Catalytic activity of {111}-facet-enclosed Pd nanoparticles for the direct synthesis of hydrogen peroxide from hydrogen and oxygen

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In this work, we studied the use of octahedral Pd nanoparticles in the direct synthesis of hydrogen peroxide by oxidation of hydrogen with molecular oxygen. {111}-facet-enclosed Pd octahedrons with different sizes (7.5, 13, 18, 26 nm in edge length) were synthesized via seed-mediated growth of the Pd nanocube. It is well known that the Pd {111} facet is more favorable than {100} facet in hydrogen peroxide synthesis. It was expected that the Pd {111} facet would be inferior to the Pd {100} facet in dissociation of O-O bonds in O2, OOH, and HOOH. In the reaction test, we have confirmed that the hydrogen peroxide productivity increased with decreasing Pd nanooctahedron size. The fraction of {111} terrace atoms increased as the Pd octahedron size decreased (26, 18, 13, 7.5 nm) and this affect the higher hydrogen peroxide productivity. So, it is thought that catalyst with selective exposure of Pd {111} facet with various size is one of a design strategy for the direct synthesis of hydrogen peroxide from hydrogen and oxygen.