

Understanding the mechanism of H_2O_2 direct synthesis from H_2 and O_2 via H_3O^+ ion using DFT calculation

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Hydrogen peroxide (H_2O_2) is a green oxidant used in various industrial applications. Direct synthesis of hydrogen peroxide (DSHP) which exclusively produces water as a by-product can be a potential alternative to the auto-oxidation of anthraquinone. However, productivity of DSHP has not surpassed the current process due to its low H_2O_2 selectivity. Thus, enhancing H_2O_2 selectivity has been a major challenge.

Palladium(Pd)-based catalysts are most effective in DSHP due to its superior H_2 conversion and fine H_2O_2 selectivity compared to those of other catalysts. Several studies have been conducted on the effects of the morphology, size, and alloying of Pd-based catalysts to improve the H_2O_2 selectivity.

In particular, it is reported that H^+ in reaction medium promotes hydrogenation in DSHP mechanisms in terms of proton-electron transfer. Herein, we tried to figure out reaction mechanisms and energetics of DSHP via H_3O^+ on Pd surface using density functional theory (DFT) calculation.