

Modification of the Pd surface electronic structures for selective hydrogen production from formic acid

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Catalysts that are highly selective and active for H₂ production from HCOOH decomposition are indispensable to realize HCOOH-based hydrogen storage and distribution. In this study, we identify two effective routes to promoting the Pd catalyst for selective H₂ production from HCOOH by investigating the effects of early transition metals (Sc, Ti, V, and Cr) incorporated into the Pd core using the density functional theory calculations. First, the asymmetric modification of the Pd surface electronic structure can be an effective route to accelerating the H₂ production rate. Second, in-plane lattice contraction of the Pd surface can be an effective route to suppressing the CO production. The unraveled atomic-scale factors underlying the promotion of the Pd surface catalytic properties provide useful insights into the efforts to overcome limitations of current catalyst technologies in making the HCOOH-based H₂ storage and distribution economically feasible.