# Tunning of electron configurations in transition metal oxides for higher OER

*Zhenxiang Cheng*

Institute for Superconducting and Electronic Materials, Australia Institute for Innovation Materials, Innovation Campus, University of Wollongong, North Wollongong, NSW 2500, Australia
Email: cheng@uow.edu.au

Electrocatalytic water splitting holds great promise for the future energy conversion devices, but the kinetics of the sluggish oxygen evolution reaction (OER, $4OH^- = O2 + H2O + 4e^-$) is the rate-determining step and deserves to be studied extensively. The oxygen evolution reaction process not only requires four sequential proton-coupled electron transfers, but also includes a transition of the spin states. Such a spin transition needs to be promoted by an additional energy to occur, enough voltage together with spin orbital coupling.

Considering the scarcity and high cost of commercial OER catalysts, such as Pt and magnetic RuO2/IrO2, a great deal of effort has been expended on possible alternatives. Transition metal-based perovskite is one of the most excellent candidates, owing to its abundance, relatively good stability, and benign electrocatalytic activity. In 2011, a volcano-shaped curve of OER efficiency against the number of $e_g$ electrons of surface transition metal cations has been proposed by Yang Shao-Horn et al. Following this rule, the fastest OER is observed on $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), of which the magnetic ions are in the intermediate spin state, that is, the number of $e_g$ electrons is around 1.2. Since then, this principle has become an effective guideline to improve the efficiency of perovskite oxide OER catalysts.

Since then the $e_g$ electron rule has fully demonstrated its power in OER process. However the electron configuration of transition metals also decide the magnetic property of the compounds and finally the electron transfer in the catalytic process. In this talk, using layered multiferroic perovskite derivates as example, which preserve multiple perovskite physical parameters, such as couplings between charge, spin, orbitals, and the lattice, I will demonstrate how the electron configuration of transition metal based OER catalyst decides its catalytic behaviour and how to design materials for high OER efficiency.

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## References

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