FIRST-PRINCIPLES GUIDED DISCOVERY OF NOVEL BIMETALLIC NANO-CATALYSTS FOR H2O2 DIRECT SYNTHESIS

Dr. Sang Soo Han, e-mail: sangsoo@kist.re.kr
Computational Science Research Center, Korea Institute of Science and Technology (South Korea)

The direct synthesis of hydrogen peroxide (H_2O_2) from H_2 and O_2 represents a potentially atom-efficient alternative to the current industrial indirect process. And, Pd has been currently used as an efficient catalyst for direct H_2O_2 synthesis, although it has not been commercialized yet due to its expensive cost and still unsatisfied catalytic performances. In this regard, it is imperative to discover an inexpensive alternative with a superior catalytic property. For this purpose, we have designed several bimetallic catalysts replacing Pd through first-principles calculations, in particular, a high-throughput approach combining a calculation automation. Moreover, the designed catalysts were experimentally confirmed.

Electronic structure of a material is one of key features to determine catalytic properties as like *d*-band center theory. In the extension line of the theory, we screened 4350 bimetallic alloys by first-principles calculation and calculated similarities of their electronic densities of states (DOS) by comparing with that of Pd. Then, we filtered 10 potential catalysts (thermodynamically miscible) with the highest DOS similarities. And then, we synthesized the 10 candidates and experimentally measured their catalytic properties for H_2O_2 direct synthesis. After the experimental confirmation, it is found that, of the 10 candidates, three bimetallic alloys indeed show similar or superior catalytic properties to Pd. In addition, we suggest a new design scheme using “immiscible” bimetallic systems based on first-principles calculation, and the scheme is also successfully confirmed by an experiment. In this talk, I will also discuss the scheme.

Acknowledgment

This work was supported by the Creative Materials Discovery Program through the National Research Foundation of Korea (NRF-2016M3D1A1021140). We are grateful to experimental teams of KIST (Dr. Seung Yong Lee, Ms. Hyobin Nam, and Dr. Jae-Pyung Ahn) and Korea University (Prof. Kwan-Young Lee, Mr. Young-Hoon Cho).