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Tuning the Electronic Structure of NiO by Li doping for Electrocatalytic Water Oxidation

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Earth-abundant transition metal (TM) oxides are excellent materials as electrocatalysts for oxygen evolution reaction (OER). It has been proposed that similar to the d-band theory in metal catalysts, the intrinsic OER activity of TM oxides is strongly linked with their electronic structures, i.e., transition metal cations with an occupation of eg=1 showing a high OER activity. This provides guideline for rational design of electrocatalysts.1 We have synthesized Li doped NiO (LixNi1-xO, x= 0, 0.09, 0.17, 0.33 and 0.5) powders and found the materials show increasing catalytic activity for OER as x increases, with comparable OER activity to that of precious IrO2 when x=0.5. The dependence of structure and electronic properties on composition were systematically investigated using high-resolution X-ray photoemission spectroscopy (XPS) and X-ray absorption (XAS) at synchrotron, and density functional theory (DFT) calculations. NiO is a wide bandgap (Eg=3.6 eV) semiconductor with a nominal charge state of Ni2+ (eg2), while Ni in the other end member Li0.5Ni0.5O has a nominal charge state of Ni3+ (eg1). O-K edge XAS indicates development of unoccupied states at 0.5 eV above the top of valence band (VB) with increasing Li doping. These experimental results supplemented with DFT calculations established a direct correlation between the enhancement of catalytic activity with the change of electronic structure.
[1] J. Suntivich, K. J. May, H. A. Gasteiger, J. B. Goodenough and Y. Shao-Horn, Science 334 (6061), 1383-1385 (2011).

Primary author(s) : Mr FU, Gaoliang; Prof. ZHANG, Kelvin H.L. (Xiamen University)

Presenter(s) : Prof. ZHANG, Kelvin H.L. (Xiamen University)

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