Alternative mechanism of H_2O_2 direct synthesis from H_2 and O_2 via H_3O^+ ion in acidic medium

이민우, 이관영†
고려대학교
(kylee@korea.ac.kr†)

H_2O_2 is a well-known green oxidant used in industrial applications. Direct synthesis of H_2O_2 from H_2 and O_2 which produces only water as a byproduct can be a promising process. Direct synthesis of H_2O_2 are composed of following reactions; $H_2+O_2 \rightarrow H_2O_2$, $H_2+1/2O_2 \rightarrow H_2O$, $H_2O_2 \rightarrow H_2O+1/2O_2$, and $H_2O_2+H_2 \rightarrow 2H_2O$. Since all of those reactions occur spontaneously, developing a catalyst with high H_2O_2 selectivity has become a challenge for researchers. Palladium(Pd)-based catalysts has been adopted to direct synthesis of H_2O_2 due to its superior hydrogenation/dehydrogenation ability. Moreover, Pd showed fine H_2O_2 selectivity since it inhibits H_2O_2 decomposition via O-O bond dissociation. Additionally, acidic conditions in reaction medium is known to enhance H_2O_2 selectivity. As several researchers suggested that H^+ ions may take part in the reaction in terms of proton-electron transfer. Herein, we tried to figure out alternative mechanism of H_2O_2 synthesis on Pd (111) surface in acidic medium using DFT calculation.