Developing efficient Water Oxidation Catalyst

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Abstract

Recently, the global warming due to rapid energy usage has accelerated the development of renewable energy. Splitting water into hydrogen and oxygen molecules is an environmentally-friendly solar-to-energy conversion method which could produce hydrogen energy. However, it shows inferior property because the oxygen evolution reaction remains a bottleneck during this process. Therefore, development of efficient and inexpensive water-oxidation catalyst is necessary for the realization of practically viable water-splitting systems.

Until now, it has been difficult to understand whether the catalytic capability originates mainly from either the Mn arrangement or the Mn valency, since the structure of the catalyst always changed significantly as the valency changed. Therefore, I selected $Li_{2-x}MnP_2O_7$ as a model system since the Mn valency can be carefully tuned from 2 to 3 by removing the controlled amount of Li-ion within minimal crystal structural change. We observed that as the averaged oxidation state of Mn in $Li_{2-x}MnP_2O_7$ increases from 2 to 3, the catalytic performance enhanced in the series of $Li_2MnP_2O_7$ $_{1.7}MnP_2O_7$ $_{1.5}MnP_2O_7$ $_2O_7$. Moreover, as a platform to better understand the structural effect in catalysis, I selected four catalysts with various local geometries. Although they exhibit various catalytic activities and stabilities during water oxidation, $Na_2CoP_2O_7$ with distorted cobalt tetrahedral geometry shows high activity under neutral conditions, along with high structural stability. First-principles calculations suggest that the surface reorganization by the pyrophosphate ligand induces a highly distorted tetrahedral geometry, where water molecules can favorably bind, resulting in a low overpotential.

In conclusion, we observed the role of Mn(III) state and the importance of local coordination in the catalysis and suggested the possible effects of polyanions on the water oxidation chemistry.

Biography

Hyunah Kim is currently a Ph.D student in Materials Science and Engineering at Seoul National University (SNU), supervised by Prof. Kisuk Kang. Hyunah's research interests focus on developing advanced energy materials to tackle current issues, such as efficient electrocatalysts for hydrogen energy production and new rechargeable battery materials. Through her six years of research at SNU, she revealed the fundamental mechanism of natural photosynthesis, and demonstrated the feasibility of batter