Study of the electronic structures of transition metal (Ni, Co, Fe) oxides by hole doping for oxygen evolution reaction

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Abstract: This talk reports a study on the correlation of the electronic structures of complex oxides with their electrocatalytic activity for oxygen evolution reaction (OER). In particular, we modulated the electronic states of complex oxides using hole doping strategy, e.g., Li doped NiO, Sr doped $LaFeO_3$ and $LaNiO_3$. Photoemission spectroscopy and x-ray absorption spectroscopy (XAS) were used to study both the occupied and unoccupied density of states around the Fermi level. The electronic structures determines the adsorption strength of reaction intermediates for OER. Our results reveal two important change in the electronic structures induced by hole doping are crucial for improving OER activity: (1) upshift of the occupied valence band center to enhance the surface absorption; (2) creation of a new hole (unoccupied) state just above the Fermi level to reduces the energy barrier for electron transfer. Our results supplemented with DFT calculations established a direct correlation between the enhancement of activity with electronic structure, providing guideline for design of highly active electrocatalysts.

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Biography:

Kelvin Zhang is a professor at college of Chemistry and Chemical Engineering, Xiamen University. His current research interest focus on the electronic properties of metal oxide thin films and heterostructures relevant to application in oxide electronics and electrocatalysts. His group have expertise in using molecular beam epitaxy and pulsed laser deposition to grow high quality single-crystalline thin films with well-controlled surface and interfaces, and studying their electronic structures using a range of x-ray spectroscopic techniques available at world-wide synchrotron facilities. He obtained his PhD degree in chemistry from University of Oxford in 2012, followed by working as a postdoc at Pacific Northwest National Laboratory and as a Herchel Smith Fellow at University of Cambridge from 2015 to 2017.