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 $\beta$-C$_4$H$_9$ with H atom on different site.