

이론에 기반한 전기화학적 H₂O₂ 생산을 위한
고성능 단원자 촉매 개발

유종석[†]

서울시립대학교

(jsyoo84@uos.ac.kr[†])

The industrial production of H₂O₂ is heavily dependent on the anthraquinone process, which is a multi-step process that involves the organic solvent separation after the hydrogenation and subsequent oxidation of anthraquinone using expensive palladium catalysts. Therefore, an electrochemical route to H₂O₂ production under ambient conditions is highly desirable. In this study, first-principles calculations are employed to identify the optimized structure of the single-atom catalyst for the electrochemical reduction of water, which is then successfully synthesized and tested experimentally to result in the record-high activity of 2.8 mA/cm² at 0.65 V vs RHE with extremely high selectivity.