

The Relationship between Metal Ionic Electronegativity and Oxygen Evolution Reaction

Pascale Ougier*

Department of Chemistry, Warsaw University of Technology, Noakowskiego, Warsaw, Poland

DESCRIPTION

Oxygen Evolution Reaction (OER) plays a crucial role in several renewable energy technologies as well as electrolyzers and reversible metal-air batteries. However, the sluggish dynamics of OER catalysts seriously impede the potency of those clean devices. Herein, a series of bimetallic Metal-Organic Frameworks (MOFs) with tunable electronegativity (Metal Ionic Electronegativity (MIE)) are ready by exactly controlling the metal composition for economical OER. Moreover, an experimental result-derived volcano plot is initially unveiled by presenting the correlation of the MIE and OER kinetic rate (Tafel slope) on the surface of the MOFs-based electrocatalysts.

Remarkably, a $\text{Ni}_{0.9}\text{Fe}_{0.1}$ MOF fictional and supported by the planned electronegative equilibrium rationales delivers a low overpotential of 206 mV at 10 mA cm^{-2} and 270 mV at 50 mA cm^{-2} along with long stability in 1 M KOH, superior to the previously reported catalysts. The excellent performance is assigned to the MIE-induced interface charge transfer resistance and intermediate adsorption resistance adjustment [1,2]. The second metal introduction causes the formation of unsaturated metal sites throughout the electronegative equilibrium method, resulting in an adjustable OER kinetic rate. These findings pave the way to coming up with extremely active MOF-based OER catalysts.

The development of efficient energy conversion and storage devices like electrolyzers, regenerative fuel cells, and reversible fuel cells is important to solve the deteriorating environmental issue caused by the consumption of fossil fuels. But, the performance of those devices is still hindered, because of the sluggish kinetics of Oxygen Evolution Reaction (OER) which may be a complex four-electron transfer reaction. To promote OER within the electrocatalytic overall water splitting, electrocatalysts supported metals and/or noble metal oxides are needed. However, the large-scale production and commercial applications have been obstructed by the high price and poor stability of metal catalysts. Thus, it's extremely fascinating to take advantage of readily available and cost-efficient OER electrocatalysts that may replace noble-metal-based catalysts.

Metal-Organic Frameworks (MOFs) formed by coordination bonds between metal atom nodes and organic ligands with periodic structural units have a larger surface area (up to quite $10\,000 \text{ m}^2 \text{ g}^{-1}$), a lot of chemical action sites, and easier adjustment of structure (the metal sites and/or the organic linkers). Altogether, MOFs mix the benefits of homogeneous catalysts (e.g., well-defined structure and/or ligand environment) and also the heterogeneous catalysts (e.g., site isolation and/or recyclability). Hence, MOFs became promising candidates for electrocatalysts but, because of the poor charge transport and inappropriate intermediates adsorption energy, the electrocatalytic performance of MOF materials has long been unsatisfactory. To beat these obstacles, it's promising to introduce a second metal to modulate the adsorption capability of reaction intermediates and accelerate the interface charge transfer with the MOFs structure unchanged. Previous research has reported that the bimetallic synergistic result would cause the coordination of unsaturated actives that greatly improves the interface charge transfer and the adsorption of the intermediates [3]. The coupling result of the bimetal might induce that the oxidized metal sites could more easily participate in the electron transfer from the water. But, the principle to work out the metal type and doping quantity remain lacking convenient and reliable descriptors to screen excellent bimetallic or polymetallic MOFs electrocatalysts.

Here, we have a tendency to synthesize a series of bimetal MOFs with terephthalic acid. The improved electronegativity that is calculated by totally different valence states, coordination numbers, ionization energy, and ionic radius, we calculated the common Metal Ionic Electronegativity (MIE) of these bimetal MOFs to explore the connection between MIE and also their OER kinetic rate that's the adsorption capability of the intermediates and the interface electron transfer capability. Later on, the $\text{Ni}_{0.9}\text{Fe}_{0.1}$ MOFs (MIE = 1.376) electrocatalyst foretold by the model showed the simplest OER performance among all MOFs-based electrodes studied here [4]. Through Electrochemical Impedance Spectroscopy (EIS) technology, the connection between MIE and their OER kinetic rate was associated with the MIE-induced interface charge transfer resistance and intermediate adsorption resistance adjustment.

Correspondence to: Pascale Ougier, Department of Chemistry, Warsaw University of Technology, Noakowskiego, Warsaw, Poland, E-mail: claus.streycek@chem.gu.se

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The analysis of X-ray Photoelectron Spectroscopy (XPS) results, the bimetal synergistic result caused the formation of unsaturated metal sites throughout the electronegative equilibrium method, resulting in adjustable OER kinetic rate.

A series of bimetal MOFs with the terephthalic acid as the ligand was synthesized. We have a tendency to demonstrate an optimum volcano-type activity trend between MIE and also the OER kinetic rate of all samples, particularly the adsorption capability of the intermediates and also the interface electron transfer capability on the surface of the bimetallic MOFs-based electrocatalysts. According to the volcano model, a predicted $\text{Ni}_{0.9}\text{Fe}_{0.1}$ MOF is built, with the experimental result confirming the excellent consistency with the theoretical prediction. Some studies indicate that the origin of OER activity for various MOFs electrodes is powerfully associated with the interface charge transfer resistance and intermediate sorption resistance that square measure influenced by the bimetallic tendency distinction in MOFs. The bimetal synergistic result caused the formation of unsaturated metal sites throughout the

electronegative equilibrium method, resulting in an adjustable OER kinetic rate. This analysis hints at the potential that the event of an efficient descriptor might predict extremely active MOFs-based OER electrocatalysts.

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