

Supporting Information for

Partial Hydrogenation of 1,3-Butadiene on Hydrogen-Precovered Pd(110) in the Balance of π -bonded C₄ Hydrocarbon Reactions

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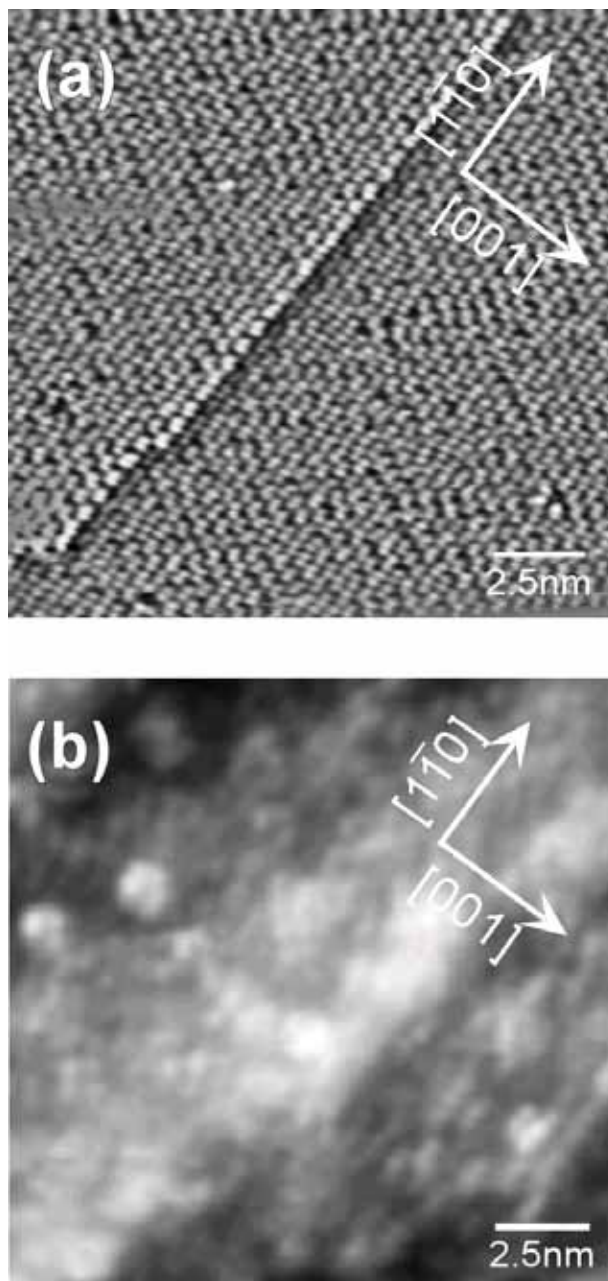


Figure S1. STM images of 1,3-butadiene adsorbed on H(1.0 ML)/Pd(110) surface at 100 K, followed by heating to (a) 130 K (below the decomposition temperature of 1,3-butadiene) and (b) 450 K (above the decomposition temperature of 1,3-butadiene). Both STM images were obtained by the constant current mode with the tunneling current of 0.9 nA and sample bias of -100 mV.

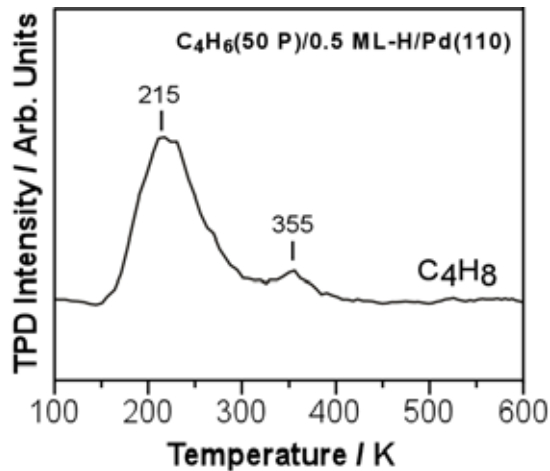


Figure S2. TPD spectrum of butene (C_4H_8) obtained from 1,3-butadiene (C_4H_6) adsorbed on less hydrogen-preadsorbed Pd(110) surface, i.e., H(0.5 ML)/Pd(110). The spectrum was obtained at the heating rate of 6 K/s. The peak appeared at 215 K is assigned to the interaction with pre-adsorbed hydrogen atoms. On the other hand, the desorption peak appeared at 355 K is assigned to self-hydrogenation of 1,3-butadiene, which is close to the decomposition temperature of 1,3-butadiene. The intensity of latter peak is decreased when TPD experiments were performed at higher H coverages (as shown in Figure 5(a)).

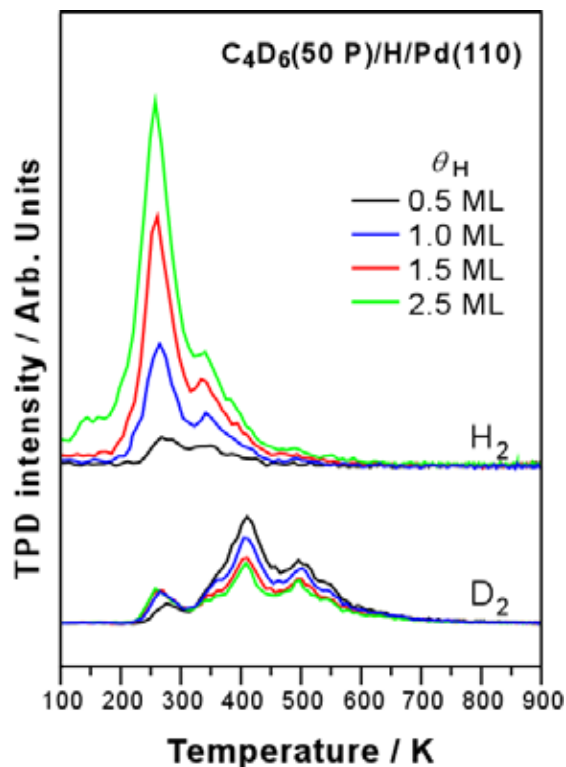


Figure S3. TPD spectra of hydrogen (H_2 and D_2) obtained from deuteride 1,3-butadiene (C_4D_6) adsorbed on $\text{H}(0.5, 1.0, 1.5 \text{ and } 2.5 \text{ ML})/\text{Pd}(110)$ surface. All spectra were obtained at the heating rate of 6 K/s. We have used deuteride 1,3-butadiene (C_4D_6) to discriminate between the hydrogen desorption from pre-adsorbed hydrogen atoms and that from the 1,3-butadiene decomposition. The peak observed at 260 K in H_2 desorption spectra is assigned to the hydrogen desorbed from the subsurface (β_1 state) site. The intensity of the desorption peak at 260 K was monotonously increased with increasing the coverage of pre-adsorbed H, suggesting that excess hydrogen were desorbed from the subsurface site. The desorption peak at 260 K was decreased when 1,3-butadiene coverage was increased and hydrogen coverage retained constant, which suggests that subsurface hydrogen atoms react with 1,3-butadiene. Meanwhile, the decrease in the desorption amount of D_2 with increasing the H coverage can be explained by the unreacted 1,3-butadiene molecules remained on the surface below decomposition temperature.