The First-Principles approach to the interplay of Ligand Effect and Strain Effect in Enhanced Dehydrogenation of HCOOH on the Bimetallic M-Pd Core-Shell Catalyst

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Formic acid (HCOOH) is a low-toxic chemical that can be easily stored, transferred, and handled. Currently, it was found that among the noble metal catalysts, the activity for the H_2 production via HCOOH decomposition is enhanced on Pd catalysts, however, the selectivity to H_2 production is still to be improved. To solve such issue, the bimetallic alloy Metal-Pd Core-Shell has been proposed to improve both the catalytic activity and selectivity of Pd toward H_2 production from HCOOH decomposition. In this work, we constructed metal core, such as Ir, Pt, Au, Cu, Ag and Rh with the monolayer Pd-Shell. Our results indicate that Pdmono/Cu (111) has the best H_2 productivity and selectivity, due to the drastic transfer of charge from Cu-core to the surface Pd atoms, which ultimately modifies the electronic structure of the Pd-shell. Moreover, the electronic structure of the Pd-shell is changed by synergistic effect of the compressive strain effect and the ligand contribution. This work hints on the importance of properly engineering the surface activity of the M-Pd core-shell catalysts by the interplay between ligand and strain effects.