

**pH-Dependent Peroxidase Mimicking Activity of M-doped CeO<sub>2</sub> (M=Co, Fe, Zr): A DFT Study**

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Peroxidases (PODs) catalyze the conversion of chromogenic substrates (e.g., TMB) into colored product through the reduction reactions of hydrogen peroxide, and they have been used widely in biosensing and detection. However, due to their intrinsic limitations, such as high cost, low stability and difficulties in recovery and storage, the enzyme mimics (so-called nanozymes) have been developed. Nanoceria has the potential as nanozymes due to its facile redox cycle and observation of the peroxidase mimetic behavior. In this work, density functional theory (DFT) calculations were performed to elucidate catalytic activity and mechanism of peroxidase-like reaction on CeO<sub>2</sub> and M-doped CeO<sub>2</sub> (M=Co, Fe, Zr) according to pH conditions. As a result, we found that Co-doped CeO<sub>2</sub> has high peroxidase-mimicking activity in a neutral pH condition. Our result will provide insight into the design of peroxidase-mimicking nanozyme catalysts.