

## Current Challenge in Design for Water Oxidizing Electrocatalysts

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### Abstract

Water splitting is regarded as a promising step towards environmentally sustainable energy schemes. The oxygen evolution reaction (OER) requires extremely high overpotential due to its slow reaction kinetics. The water oxidizing cluster in photosystem II, in the form of cubical  $\text{Mn}_4\text{CaO}_5$  cluster, efficiently catalyzes water oxidation. Inspired by  $\text{Mn}_4\text{CaO}_5$  cluster, we previously identified a new crystal structure,  $\text{Mn}_3(\text{PO}_4)_2 \cdot 3\text{H}_2\text{O}$ , and demonstrated its superior catalytic performance at neutral pH. We revealed that structural flexibility can stabilize Jahn-Teller distorted Mn(III), and thus facilitate Mn redox during catalysis. Additionally, we verified influence of Mn valency and asymmetric geometry on water oxidation catalysis using  $\text{Li}_2\text{MnP}_2\text{O}_7$  and its derivatives.

Specific questions that we intensively focus for further applications include how to translate the underlying principles in  $\text{Mn}_4\text{CaO}_5$  cluster into synthetic heterogeneous catalysts. Toward this vision, we have been developing a new catalytic platform based on sub-10 nm-sized MnO nanoparticles (MnO NPs) to bridge the gap between atomically defined biological catalysts, their metalloenzyme counterparts and the heterogeneous materials. In this approach, the local atomic geometry is controlled by the nitrogen surface modification by the specific ligand and the heterogeneous atom doping, that enhance the catalytic activity and selectivity. Furthermore, we detected key intermediate species,  $\text{Mn(IV)=O}$ , based on comprehensive electrokinetic and *in-situ* spectroscopic analysis. We revealed unique water oxidizing mechanism mediated by MnO different from bulk counterparts.

### Biography

Prof. Ki Tae Nam is an associate professor in the Department of Materials Science and Engineering at Seoul National University. He received BS and MS degree on Materials Science and Engineering at Seoul National University and Ph.D at Massachusetts Institute of Technology. His research interests mainly focus on the bio-inspired nanomaterials for chirality control and water oxidation.