

# Computational design of the catalyst for hydrogen generation and energy storage materials

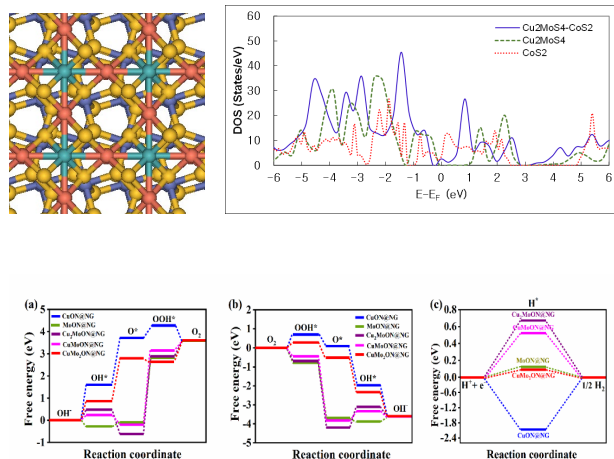
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\*E-mail: [dhk201@jbnu.ac.kr](mailto:dhk201@jbnu.ac.kr)**Keywords:** hydrogen evolution, density of states, Gibbs free energy

## 1. Introduction

To The design and development of an active trifunctional catalyst for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR) are critical for the innovative renewable energy conversion and storage technologies. We used density functional theory (DFT) to investigate how hierarchical design of the catalytic surface and the support layer influences the trifunctional behavior of the catalysts in HER, OER, and ORR. In particular, the promising catalyst significantly enhances density of states (DOS). Gibbs energy change for hydrogen adsorption on the catalyst surface ( $\Delta G_H$ ) is nearly zero. The oxygen evolution has lower overpotential ( $\eta_{OER}$ ) with appropriate energy barriers in overall reaction steps. According to theoretical calculations, the new catalyst reduces the overpotential by increasing the binding energy of water oxidation intermediate species, and enhances electric conductivity with higher DOS around the Fermi level. Thereby, it exhibits greater activity toward HER, OER, and ORR than conventional catalyst. This study emphasizes the need for clear guidelines via optimized electronic structure and the adsorption property of the intermediate species towards the development of trifunctional electrocatalysts.



The catalyst has nearly zero  $\Delta G_H$ , presumably due to the balance between hydrogen adsorption and desorption. Theoretical inspection was consistent with the experimentally optimized catalyst with enhanced active sites towards water splitting.

## 4. Conclusions

Calculation results clearly explain that the doping effect may reason for greater activity over the structures. The DOS at Fermi level confirms enhanced conductivity and the Gibbs free energy change upon hydrogen adsorption ( $\Delta G_H$ ) is nearly zero. The synergistic doping effect enables the efficient electrocatalyst for cost-effective hydrogen production through water splitting

## References

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## 2. Computational Methodology

DFT calculations were performed by using Vienna Ab initio Simulation Package (VASP). The Projected Augmented Waves (PAW) was implemented to illustrate the ion- electron interactions, and the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional was applied in this system, with k-point meshes of  $8 \times 8 \times 1$  for the (DOS) and energy calculations.

## 3. Results and Discussion

**1. Density of States:** Catalytic materials delivers improved conductivity and higher density due to effect of combination of transition metal atoms and non-metal elements. ( Fig.1)

### 2. Gibbs free energy and Hydrogen Evolution Reaction

The formation energy, Hydrogen adsorption energy ( $\Delta H_{ads}$ ) and Gibbs free energy change ( $\Delta G_H$ ) was calculated for the  $H^*$  adsorbed active site of the material based on the number of atoms in the unit cell.