Supporting Information

The Role of H_2S Addition on Pt/Al_2O_3 Catalyzed Propane Dehydrogenation: A Mechanistic Study

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S1.The adsorption of sulfur species on Pt(111) and Pt(211) surfaces

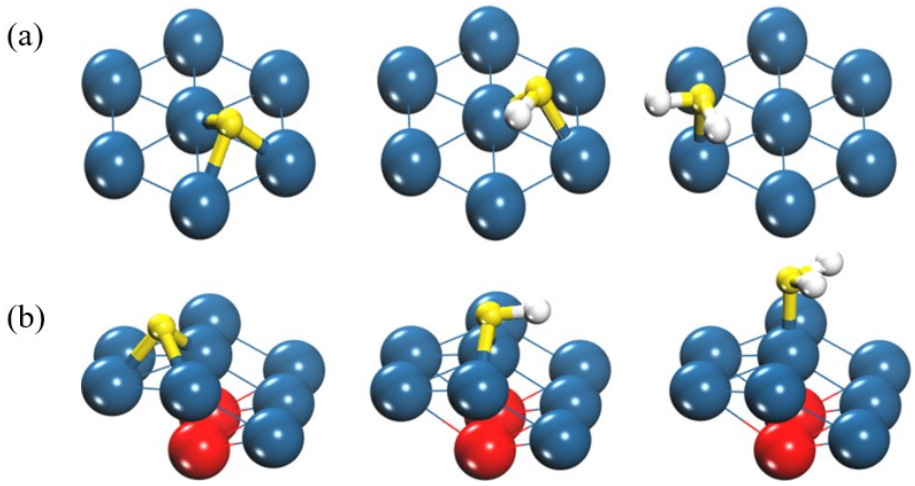

Figure S1. Configurations of sulfur species adsorbed on (a) Pt(111) and (b) Pt(211).

S2. Activation energies for elementary reaction steps

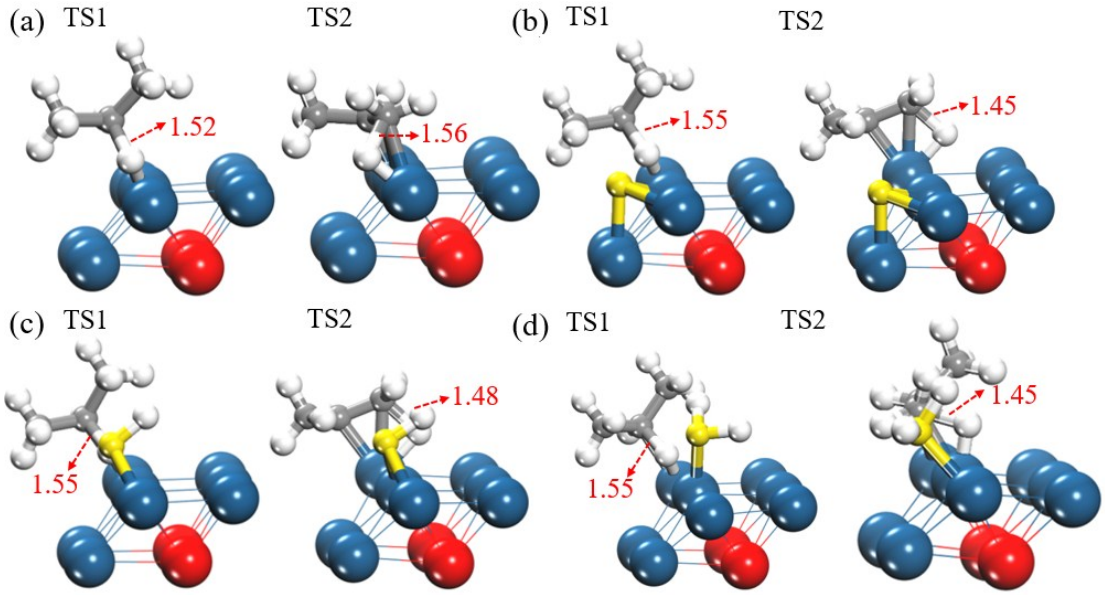

Figure S2. Transition state structures for PDH reaction over (a) the clean Pt(211) surface, (b) the Pt(211)&S surface, (c) the Pt(211)&SH surface, and (d) the Pt(211)&H_2S surface.

S3. The effect of hydrogen on catalytic performance for PDH

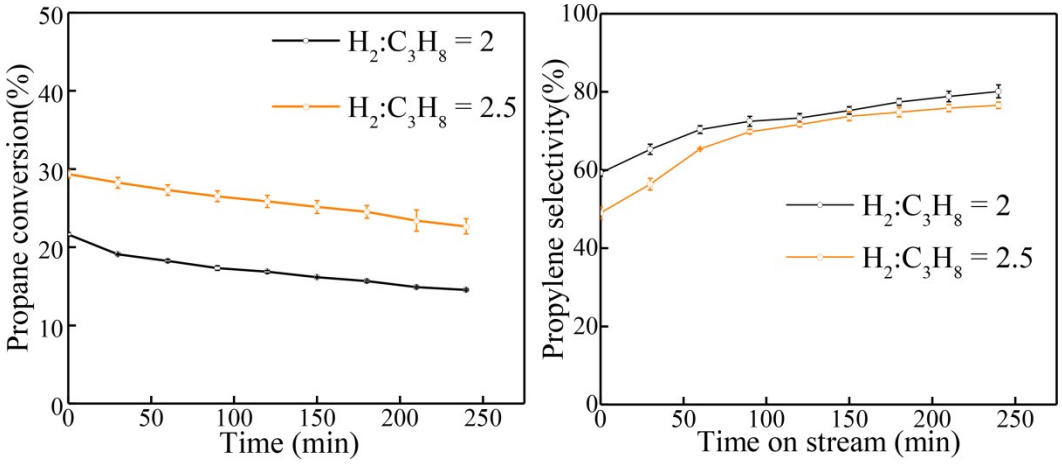

Figure S3. (a) Propane conversion and (b) propylene selectivity of Pt/θ-Al_2O_3 with different molar ratios of H_2 to propane in the reaction feed. Reaction conditions: 0.1 g catalyst, P_t = 1 atm, and T = 575 °C.