Figures

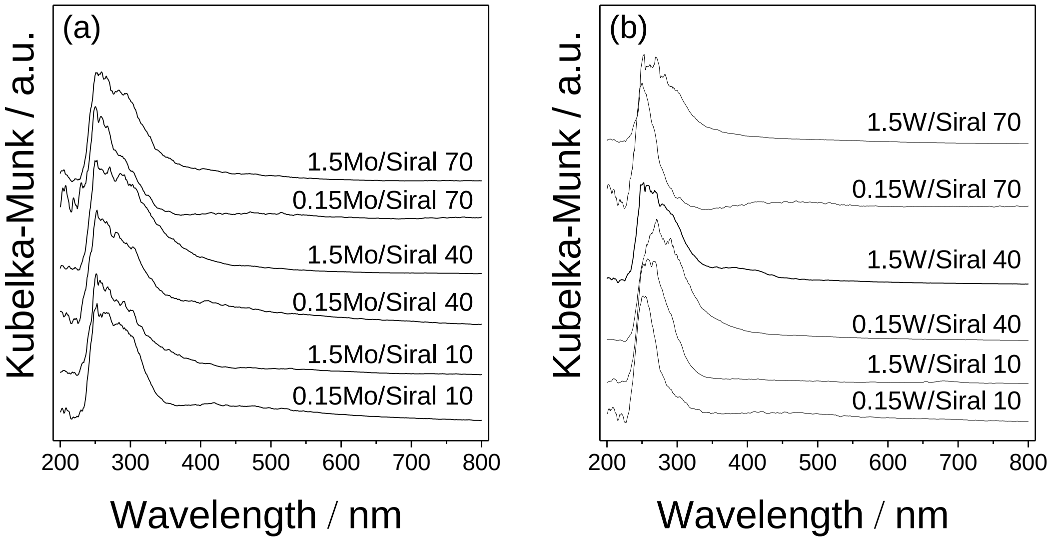

Figure S1 UV-Vis spectra of (a) XMo/Y and (b) XW/Y catalysts.

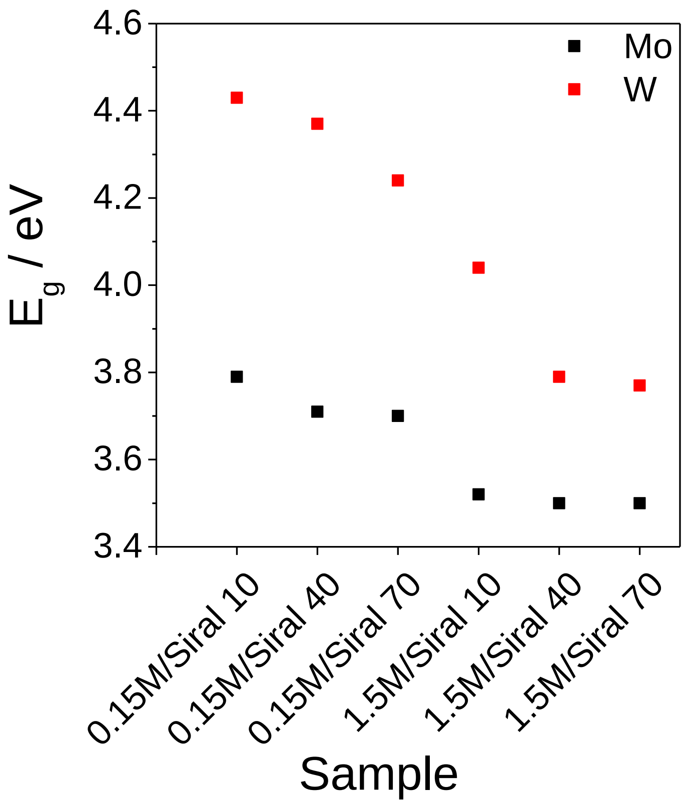

Figure S2 UV-Vis Edge energies (E_g) determined for XMo/Y (■) and XW/Y (■) catalysts.

The E_g values were obtained from the Tauc plots ($[F(R)\cdot h\upsilon]^2$ versus photon energy ($h\upsilon$)) by extrapolation of linear region to the photon energy axis.

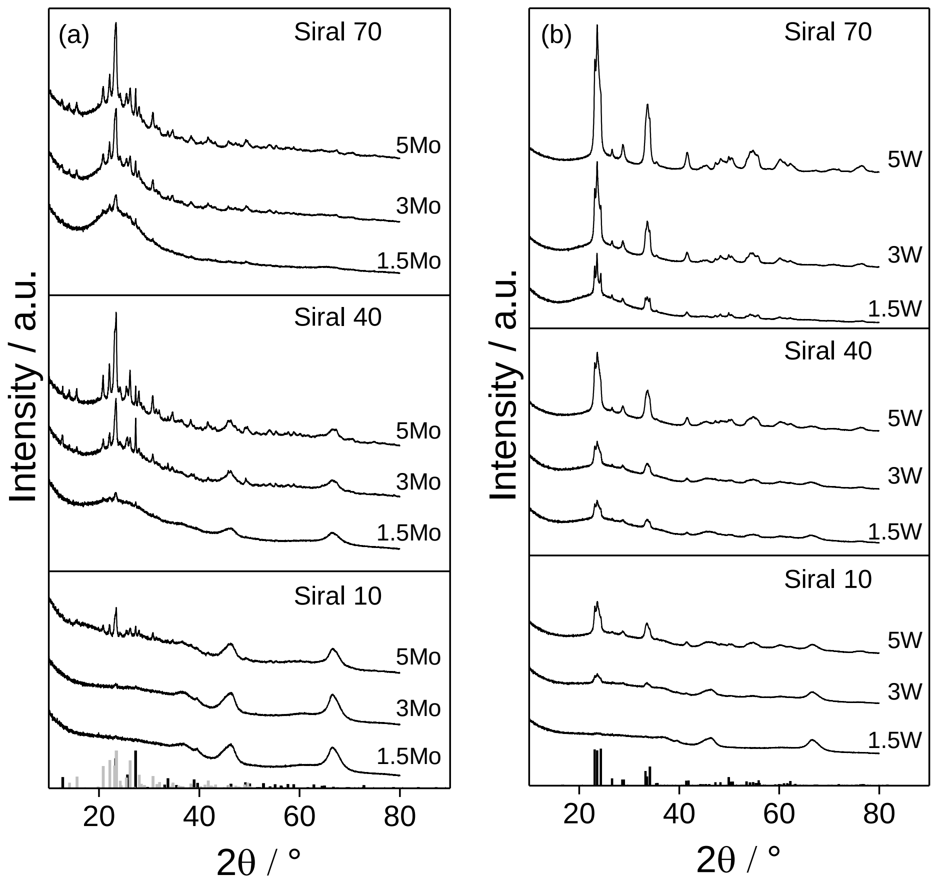

Figure S3 (a) XRD patterns of Mo/Siral 10, Mo/Siral 40 and Mo/Siral 70 with the nominal atomic surface density of Mo of 1.5, 3 and 5 nm^{-2}. Black and grey bars are related to orthorhombic MoO_3 and monoclinic $Al_2(MoO_4)_3$ phases respectively; (b) XRD patterns of W/Siral 10, W/Siral 40 and W/Siral 70 with the nominal atomic surface density of W of 1.5, 3 and 5 nm^{-2}. Black bars are related to monoclinic WO_3 phase.

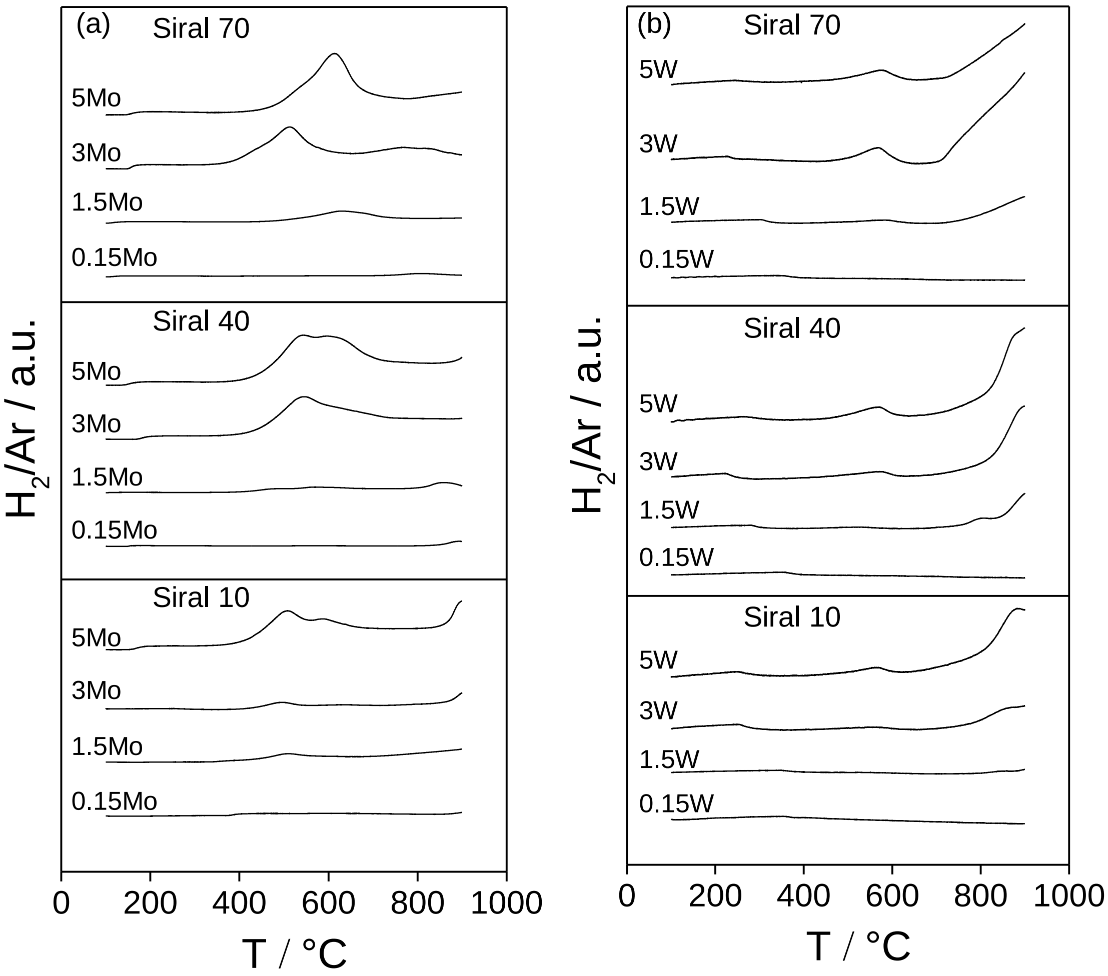

Figure S4 H_2-TPR profiles of (a) Mo-containing or (b) W- containing catalysts.

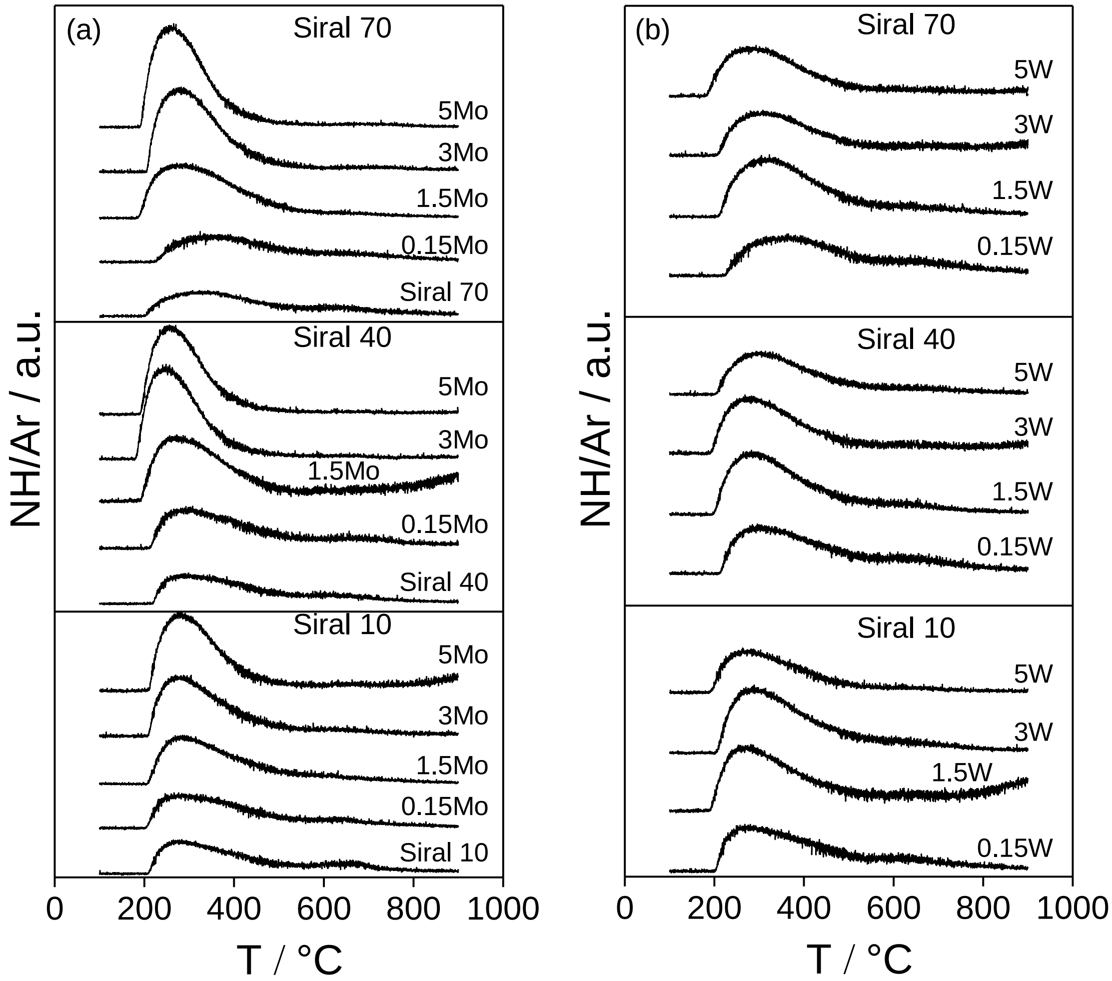

Figure S5 NH_3-TPD profiles of (a) bare supports and Mo-containing or (b) W-containing catalysts.

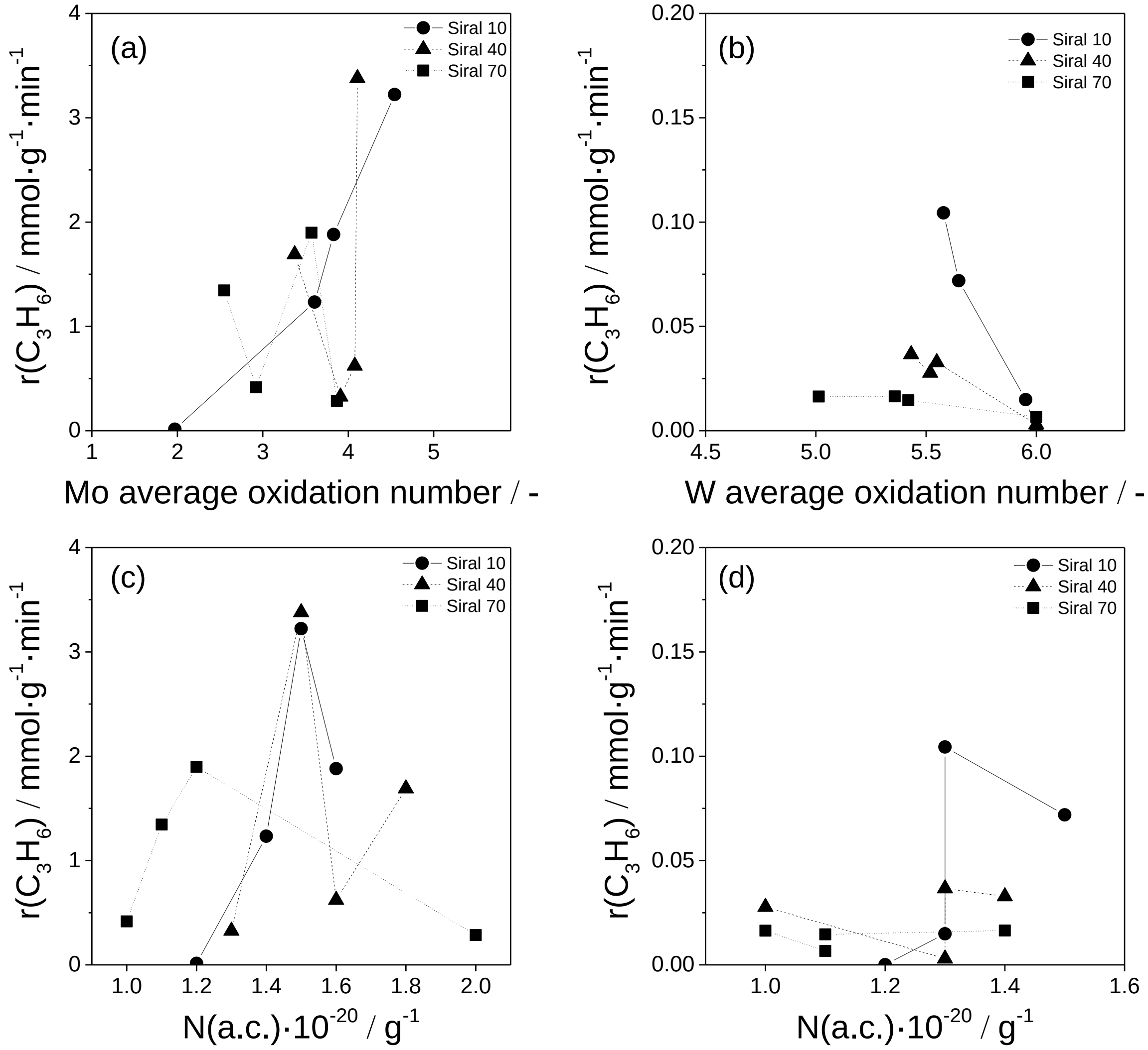

Figure S6 Rate of propene formation at 50°C as a function of (a) Mo reducibility, (b) W reducibility, (c) number of acidic sites in Mo-containing catalysts and (d) number of acidic sites in W-containing catalysts.

Reducibility of the catalysts is expressed as an average oxidation number of Mo or W (ON). This number was estimated from the amount of H_2 consumed during TPR experiment assuming that Mo or W existed in a form of M^{6+} in freshly prepared catalysts. Removal of oxygen from Al_2O_3 was not assumed to play an important role.

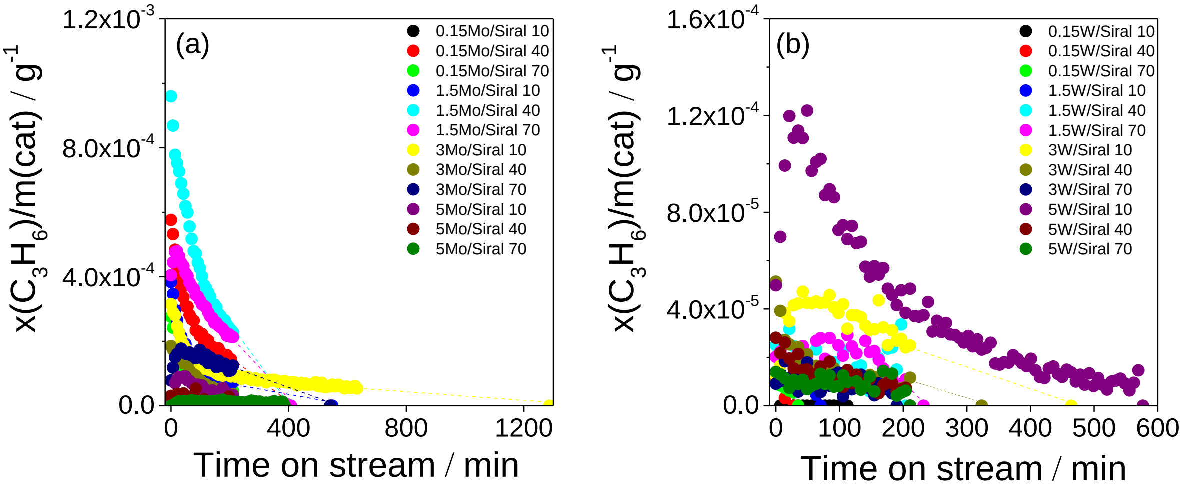

Figure S7 Change of molar fraction of registered propene related to catalyst amount with time on ethylene stream for (a) Mo-containing and (b) W-containing catalysts.

References

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