

### Effect of iridium dopant on reduction and exsolution of Ir@WO<sub>3</sub>

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Exsolution is one way to improve the efficiency (intrinsic activity) of catalysts. It can be useful for rare metal catalysts like iridium (Ir), which is good candidate for oxygen evolution reaction (OER) due to its high performance and stability despite of its high cost and scarcity. Using density functional theory calculations, we investigated Ir exsolution supported on WO<sub>3</sub>, which is well-used material as the support for other noble metals.

We studied room temperature monoclinic and tetragonal structure for WO<sub>3</sub>, and monoclinic structures for WO<sub>2.9</sub> and WO<sub>2</sub>. Ir extraction energy and oxygen vacancy formation energy of all structures were calculated to show that Ir dopant decreases the oxygen vacancy formation energy and Ir extraction energy was dramatically lowered in WO<sub>2</sub> structure compared with other structures. In addition, the addition of Ir induced the reduction and phase transition of WO<sub>3</sub> into WO<sub>2</sub>. In addition, it is found that there is a chain process from the reduction of WO<sub>3</sub> to Ir exsolution in Ir<sub>x</sub>W<sub>1-x</sub>O<sub>3</sub> system.