Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

DFT Studies of Selective Oxidation of Propene on MoO_3(010) Surface

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Path 1-a3

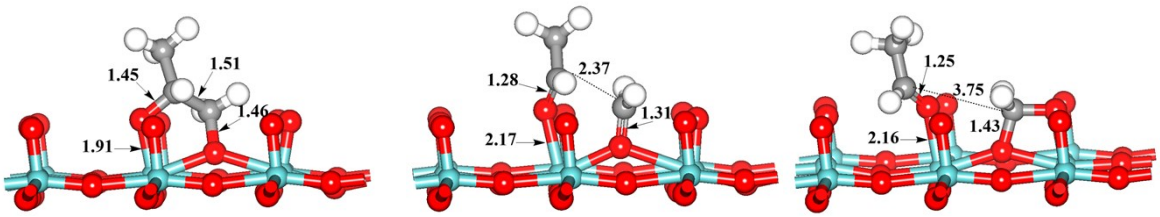
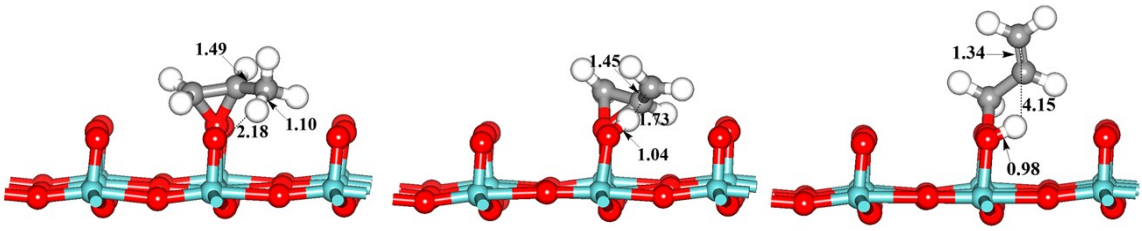


Fig. S1 C-C bond cleavage from the di-σ bonded propene.

Path 1-b1



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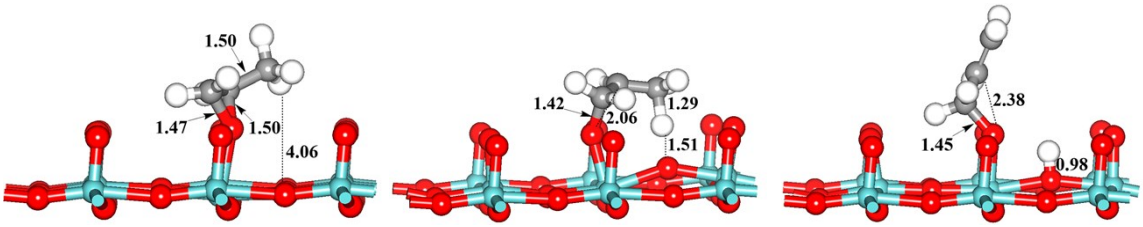
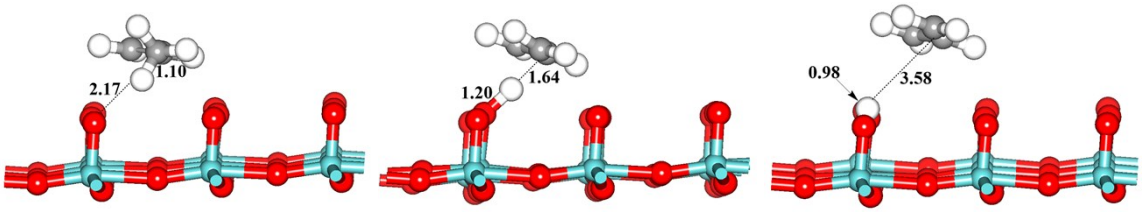


Initial State Transition State Final State

Fig. S2 Dehydrogenation from the π-bonded propene.

Path 1-c1



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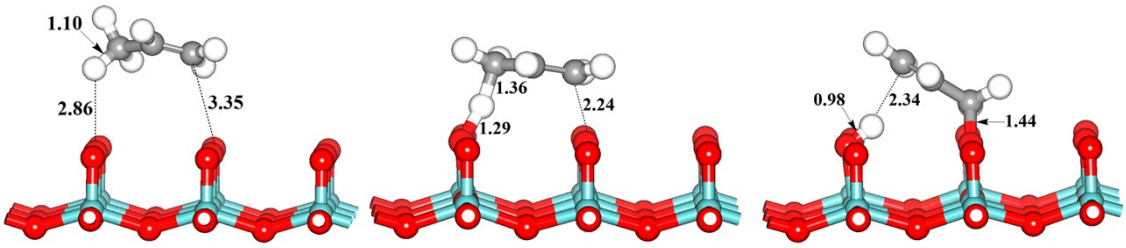
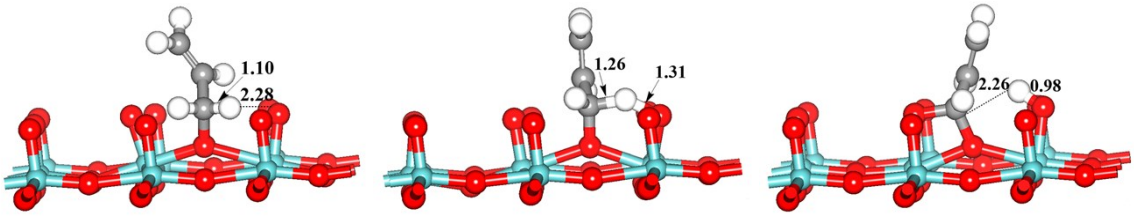


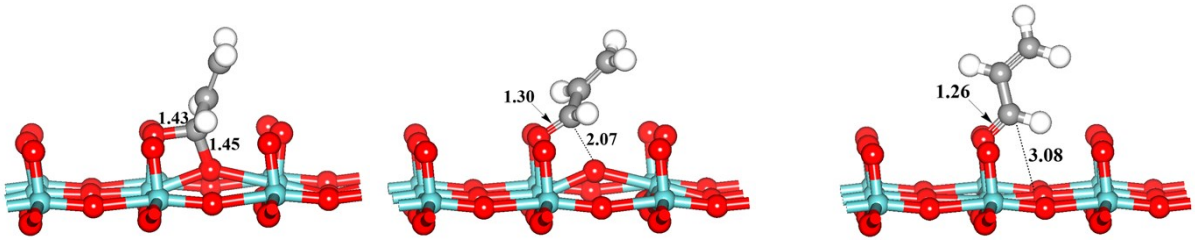
Initial State Transition State Final State

Fig. S3 The first hydrogen abstraction from physically-adsorbed propene.

Path 2-b1



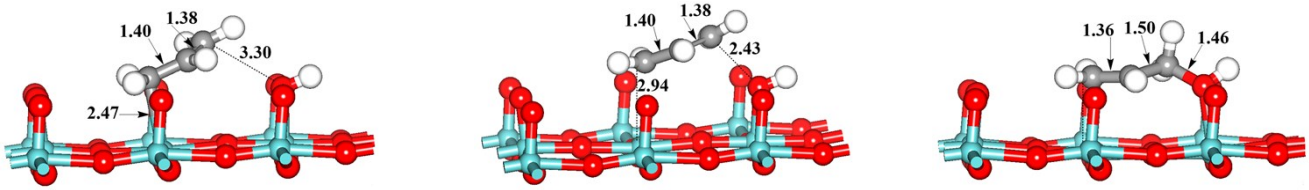
Path 2-b2



Initial State Transition State Final State

Fig. S4 Hydrogen abstraction of allyl on the asymmetric oxygen atom of MoO_3 (010) surface.

Path Def-a3



Initial State Transition State Final State

Fig. S5 Allyl migration from defective Mo atom to the hydroxyl group.

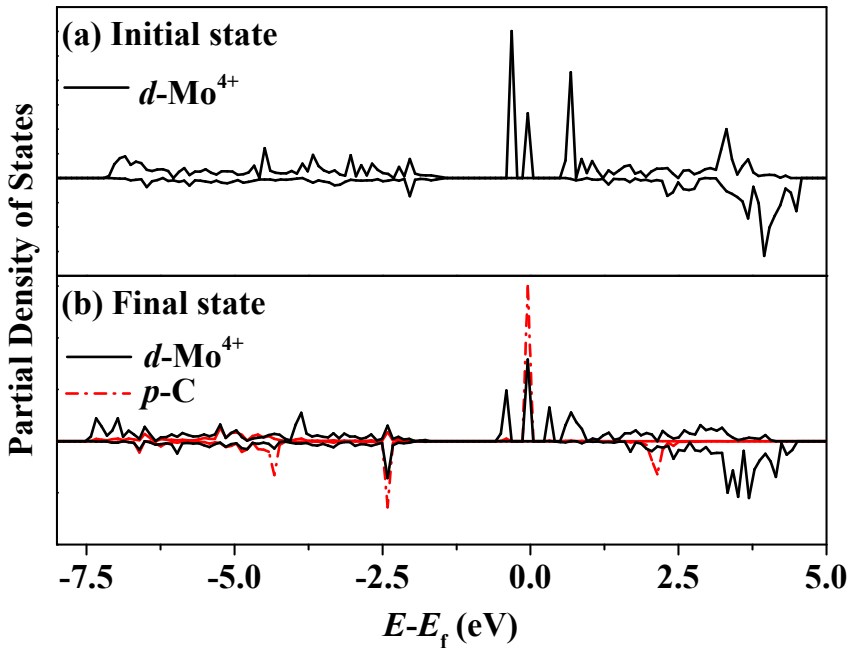


Fig. S6 The partial density of states for the initial state and final state in the first hydrogen abstraction of propene.