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## Developing highly efficient Water-splitting Catalyst and Revealing the Mechanism using Rechargeable Battery Materials

Recent global warming and exhaustion of fossil fuels have accelerated advancements to develop renewable energy sources and its applications. Among various alternative energy sources, splitting water to generate hydrogen and oxygen molecules is an environmentally friendly solar-to-energy conversion method for hydrogen energy production. However, because of inferior performance, development of inexpensive water-oxidation catalyst is necessary. **Ref [1-5]**

### [Discovery on the role of Mn valency on oxygen evolution reaction catalysis]

Although intensive studies have explored the role of Mn in water oxidation, it has been difficult to understand whether the catalytic capability originates mainly from either the arrangement or the valency, since the structure of the catalyst changed significantly as the valency changed. To decouple these two factors, we selected a new pyrophosphate-based Mn compound as a model system. Notably, we observed that as the averaged oxidation state of Mn increases from 2 to 3, the catalytic performance enhanced. This study provides valuable guidelines for developing an efficient Mn-based catalyst with controlled Mn valency and atomic arrangement. Ref [1]

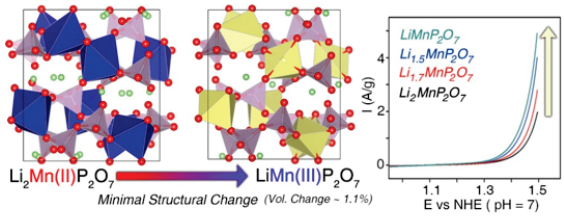


**Figure 1.** The effect of the Mn valency on oxygen evolution reaction catalysis. Ref. [1]

### [Development of efficient catalyst by changing the structure and revealing the mechanism]

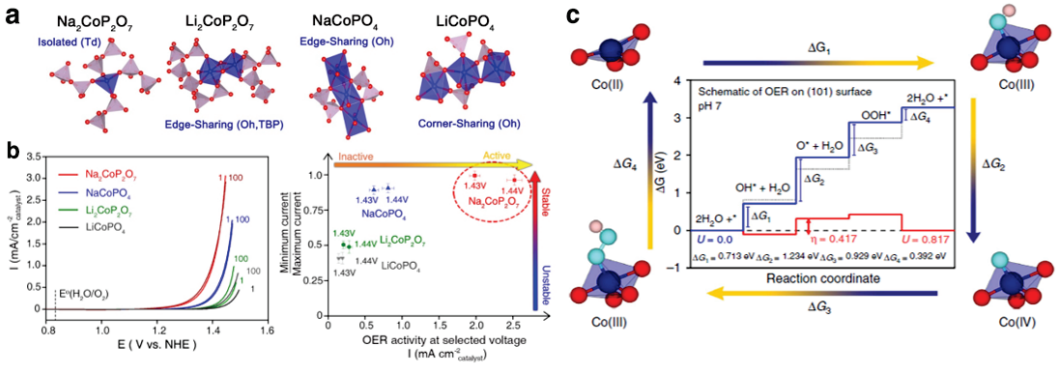


**Figure 2. (a)** Local structure of cobalt phosphate catalysts. **(b)** Oxygen evolution performances of cobalt phosphate catalysts. **(c)** Density functional theory calculation for OER mechanism of $Na_2CoP_2O_7$. Ref. [3]

Here, as a platform to better understand the effect of metal-coordination on the catalytic

ability, we selected four cobalt-based phosphate catalysts with various cobalt and phosphate-group coordination. Among them, $Na_2CoP_2O_7$ with distorted cobalt tetrahedral geometry shows high activity along with high structural stability. First principles calculations suggest that the surface reorganization induces a highly distorted tetrahedral geometry where water-molecules can favorably bind, resulting in a low overpotential (~0.42eV). Our findings emphasize the importance of local cobalt coordination in the catalysis and suggest the possible effect of polyanions on the water-oxidation chemistry. Ref [2]

**[Recent progress on multi-metal oxide catalysts for the oxygen evolution reaction]**

In water splitting, the use of multi-metal has been demonstrated to enhance the catalytic performance. Herein, we studied recent progress and accomplishments of multi-metal catalytic systems, including several important groups of catalysts along with the theoretical principles. Finally, we conclude by discussing remaining challenges to achieve further improvements of OER catalyst activities. Ref [3]

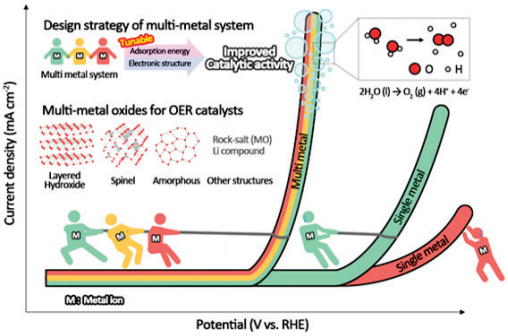


**Figure 3.** Strategies for the development of efficient multi-metal catalyst for the OER. Ref. [1]

I continuously have attempted to develop efficient water splitting catalyst with efficient rechargeable battery materials. I believe that this systematic approach can be extended to other chemical reactions which uses transition metals, and be a basis for the significant development in alternative energy area.

## References ( † denotes equal contributions )


[1] **H. Kim**† & J. Park† *et al.* ***Journal of American Chemical Society*** 136, 4201–4211 (2014)

[2] **H. Kim**† & J. Park† *et al.* ***Nature Communications*** 6, 8253 (2015)

[3] **H. Kim**†, J. S. Kim†, B. Kim†, K. Kang, ***Advanced Energy Materials*** 1702774 (2018)

[4] J. Kim†, B. Lee†, H. Kim, **H. Kim**, K. Kang, ***Chemistry of Materials*** 28, 6894-6899 (2016)

[5] J. S. Kim†, I. Park†, E. Jeong, K, Jin , W. M. Seong, G. Yoon, **H. Kim**, B. Kim, K. T. Nam, K. Kang, ***Advanced Materials*** 46, 1606893 (2017)