Supporting Information

Active Sites in Olefin Metathesis over Supported Molybdena Catalysts

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Figure S1. Time trend of the propene metathesis activity of MoO x/SBA-15 normalized by BET surface area: (a) Fresh catalysts, and (b) regenerated catalysts. Reaction conditions: T = 323 K, contact time = 0.75 s g ml -1 , p = 0.1 MPa, neat propene. Pretreatment or regeneration: T = 823 K, 0.5 h in 20% O2-Ar, subsequent purge with pure Ar at 323 K.

Figure S2. Relationship between the propene adsorption microcalorimetry data and the density of active carbene (Mo=CHR) sites found after propene metathesis. a) Density of the Mo=CHR sites as a function of the initial heat of propene adsorption, and b) density of the Mo=CHR sites as a function of the density of propene adsorption sites exhibiting heat of adsorption higher than 30 kJ mol -1 . See also Figures 1, and 2b in the main text.
Figure S3. IR spectra of MoO<sub>x</sub>/SBA-15 recorded after ammonia dosing (7 hPa, 353 K) and subsequent evacuation for 1h. The catalysts were pretreated in O<sub>2</sub> (20 kPa) at 823 K for 0.5 h. Spectra before ammonia dosing were used as reference.

Figure S4. Profiles of temperature-programmed desorption of ammonia (NH<sub>3</sub>-TPD) for MoO<sub>x</sub>/SBA-15 at a heating rate of 10 K min<sup>-1</sup>. The similar profiles suggest no significant variation in average acid strength. The catalysts were pretreated in 20% O<sub>2</sub> in Ar at 823 K for 0.5 h, which was followed by ammonia adsorption at 353 K by feeding 1% NH<sub>3</sub> in Ar and subsequent purge in a He stream at 353 K for 0.5h.
Figure S5. Temperature programmed desorption (TPD) profile after propene metathesis over MoO\textsubscript{x}/SBA-15 (1.1 Mo atoms \textpercm\textsuperscript{2}). The concurrent occurrence of m/e = 58 and 43 with an intensity ratio of approximately 1:4 indicates desorption of acetone. Besides, desorption of propene (m/e 41) and butenes (m/e 55) was observed. Metathesis reaction conditions: $T = 323 \text{ K}$, contact time = 0.75 s g ml$^{-1}$, $p = 0.1 \text{ MPa}$, neat propene, 16 h of reaction time. Pretreatment: $T = 823 \text{ K}$, 0.5 h in 20% O\textsubscript{2}-Ar, subsequent purge with pure Ar at 323 K. Post-reaction TPD: ramp rate of 10 K min$^{-1}$ in Ar.

Figure S6. Raman (excitation at 1.96 eV) and IR spectra of MoO\textsubscript{x}/SBA-15 measured at 40°C after pretreatment in 20% oxygen at 823 K for 0.5 h. The bands at 993 and 816 cm$^{-1}$ in the Raman spectrum of 2.5Mo are due to small amount (ca. 3% of total Mo) of MoO$_2$ phase giving very intense signal due to its high Raman sensitivity.