Supporting Information

First-Principles Study of Electronic Structure and Hydrogen Adsorption of 3d-Transition Metal Exposed Paddle Wheel Frameworks

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**Figure S1.** Comparison of local density of states (LDOS) for Co$_2$-(HCOO)$_4$ and Co$_2$-TBC before and after the dihydrogen adsorption. The Fermi level is marked by the dashed line. The projected H$_2$ and TM$_2$ states are represented by the red and black solid lines, respectively.
Figure S2. Initial dihydrogen binding configurations of Co$_2$-TBC: (a) and (b) are side-on fashion, while (c) is on-top. Cobalt, carbon, oxygen, and hydrogen are depicted in cyan, grey, red, and white, respectively.
Figure S3. Local density of states (LDOS) of Sc2-PW before and after the dihydrogen adsorption. The Fermi level is marked by the dashed line. The projected H\textsubscript{2} and TM\textsubscript{2} states are represented by the red and black solid lines, respectively.
Figure S4. Local density of states (LDOS) of V$_2$-PW before and after the dihydrogen adsorption.
Figure S5. Local density of states (LDOS) of Mn2-PW before and after the dihydrogen adsorption.
Figure S6. Local density of states (LDOS) of Ni$_2$-PW before and after the dihydrogen adsorption.
Figure S7. Local density of states (LDOS) of Cu$_2$-PW before and after the dihydrogen adsorption.