

I²CNER Seminar Series

Recent development of complex metal oxide electrocatalysts for oxygen evolution reaction

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Abstract. The need for green hydrogen product using water electrolyzer has attracted much attention in re-examining the electrocatalysis for oxygen evolution reaction (OER). Numerous studies have been carried out in recent years to better understand the mechanisms of catalysts that are made of metal oxides. Adsorbate evolution on the active sites of metal cations has long been the essential concept for understanding the OER catalytic activity. Based on this adsorbate evolution mechanism (AEM), only adsorption and desorption of oxygen species on the metal centers need to be considered and a limit of the overpotential for OER was suggested to be around 370 mV. The recent body of publications in the area however have often reported OER activity of electrocatalysts well below this overpotential value, thus a fresh look of the AEM-based OER mechanism is needed.

Previously, we reported oxygen deficient perovskite of $\text{Ca}_2\text{Mn}_2\text{O}_5$ could exhibit greatly enhanced OER activity when compared to its perovskite structure. The ABO_x type metal oxides may have lattice oxygen vacancies, which could facilitate the creations of mobile oxygen. Such defects change the elemental composition of the solids and valence of metal cations, thus the activity of catalysts. We further developed oxygen-defected electrocatalysts of pyrochlore-type $\text{Y}_2\text{Ru}_2\text{O}_{7-\delta}$ for OER in acid, which exhibited high activity and stability. Lattice oxygen-mediated mechanism (LOM) was proposed to account for the observed high OER activities that often exceed the prediction based on the AEM. In LOM, lattice oxygen is considered as a part of catalytic structures for OER, which involves the adsorption of hydroxyl groups as well. The formation of oxygen vacancies is an essential step in LOM, thus oxygen deficiencies often facilitate the fast OER kinetics of electrocatalysts made of metal oxides. Although AEM and LOM have gained popularity in explaining the experimental results, the real reaction mechanism is still quite complicated and needs to be analyzed experimentally and computationally.

In this presentation, I will focus on complex metal oxides with the general formula of $\text{A}_x\text{B}_y\text{O}_z$, where A and B can be single or mixed metal cation sites. The flexibility in composition of such metal oxides allows us to change the crystal structures and electronic configurations, and to examine the corresponding OER performance. By varying A-site and B-site metal cations, metal substitution and defect engineering, we have uncovered some structural cues for the design of OER catalysts. This talk will focus on the relationship between structures and OER performance of these metal oxide electrocatalysts, including perovskite, pyrochlore, Ruddlesden-Popper, and spinel structures.