Highly Active and Stable NiCoIr Oxyhydroxides for Electrochemical Oxygen Evolution Reaction

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ABSTRACT

- It is essential to develop efficient and durable electrocatalysts for oxygen evolution reaction (OER) to achieve practical application of fuel production technologies from water. Herein, we report a design strategy for a catalyst that exhibits excellent catalytic activity and durability for OER, using mostly non-noble metal based materials. We synthesized Ir-modified NiCo oxyhydroxide (NCI) nanosheets with various concentrations of Ir using a photodeposition method. This synthesis results in deposition of catalyst layers with uniform and large catalytic active area, leading to enhanced catalytic activity. Based on structural, electrochemical analysis and density functional theory calculations, we found that the most efficient OER activity is observed from the NCI-8 nanosheets in which 8% Ir and 46% Co play essential bifunctional roles in stabilizing the key O radical intermediate on Ir and promoting the O-O bond coupling on Co, respectively. In addition, NCI-8 shows significant stable performance for 70 hours in alkaline media.

METHODS

[Synthesis]

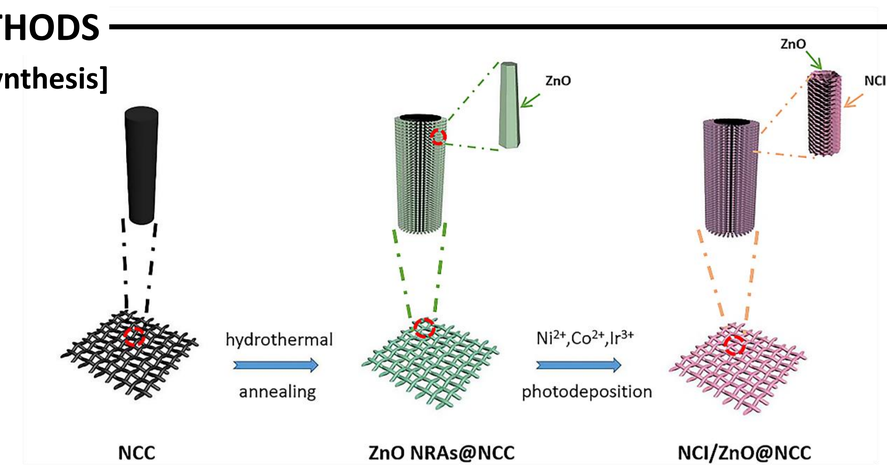

Figure 1. Schematic illustration for the fabrication of hierarchical layered Ir-modified NiCoOOH/ZnO@NCC composite film.

[Computational Details]

- Spin-polarized density functional theory (DFT) calculations using the Vienna Ab-initio Simulation Package (VASP).
- Perdew-Burke-Ernzerhof (PBE) flavor of DFT including the D3 empirical van der Waals correction.
- Phonon contribution (*Zero-point energy (ZPE), S, H*)

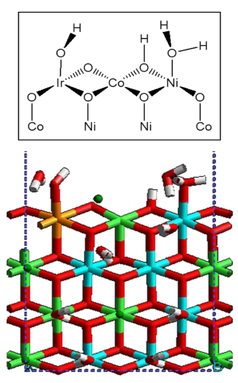

Figure 2. Slab model with one explicit water layer for NCI-8 (atomic ratio: Ni 50%/ Co 42%/Ir 8%).

RESULTS AND DISCUSSION

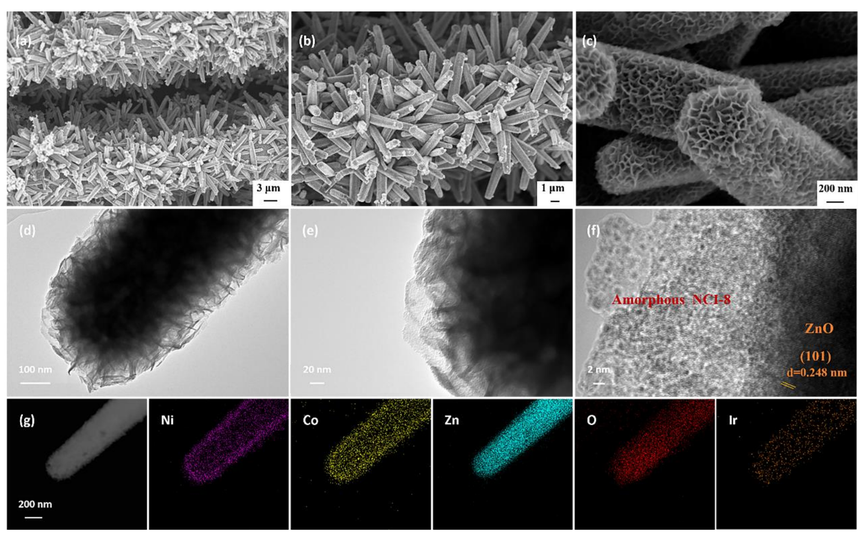

Figure 3. (a-c) SEM, (d, e) TEM and (f) HRTEM images of NCI-8. (g) Elemental mappings of Ni, Co, Zn, O and Ir in NCI-8.

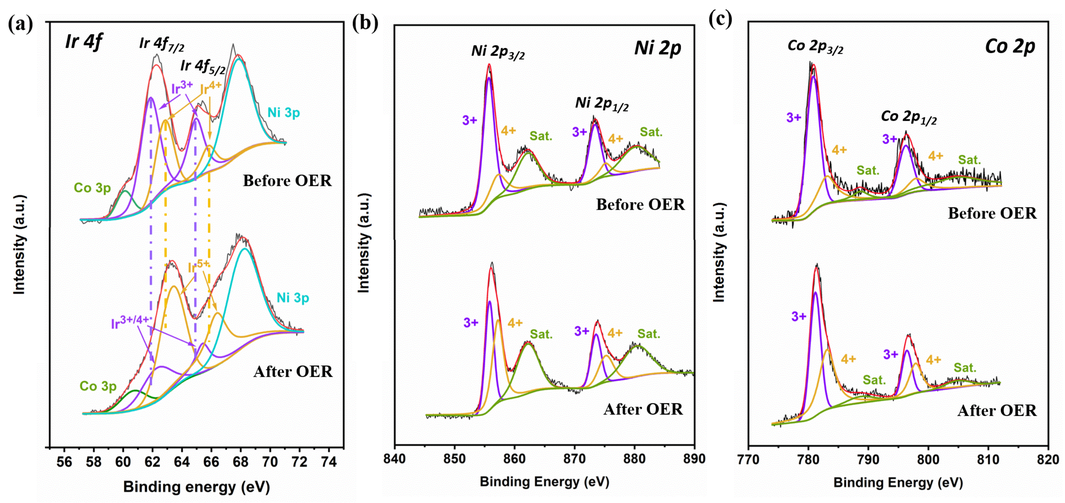

Figure 4. High-resolution XPS patterns of NCI-8 before and after OER. (a) Ir 4*f*, (b) Ni 2*p* and (c) Co 2*p*.

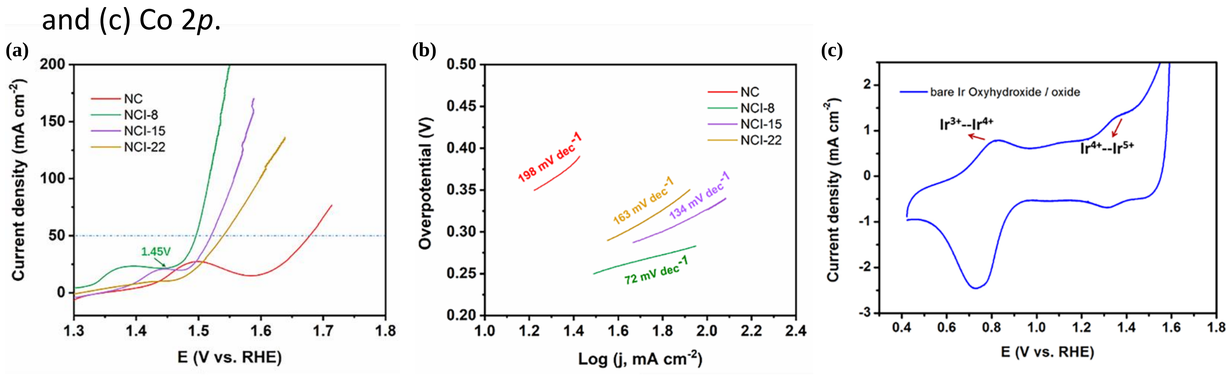

Figure 5. (a) LSV curves of NC, NCI-8, NCI-15 and NCI-22 for OER at a scan rate of 5 mV/s in 1 M KOH; (b) The corresponding Tafel plots; (c) And the CV curve of bare Ir oxyhydroxide/oxide at 5 mV s-1 in 1 M KOH.

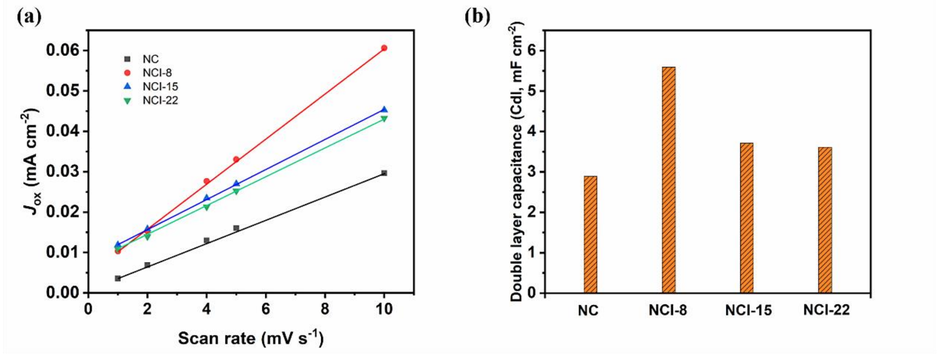

Figure 6. The relationship between scan rate and charge current density of double layer capacitor (a) and the corresponding electrochemical double-layer capacitances (b) of NC, NCI-8, NCI-15 and NCI-22.

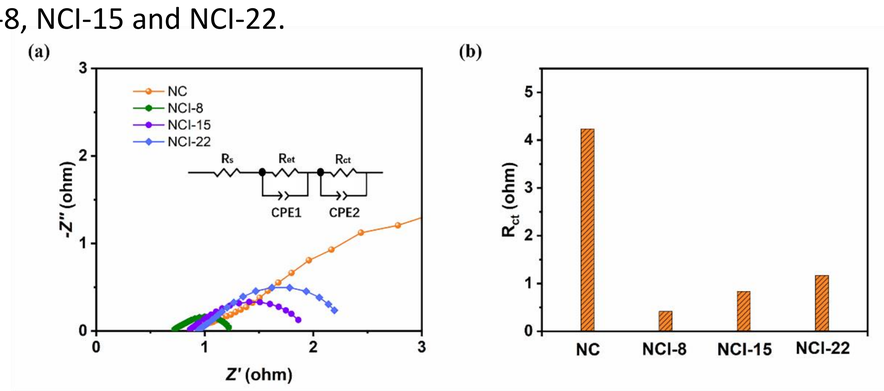

Figure 7. Nyquist plots (a) and charge transfer resistance (b) of NC, NCI-8, NCI-15 and NCI-22 at 1.54 V vs. RHE. Inset in Fig. 7a is the corresponding equivalent circuit model for the Nyquist plots.

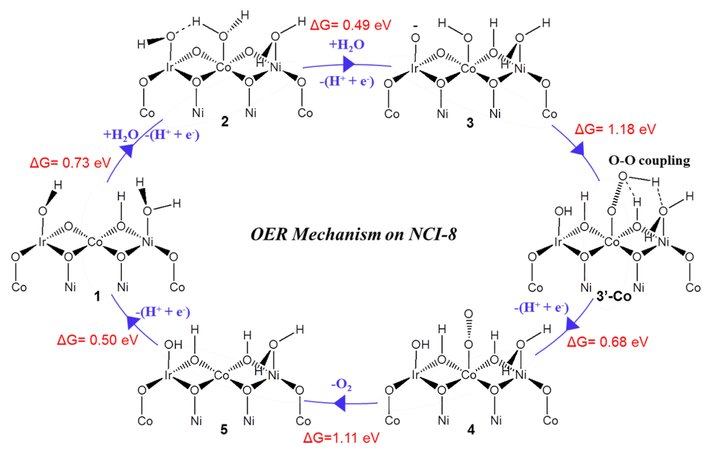

Figure 8. Mechanism for OER on NCI-8 catalyst.

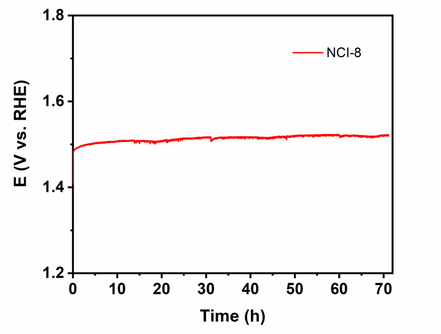

Figure 9. Durability test at 20 mA cm-2

CONCLUSION

- NCI-8 (with 8% Ir and 46% Co) shows highly efficient oxygen evolution reaction activity (20 mA cm-2 at an overpotential of 0.27 V) and stable performance for 70 hours in alkaline media.
- Ir and Co play essential bifunctional roles in stabilizing the key O radical intermediate on Ir and promoting the O-O bond coupling on Co, respectively.

ACKNOWLEDGMENT

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