First-principles design of Pd-based alloy catalysts for H_2 production from HCOOH decomposition

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Multi-metallic catalysts have been found to significantly increase catalytic efficiency, compared to the monometallic counterparts. This enhancement can be attributed to various alloying effects: i) the existence of unique mixed-metal surface sites [the so called ensemble (geometric) effect]; ii) the modification of electronic state due to metal-metal interactions [the so called ligand (electronic) effect]; and iii) strain caused by lattice mismatch between the alloy components [the so called strain effect]. In addition, the presence of low-coordination surface atoms and preferential exposure of specific facets in association with the size and shape of nanoparticle catalysts [the so called shape-size-facet effect] can be another important factor for modifying the catalytic activity. In this talk, I will present the underlying principles that govern catalytic reactions (such as formic acid decomposition) occurring on Pd-based multi-metallic catalysts using the first-principles density functional theory calculations. This work highlights the importance of knowing how to properly tailor the surface reactivity of multi-metallic catalysts for achieving high catalytic performance.