

## Perovskite oxides: application in oxygen evolution reaction.

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Hydrogen, as a kind of green renewable energy, can greatly alleviate the current energy crisis and environmental pollution problems. As the focus and front of scientific research, splitting of water into hydrogen and oxygen by solar energy is considered to be one of the most ideal means to obtain the hydrogen energy. However, the oxygen evolution reaction (OER) is more difficult to occur, which greatly limits the application of water splitting. This is because OER is a 4 electron transfer reaction with a higher reaction barrier, requiring additional over-potential to drive the reaction. The additional over-potential will cause higher efficiency loss, thus reducing the practicability of the water splitting. The ideal OER catalyst should have an appropriate band gap, high efficiency in converting solar energy, chemical inertness and reduces the consumption of precious metals. Although  $\text{IrO}_2$  and  $\text{RuO}_2$  show a high OER catalytic activity, but for economic reasons, researchers are still working on finding highly active OER catalysts based on cheaper metals.

The crystal structure of  $\text{ABO}_3$  endows perovskite materials with unique photoelectric response and excellent carrier transportation. This accelerates the research of its application in solar battery, metal-air battery and water splitting. This not only reduces the use of noble metals, but also greatly improves the electronic structure of the catalyst by its flexible crystal structure, thus providing an effective way to enhance the catalytic activity of OER. It has been proved that the essential activity of perovskite material is even higher than that of  $\text{IrO}_2$  or  $\text{RuO}_2$  [1].

In the  $\text{ABO}_3$ -type crystal structure of perovskite, site of A and B can be replaced by metal cations with different valence and ionic radius. This provides an effective method for promoting the OER catalytic activity by partial substitution or doping to change their physical and chemical properties. Nanocrystallization of materials is also a useful method for improving their catalytic performance because nanomaterials have larger surface area to expose more catalytic active centers. As we all know, only the transition-metal ions at B-site are catalytic active centers. Fabricating nanocrystals terminated with high index crystallographic plane through crystal-facet tailoring [2] will be beneficial to expose the transition-metal ions. However, these methods do not change the kinetic process of OER in essence, and the high over-potential and efficiency loss remain to be the bottleneck for designing high performance OER catalysts.

The relationship between the electronic states of materials and their catalytic properties has been well demonstrated in noble metals. The surface structures, bonding modes and valence states of the materials have a great influence on their properties. In the perovskite structure, professor Yang Shao-Horn from MIT found

that perovskites with transition metal  $e_g$  orbital filling number slightly greater than 1 exhibit the best OER catalytic activity through comparing with different electronic configurations of catalyst on a series of OER catalytic activity [3]. According to molecular orbital theory, the  $e_g$  orbitals of the surface transition metals are directly involved in the formation of the  $\sigma$  bonds between the metal and the adsorbed anion. Obviously, it requires a strict regulation of  $e_g$  orbitals filling number. This makes the materials that we can select become rare.

Base on structure and defect, it is a simple and suitable method to design and control the electronic states of materials. Compared with metal cations, the regulation of oxygen ions is more convenient. And the formation of impurities or defect complexes can be reduced to the greatest extent [4]. This themed issue demonstrates to find a simpler way to improve the catalytic activity of OER, and to make it applicable to most of the material systems.

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