

Role of Pt atoms on Pd(111) surface in the direct formation of hydrogen peroxide: catalytic experiments and DFT calculations

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Pd-Pt catalysts have been studied for improvement of selectivity in direct formation of hydrogen peroxide, but the roles of Pt has not yet been identified. Therefore, we investigated the roles of Pt atoms on Pd(111) surface and realized the surface in two methods: nano-catalyst synthesis and density functional theory (DFT) calculation model. Modification of Pd(111) surface was conducted to make 3 kinds of Pd-Pt-alloyed surfaces, a minor Pt-substituted Pd, a major Pt-substituted Pd and a Pt-shell Pd. Reaction tests of the minor Pt-substituted Pd(111) had the highest peroxide selectivity, production rate and the lowest peroxide decomposition rate. These are consistent with the lowest activation barrier for the O<sub>2</sub> hydrogenation step and the highest one for the H<sub>2</sub>O<sub>2</sub> dissociation step on the minor Pt-substituted Pd. We also suggested the electronic property of surface in terms of the DOS distribution of the d-band electrons and the surface bader charge in the DFT region. It is regarded that we succeeded in producing a target nanoparticle with convincing experimental results by controlling the adsorbates, furthermore making the correlation between experimental and calculational results.