Coverage and location of hydrogen for understanding ultra-small

Pt nanoparticles towards 1,3-butadiene hydrogenation

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Supporting Information



Fig. S1. Energy reaction profiles for hydrogenation of 1,3-butadiene with tetra- σ and di- π structures to 1B4R, and the optimized structures of reactants, transition states, and products involved.



Fig. S2. The co-adsorption of β -C₄H₉ with H atom on different site.