

# Hydrogen Production via Electrocatalysis: From Nanoclusters to Single Atoms

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## Extended Abstract

Water electrolysis powered by renewable energy sources represents a sustainable and environmentally-friendly way of producing “green” hydrogen that can be used to decarbonize the power and transport sectors as well as industry. Proton exchange membrane water electrolysis (PEM-WE), compared to conventional alkaline water electrolysis (AWE), shows many advantages such as more compact configuration, higher energy efficiency, larger current densities, higher H<sub>2</sub> purity, and dynamic flexibility of operation [1], and therefore shows substantial potential for green hydrogen production. However, the rapid degradation of catalysts in the strongly acidic and highly oxidative environment severely limit the materials of choice. By far, platinum group metal (PGM) catalysts are usually indispensable to be used to catalyze the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) for PEM-WE. To enable widespread deployment of PEM-WE technology, reducing the utilization of PGM in catalysts has become a pressing need given they are expensive, scarce and geographically unevenly distributed in the world.

In this presentation, our effort toward reducing PGM utilization for hydrogen production via water electrolysis will be presented. We developed one-pot hydrothermal synthesis of ultrafine IrRu intermetallic nanoclusters loaded on conductive, acid-stable, amorphous tellurium nanoparticle support (IrRu@Te) [2]. Benefiting from the large exposed electrocatalytically active surface of ultrafine IrRu clusters and the strong electronic coupling between IrRu and Te support, the as-obtained IrRu@Te catalysts show good catalytic performance for the OER in strong acidic electrolyte (i.e., 0.5 M H<sub>2</sub>SO<sub>4</sub>), requiring overpotentials of only 220 and 303 mV to deliver 10 and 100 mA cm<sup>-2</sup> and able to sustain continuous OER electrolysis up to 20 hours at 10 mA cm<sup>-2</sup> with minimal degradation. Moreover, IrRu@Te exhibits high specific activity, illustrating intrinsically better performance compared to that of unsupported IrRu and other commercial Ir and Ru based catalysts. It also demonstrates high mass activity of 590 A gIrRu<sup>-1</sup> at an overpotential of 270 mV. Furthermore, we managed to anchor IrRu nanoclusters on a MOF-derived carbon support (IrRu@CoNC) [3], which shows outstanding OER catalytic performance with high mass activities of 2041, 970 and 205 A gIrRu<sup>-1</sup> at an overpotential of 300 mV and can sustain continuous OER electrolysis up to 40, 45 and 90 hours at 10 mA cm<sup>-2</sup> with minimal degradation in 0.5 M H<sub>2</sub>SO<sub>4</sub>, 0.05 M H<sub>2</sub>SO<sub>4</sub> and PBS electrolytes, respectively, outperforming most Ir and Ru based OER catalysts reported in the literature. Furthermore, we will show our recent progress in preparing atomically dispersed PGM catalysts. The rhodium (Rh) single-atom catalysts exhibit a mass activity for HER more than 8 times higher than the benchmark Pt/C catalysts [4]. Moreover, the atomically dispersed Ru catalysts we developed recently show bifunctionality, being active for both HER and OER [5]. When used together with a bipolar membrane, overall water electrolysis can be accomplished at a low cell voltage saving substantial energy needed for electrolysis.

## References

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