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Essential role of CO coverage in CO<sub>2</sub> hydrogenation over Pt(111)

We show that CO and hydrogen can be deposited on Pt(111) during CO<sub>2</sub> hydrogenation and the reaction will proceed by maximizing the adsorption free energy of CO and hydrogen. The role of CO coverage is manifested in two aspects. First, the CH-CO coupling and CH hydrogenation are facilitated by the increase of CO coverage. Second, the adsorption of CO on Pt(111) makes the coadsorbed H relatively positively charged, which is favorable for the H-assisted dehydroxylation of CHOH that produces CH, a key intermediate for the production of C<sub>2</sub>H<sub>5</sub>OH or CH<sub>4</sub>.

As featured in:



See Yongjie Xi, Fuwei Li *et al.*,  
*Catal. Sci. Technol.*, 2023, **13**, 6153.