Role of Pd ensemble in hydrogen production from formic acid decomposition on Ag@PdAg core-shell catalysts

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Formic acid is one of the most promising hydrogen sources for low-temperature fuel cell applications, due to its high hydrogen capacity. In this study, we have elucidated the role of Pd ensembles in determining the activity of the hydrogen production from formic acid decomposition on $Ag@Pd_{16-x}Ag_x$ (x = 0, 2, 4, 8, 12) catalysts, by using density functional theory calculations. We found that the catalysis of HCOOH decomposition strongly depends on the ratio and the arrangment of Pd atoms in $Pd_{16-x}Ag_x$ surfaces, which modulates the binding energies of *H and *HCOO differently during the first step of the reaction. The higher the ratio of Pd atoms and the more Pd is gathered together on the surface, the activity of H_2 production becomes higher and $Ag@Pd_{14}Ag_2$ showed the highest activity owing to its appropriately modulated binding energies of intermediates. Our results provide a valuable clue in designing highly active catalysts, which can exhibit better catalytic performance by forming the appropriate surface Pd ensembles on Pd-Ag bimetallic catalysts.