DFT calculation for highly selective Pd/rutile catalyst in direct synthesis of H_2O_2.

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Direct synthesis of H_2O_2 from H_2 and O_2 has been attracted an attention owing to its simple process and use of eco-friendly solvents compared to commercial process. Reaction pathways are composed of following reactions; 1) $H_2 + O_2 \rightarrow H_2O_2$, 2) $H_2 + 1/2O_2 \rightarrow H_2O$, 3) $H_2O_2 \rightarrow H_2O + 1/2O_2$, and 4) $H_2O_2 + H_2 \rightarrow 2H_2O$. 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. TiO_2 support is widely known for its reducibility and strong metal-support interaction (SMSI) with various noble metal catalysts. In our work, we found out Pd metal supported on rutile TiO_2 showed an outstanding catalytic performance. It is expect that Pd^{4+} (PdO_2) species observed on Pd/rutile surface caused a high selectivity. Herein, we tried to figure out an energetics of H_2O_2 synthesis on PdO_2/rutile surface by density functional theory (DFT) calculation.