Pd nano-octahedron with Pt doped from Galvanic replacement for direct synthesis of H_2O_2

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Currently, for commercial production of H_2O_2, which is used as an oxidant in broad industrial applications, direct synthesis of H_2O_2 from H_2 and O_2 was proposed as a solution to replace the conventional AO process because of its several advantages that it is an eco-friendly and economical method for small-scale production of H_2O_2 and immediate supply of H_2O_2 as an oxidant for another on-site process (e.g. DSHP-HPPO) is possible. However, the issue is the low selectivity of direct synthesis of H_2O_2 because it includes four spontaneous reactions including three ways of side reactions.

DFT calculations can demonstrate structural effects of nanoparticle by simulating a reaction on specific structure of atoms, and the DFT results are realized by performing the experiment with the synthesized nanoparticle. A previous series of DFT calculations showed that Pd {111} facet is more effective in direct synthesis than Pd {100} facet [1] and this simulation was realized by an experimental result that Pd nano-octahedrons enclosed by {111} facets showed much higher H_2O_2 selectivity and productivity than Pd nanocubes enclosed by {100} facets did [2]. In addition, according to previous studies about Pd and Pt catalysts, when a small amount of Pt was added to Pd, H_2O_2 selectivity and productivity considerably increased as a result of electron transfer of Pd atoms affected by Pt atoms [3].

In this research, (1) we simulate direct synthesis of H_2O_2 on Pd {111} surface which is doped with Pt atoms using DFT calculations, then (2) realize the simulation by synthesizing Pt-doped Pd nano-octahedron and performing activity tests as observing how H_2O_2 selectivity/productivity change as Pt/Pd ratio increases (3) to find the optimal Pt/Pd ratio on the octahedron. To replace Pd atoms on the surface of octahedrons with Pt atoms, we performed Galvanic replacement reaction because standard reduction potential of Pd^{2+} is lower than one of Pt^{2+}. As shown in Figure 2, Pd nano-octahedrons with Pt doped from Galvanic replacement (Figure 1) showed H_2O_2 productivity almost twice as high as Pd nano-octahedrons did.

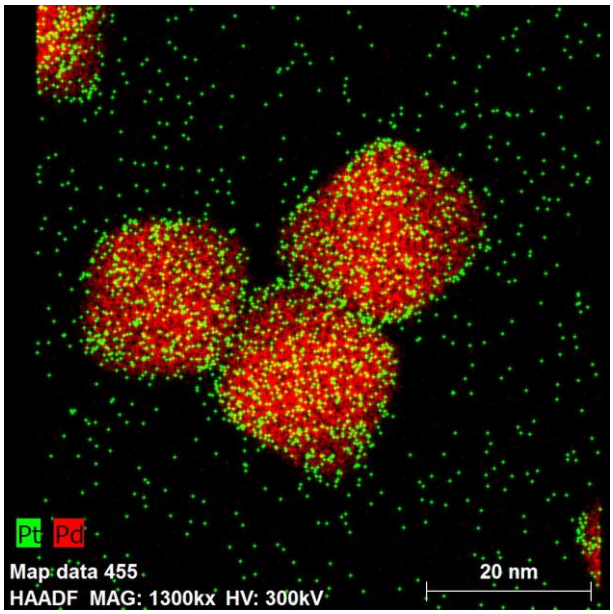

Fig.1 A HAADF-STEM map data of Pt-doped Pd nano-octahedron.

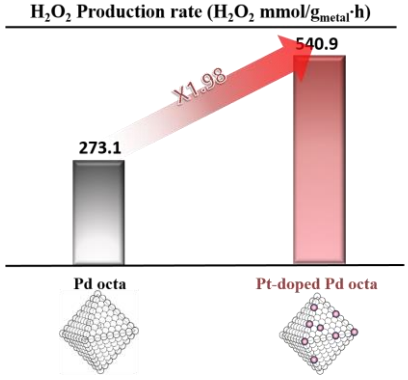

Fig.2 H_2O_2 production rates of Pd octahedron and Pt-doped Pd nano-octahedron.

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