

Br effect on different Pd surfaces in H₂O₂ direct synthesis이민우¹, 이관영^{1,2,†}¹고려대학교; ²KU-KIST Green school

H₂O₂ is a well-known green oxidant used in industrial applications. Direct synthesis of H₂O₂ from H₂ and O₂ which produces only water as a byproduct can be a promising process. However, productivity of direct synthesis has not surpassed the existing process. Thus, enhancing selectivity in the reaction has been widely studied to commercialize this process.

V. R. Choudhary et al. revealed that incorporation of Br in the Pd catalysts promoted the H₂O₂ selectivity compared to other halogen species. T. Deguchi et al. confirmed that adsorption energy of Br on the Pd cluster was the strongest among halogen species. These studies indicate that Br with the strongest adsorption results the enhanced H₂O₂ selectivity. They also showed that Br adsorbed at the edge site of the Pd cluster rather than at the terrace site. It is suggested that Br blocks the site with low selectivity, thus improves H₂O₂ selectivity.

In our study, we tried to compare the effect of Br on different Pd surfaces using DFT calculation. We found that Br not only blocks the (1 0 0) surface with low selectivity, but also improves the selectivity of (1 0 0) surface by structural effect.