

Role of heteronuclear interactions in selective H<sub>2</sub> formation from HCOOH decomposition on bimetallic Pd/M (M= late transition FCC metal) catalysts

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Formic acid (HCOOH) serves as a potential source of hydrogen since it is a low-toxicity chemical that can be easily stored and handled. HCOOH may decompose via dehydrogenation or dehydration, depending on the reaction conditions. It was found that the activity of the noble metal catalysts for the H<sub>2</sub> production via HCOOH decomposition was superior on Pd. Since the CO generated from HCOOH dehydration can poison the Pd-based electrode in a fuel cell, a highly selective catalyst toward HCOOH dehydrogenation is required and such desired selectivity can be obtained by modifying the chemical and physical properties of surface by adopting Pd shell based core-shell alloy catalysts in order to maintain the Pd surface features in such configuration. In this presentation, via Density functional theory (DFT) calculation, we revealed a fundamental mechanism towards the bimetallic Pd/M (M= Ag, Cu, Rh, Pd, Ir, Pt, Au) to find the most economical use of rather expensive noble metal and most importantly to further understand a role of alloying effect. Finally, physical and chemical intuition for the next generation bimetallic catalyst is also discussed.