

Electronic Supplementary Information

Fundamentals and application potential of synergy effect between ZnO and Mo/SiO₂ for propene production in the metathesis of ethylene and trans-2 butene

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Tables

Table S1 The surface area and the average size of crystallites of different ZnO.

Sample	Surface area / $\text{m}^2 \cdot \text{g}^{-1}$	Crystallite size / nm
a-ZnO	4	69.3
b-ZnO	35	10.3
c-ZnO	7	58.0

Table S2 Apparent activation energies of propene formation in the metathesis of ethylene with 2-butene determined in the temperature range from 100 to 200°C.

Sample	E_a , kJ/mol
Mo/SiO ₂	15.5
a-ZnO_dual-bed	94.3
a-ZnO-1	92.9
a-ZnO-5	105.8
a-ZnO-10	100.1
a-ZnO-20	99.9
a-ZnO-50	104.0
a-ZnO-100	88.1

Figures

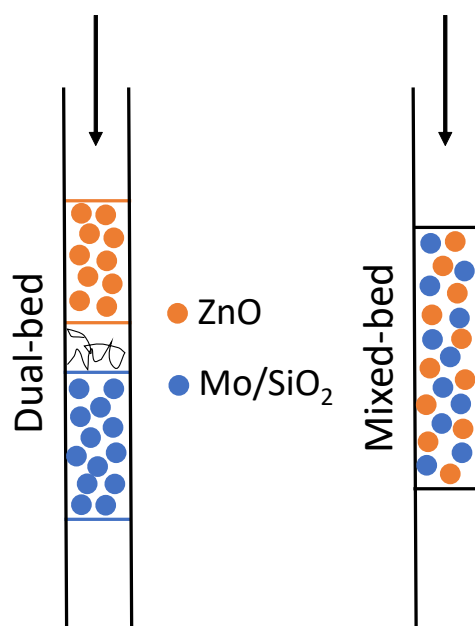


Figure S1 A schematic representation of reactor configurations with different integration manners for ZnO and Mo/SiO₂.

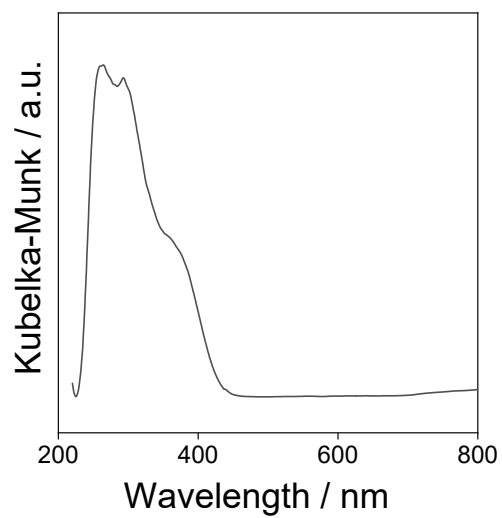


Figure S2 The UV-vis spectrum of Mo/SiO₂ at room temperature after catalyst treatment in air at 500°C for 1 h.

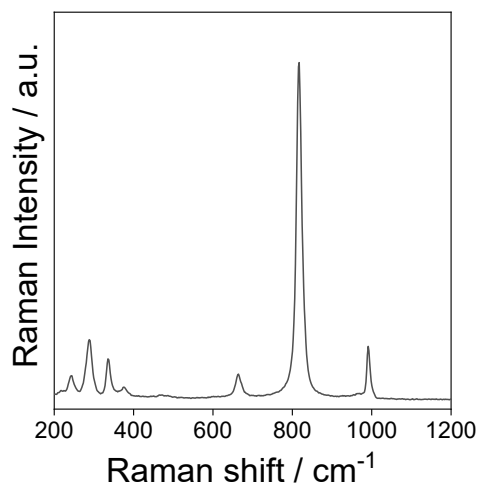


Figure S3 The Raman spectrum of Mo/SiO₂ at room temperature after catalyst treatment in air at 500°C for 1 h.

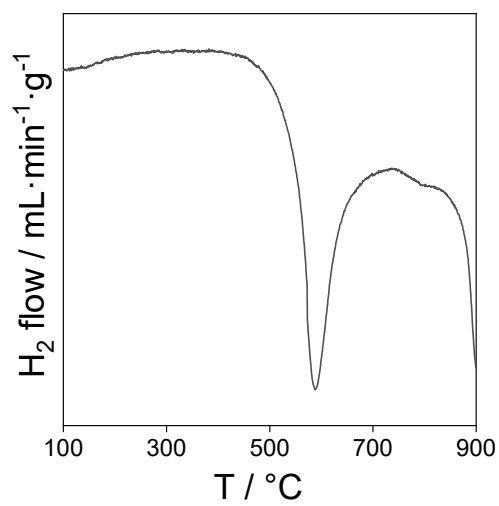


Figure S4 The profile of outlet H₂ flow in temperature-programmed reduction of Mo/SiO₂ with 5vol% H₂ in Ar.

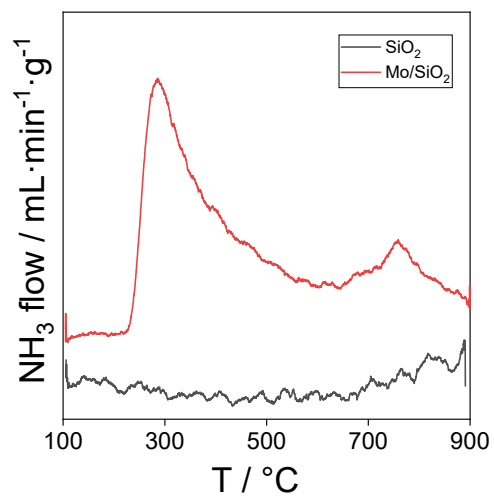


Figure S5 The profile of outlet NH₃ flow in temperature-programmed desorption of NH₃ from Mo/SiO₂ or bare SiO₂.

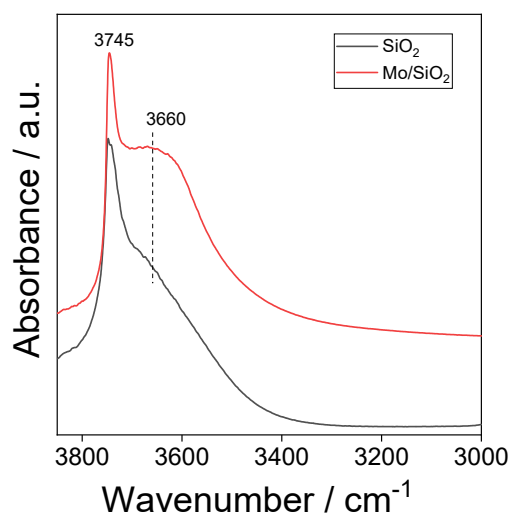


Figure S6 *In situ* DRIFT spectra of Mo/SiO₂ and bare SiO₂. The spectra were recorded at 150°C after treatment of the samples in air at 450 °C for 1h.

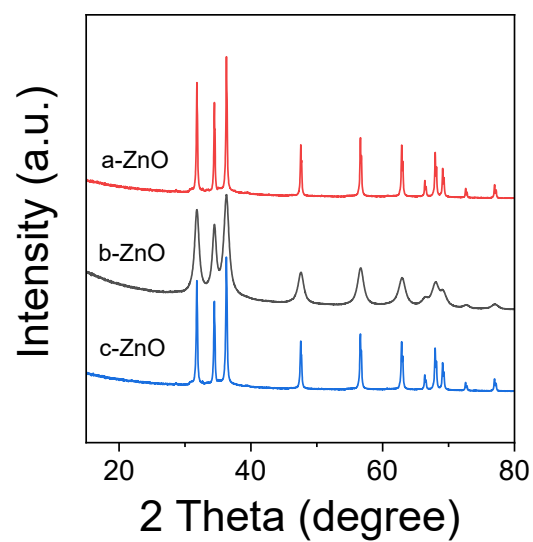


Figure S7 XRD patterns of a-ZnO, b-ZnO and c-ZnO.

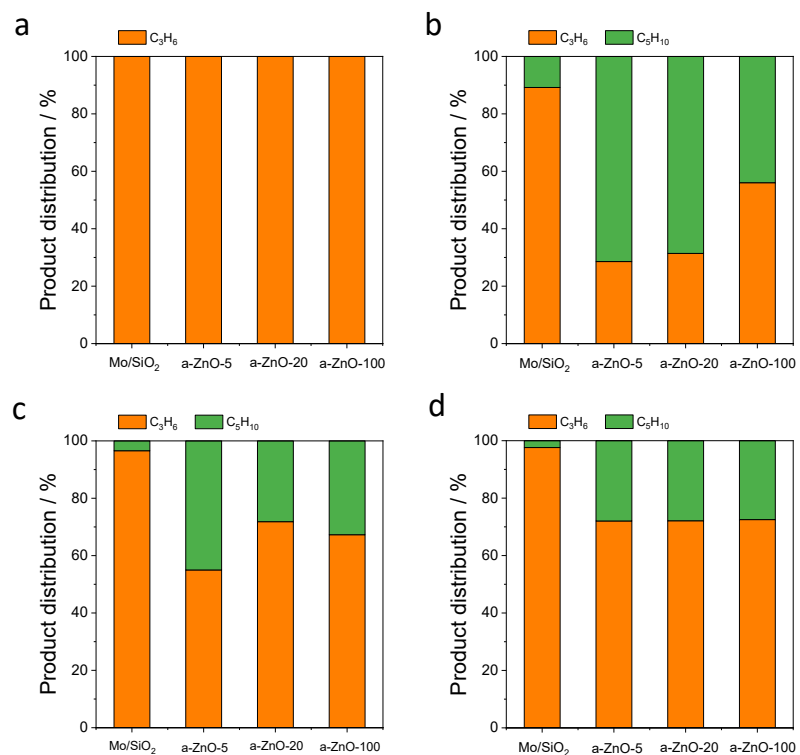


Figure S8 The effect of the presence of a-ZnO and the weight ratio of a-ZnO to Mo/SiO₂ on product distribution at (a) 50°C, (b) 100°C, (c) 150°C and (d) 200°C.

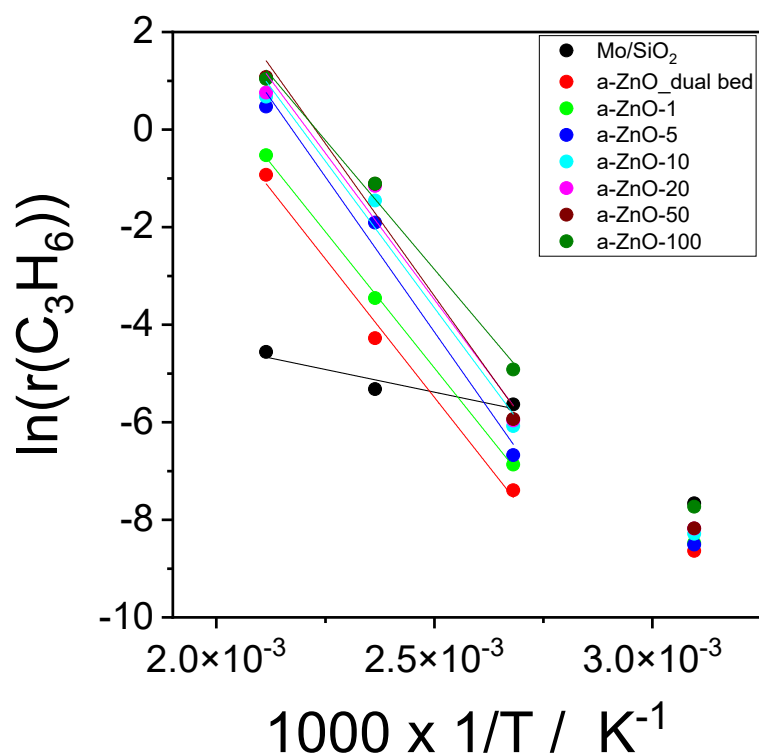


Figure S9 Arrhenius plots of the rate of propene formation in the metathesis of ethylene with 2-butene over Mo/SiO₂ and different Mo/SiO₂-ZnO combinations. Reaction conditions: T=50 – 200° C, feed composition: C₂H₄/trans-2-C₄H₈/N₂=5/5/1. The activation energy was calculated for the temperature range between 100 and 200°C.

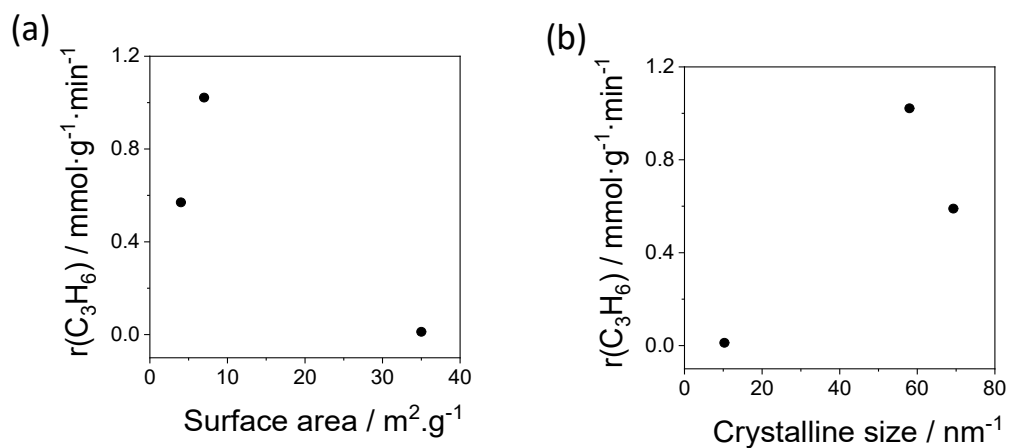


Figure S10 The dependences of the rate of propene formation over physically mixed Mo/SiO₂ and ZnO (the weight ratio of ZnO to Mo/SiO₂ of 1:1) at 200°C on (a) the specific surface area of ZnO and (b) the size of crystallites of ZnO.

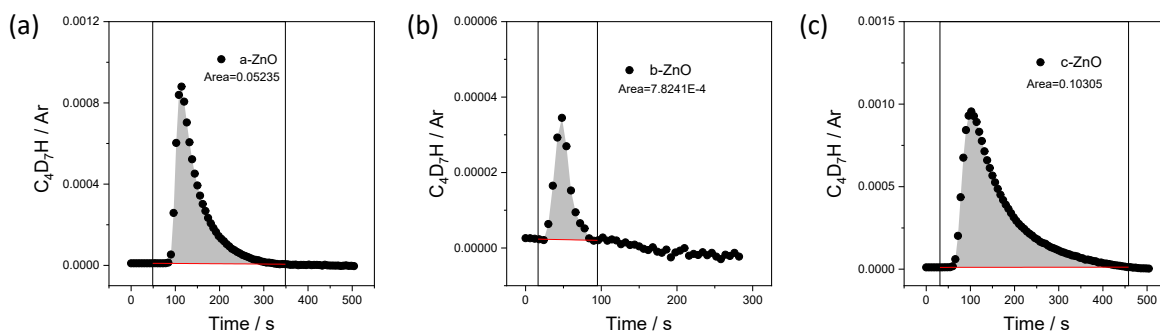


Figure S11 MS signal of C_4D_7H ($m/z=63$) collected during the H-D experiments with different ZnO samples using C_4H_8 - and 2- C_4D_8 -containing feeds.