First-principles design of effective catalysts for dehydrogenation of LOHC

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Developing effective dehydrogenation catalysts is important for liquid organic hydrogen carrier development. In this study, dehydrogenation performance of perhydro-dibenzyltoluene on subsurface alloys of Pt/M/Pt(111) (M = Pd, Cu, and Ni) was assessed using first-principles calculations. The detailed dehydrogenation mechanism of perhydro-dibenzyltoluene over each catalyst, including the rate-determining step (RDS) was systematically elucidated. In addition, the effect of strain applied to catalysts on dehydrogenation was investigated. More importantly, a practical descriptor for predicting dehydrogenation activity was proposed in this study. Overall, these studies will be valuable for designing effective LOHC-dehydrogenation catalysts.