

*Biography: Prof. Dr. Chanho Pak*

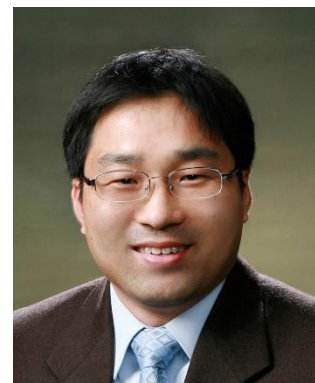
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Professional Activity

1995. 2 – 2013. 4	Master, SAIT in Samsung Electronics, Korea
1999. 3 – 2000. 4	Post-doctoral Associate, Dept. of Chemical Engineering, Yale University, USA
2000. 5 – 2001. 4	Post-doctoral Researcher, College of Chemistry, University of California at Berkeley and Lawrence Berkeley National Laboratory, USA
2013. 4 – 2016. 7	Vice President, Samsung SDI, Korea
2016. 7 – 2021. 8	Associate Professor, Gwangju Institute of Science and Technology, Korea
2021. 9 – Present	Professor, Gwangju Institute of Science and Technology, Korea

Honors and Awards

2022. 8	Award for Local Area Collaboration, GIST
2011. 4	Young Scientist for Catalysis from Catalysis Division of KICHE
2004. 10	Silver Medal in Samsung Paper Award

Current Research Topics

- Electrocatalyst for fuel cells and electrolyzer
- Electrode development for a membrane electrode assembly
- Nanoporous carbon materials for energy application
- Porous metal oxide supports

## Investigation of Porous and Supported Catalysts in the Anode of Proton Exchange Membrane Water Electrolysis

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For the efficient utilization of intermittent electricity produced by renewable energies, the proton exchange membrane water electrolyzer (PEMWE) has been attracting significant attention by converting surplus electric energy into transportable hydrogen energy. [1].

However, the high cost of noble metal (Ir and Ru) based catalysts for oxygen evolution reaction (OER) hinders the wide application of PEMWE. It is challenging to improve OER catalytic activity while decreasing the Ir amount to the level of  $0.01 \text{ g kW}^{-1}$  in the membrane electrode assembly (MEA) for wide application of PEMWE in near future [2]. Therefore, the OER catalysts, which are mainly based on Ir, have been developed in various strategies to improve the activity and stability such as mixed metal oxides [3], metal oxide supported catalysts [4], and Ir oxidation state design [5].

This study will focus on two main strategies (nanostructure and oxidation states design of Ir and metal oxide supported catalysts). First, new synthetic approaches to establishing gradient (hierarchical) distribution of the Ir oxidation states ( $\text{Ir}^0$ ,  $\text{Ir}^{3+}$ , and  $\text{Ir}^{4+}$ ) in nanosheet structure will be discussed. A novel solution process using ethylene glycol, formic acid, and sodium acetate for breaking the trade-off relationship between the activity and stability of the OER [6] is developed which is

suitable for the mass production of  $\text{IrO}_x$  catalyst owing to a simple preparation process.

For further studies to reduce Ir loading levels in the PEMWE system, mesoporous tantalum oxide ( $\text{Ta}_2\text{O}_5$ ) with a high specific surface area ( $>100 \text{ m}^2/\text{g}$ ) is developed as a stable metal oxide support. The well-dispersed Ir nanostructure on the  $\text{Ta}_2\text{O}_5$  support improved electrical conductivity and increased electrochemically active surface area. Strong metal-metal oxide support interaction effect between Ir and Ta was demonstrated using X-ray photoelectron spectroscopy and X-ray absorption spectroscopy and their contribution toward OER activity was elucidated. Owing to the electron transfer from Ta to Ir, the OER-active Ir(III) ratio was increased compared to other supported catalysts under oxidative OER conditions. The improved OER activity ( $288 \text{ mV/cm}^2$ ) and mass activity ( $876 \text{ A/g}_{\text{Ir}}$  at  $1.55 \text{ V}$ ) indicate that  $\text{Ta}_2\text{O}_5$  support efficiently reduced Ir loading levels. Also, it was demonstrated in the MEA performance under PEMWE conditions.

In summary, it is suggested the control of the oxidation states of the Ir in the OER catalyst via preparing by solution reduction method and using metal oxide support is a promising approach for practical low Ir loading MEA for PEMWE

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Professional Activity

1992. 4 – 1996. 6 National Institute of Advanced Industrial Science and Technology (AIST; formerly National Institute of Materials and Chemical Research), Japan

1994. 9 – 1995. 12 Visiting Associate, California Institute of Technology (Prof. Mark E. Davis), USA

1996. 7 – 2004. 8 Associate Professor, Department of Chemistry, Gifu University, Japan

2004. 8 – 2007. 10 Associate Professor, Division of Materials Science and Chemical Engineering, Yokohama National University, Japan

2007. 11 – Present Professor, Division of Materials Science and Chemical Engineering, Yokohama National University, Japan

2020. 6 – 2022. 6 Chairman, Japan Zeolite Association

International Academic Activity

2013. 7 – Present Member of Synthesis Commission, International Zeolite Association

Honors and Awards (Max. 7)

2001. 5 Tokai Chemical Industry Association Award

2002. 5 The Japan Petroleum Institute, Young Scientist Award

2003. 5 The Chemical Society of Japan, BCSJ Award

2019. 6 Yokohama National University, Best Teaching Award

Current Research Topics (Max. 5)

- Design and synthesis of organic structure-directing agents for zeolite synthesis
- Synthesis of ordered microporous and mesoporous materials and their catalytic applications
- Preparation of acid-base and oxidation catalysts for fine chemicals production
- Catalytic cracking and MTO/DTO reactions to produce light olefins

## Preparation of High-Performance Catalysts with MSE- and YFI Frameworks via Self-Defect-Healing

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Framework stability of zeolite as well as understanding the atomic position in the framework is important to design high performance catalyst based on microporous crystals. In the field of fine-chemicals synthesis, there is a persistent demand for zeolite catalysts that have large-pores and multi-dimensional channel systems. However, the number of such zeolites is still limited. We focused on two 3-dimensional, large-pore zeolite framework types. One is YNU-2 (**MSE** topology) with a pore system of 12-10-10-ring [1,2]; the other is YNU-5 (**YFI** topology) with a pore system of 12-12-8-ring and an isolated 8-ring channel [3] (Figure 1).

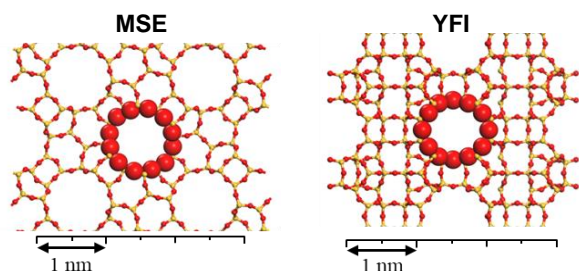


Fig. 1. **MSE** and **YFI** frameworks. Oxygens in a 12-ring are emphasized for each framework.

The properties of zeolites depend on the method of preparation including starting gel composition and synthesis conditions. For example, the synthesis using organic structure-directing agent (OSDA) usually gives high-silica zeolites while OSDA-free synthesis gives materials with much lower silica contents. In both cases, some post-synthetic modifications are necessary for preparing catalysts that have active sites, suitable hydrophobicity and stability. In this work, we used relatively hydrophilic OSDAs.

Site defects (vacancies) are useful in terms of heteroatom substitutions, whereas too many vacancies lead to framework collapse. Thus, the control of the vacancies is a main issue in

the post-synthetic modification of zeolite. Some examples of the modification consist of (1) preparation of high-performance titanosilicate Ti-YNU-2 from YNU-2P that is a zeolitic framework-OSDA composite, and (2) preparation of novel titanosilicate Ti-YNU-5 from YNU-5 zeolite that is originally an aluminosilicate with Si/Al = 9. The dealumination by careful acid-leaching enables framework stabilization. If there are too many framework Al sites and the Al atoms are removed without repairing the newly generated vacancies, then the framework is unstable and collapses along with the dealumination.

In both **MSE** and **YFI** cases, Si-migration played important roles to stabilize the frameworks by repairing the vacancies. It could be the same phenomenon as the self-defect-healing. The Si-migration is supported by several characterization results such as  $^{29}\text{Si}$  MAS NMR. Computational modeling based on DFT helped understand the preference for the formation on vacancies and the replacement of Si by Ti or Al in different crystallographic positions of the **MSE** framework [4]. TEM results have been disclosed as a powerful support [5].

These results could afford new insights into the understanding of structural stability of high-silica zeolites towards preparation of high-performance catalysts.

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#### Professional Activity

- |                    |  |
|--------------------|--|
| 2007. 10 – 2008. 3 | JSPS Post-doc, The University of Tokyo (Prof. Kazunari Domen)                                  |
| 2008. 4 – 2009. 3  | JSPS Post-doc, The Pennsylvania State University (Prof. Thomas E. Mallouk)                     |
| 2009. 4 – 2012. 7  | Assistant Professor, The University of Tokyo (Prof. Kazunari Domen)                            |
| 2010. 10 – 2014. 3 | PRESTO/JST Researcher  |
| 2012. 8 – 2022.3   | Associate Professor, Department of Chemistry, School of Science, Tokyo Institute of Technology |
| 2022. 4 – Present  | Professor, Department of Chemistry, School of Science, Tokyo Institute of Technology           |
| 2022. 6 – Present  | Leader of Grant-in-Aid for Transformative Research Areas (A) “Supra-ceramics”                  |

#### International Academic Activity

- |                   |  |
|-------------------|--|
| 2018. 3 – Present | Associate Editor in Journal of Photochemistry and Photobiology C |
|-------------------|--|

#### Honors and Awards

- |          |  |
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| 2022. 10 | Fellow of the Royal Society of Chemistry: FRSC   |
| 2021. 11 | Clarivate Analytics Highly Cited Researchers 2021  |
| 2017. 6  | Journal of Materials Chemistry A, Emerging Investigators   |
| 2016. 12 | The 13th JSPS Prize  |
| 2016. 4  | Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Young Scientist Award |

#### Current Research Topics

- Artificial photosynthesis
- Mixed-anion compounds
- CO<sub>2</sub> conversion
- Water splitting

## Artificial Photosynthetic Assemblies Constructed from Molecules and Inorganic Solids

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Metal oxide nanosheets derived from the layered solids have attracted attention in various fields of materials chemistry due to their unique physicochemical properties. The anisotropic feature of nanosheets, having a thickness of ~1 nm and lateral dimensions ranging from several hundred nanometers to a few micrometers, is advantageous for heterogeneous photocatalysis, as the diffusion length of photogenerated carriers to the surface is shortened, leading to higher activity [1].

It is also known that certain nanoparticulate metals or metal oxides on a semiconductor photocatalyst work as cocatalysts to promote water reduction and/or oxidation [2]. In heterogeneous photocatalysis, the effect of cocatalyst size on the water-splitting performance had not been examined at sizes smaller than 1 nm due to the lack of an effective preparation method and a suitable photocatalyst. We have demonstrated that metal nanoclusters (such as Pt) of <1 nm in size could be deposited on the interlayer nanospace of  $\text{KCa}_2\text{Nb}_3\text{O}_{10}$  using the electrostatic attraction between a cationic metal complex and a negatively charged  $\text{Ca}_2\text{Nb}_3\text{O}_{10}^-$  nanosheet, without the aid of any additional reagent [3]. The material obtained exhibited 8 times greater photocatalytic activity for overall water splitting under band-gap irradiation than the previously reported analog using a  $\text{RuO}_2$  promoter [4]. This study highlighted the superior functionality of <1 nm Pt nanoclusters for photocatalytic overall water splitting.

With further modification by a ruthenium(II) photosensitizer, this material also worked as a  $\text{H}_2$  evolution photocatalyst in visible-light-driven Z-scheme water splitting, in combination with a  $\text{WO}_3$ -based  $\text{O}_2$  evolution photocatalyst and a triiodide/iodide redox couple [5]. It is shown that modification of Ru dye-sensitized, Pt-intercalated

$\text{HCa}_2\text{Nb}_3\text{O}_{10}$  nanosheets ( $\text{Ru/Pt/HCa}_2\text{Nb}_3\text{O}_{10}$ ) with both amorphous  $\text{Al}_2\text{O}_3$  and poly(styrenesulfonate) (PSS) improves the STH efficiency of Z-scheme overall water splitting by a factor of ~100, relative to an analogous system that uses unmodified  $\text{Ru/Pt/HCa}_2\text{Nb}_3\text{O}_{10}$  [6]. The  $\text{Al}_2\text{O}_3$  and PSS modifiers, which have previously been shown to suppress back electron transfer reactions in a dye-sensitized  $\text{H}_2$  evolution photocatalyst (Fig. 1), enabled operation of the Z-scheme system even at low intensity of simulated sunlight without a decrease in the STH values. By using the optimized photocatalyst,  $\text{PSS/Ru/Al}_2\text{O}_3/\text{Pt/HCa}_2\text{Nb}_3\text{O}_{10}$ , a maximum STH of 0.12% and an apparent quantum yield of 4.1% at 420 nm were obtained, by far the highest among dye-sensitized water splitting systems and also comparable to conventional semiconductor-based suspended particulate photocatalyst systems.

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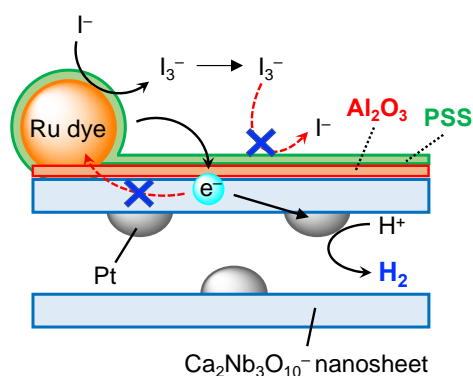


Fig. 1. Schematic reaction mechanism of  $\text{PSS/Ru/Al}_2\text{O}_3/\text{Pt/HCa}_2\text{Nb}_3\text{O}_{10}$  nanosheets during visible-light  $\text{H}_2$  evolution.

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Professional Activity

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| 1996. 12 – 1999. 10 | Research Scientist, LG Metal Research Institute of Technology  |
| 2000. 02 – 2000. 08 | Visiting Researcher, University of California, Santa Barbara, USA  |
| 2011. 12 – 2012. 11 | Visiting Scientist, Northwestern University, USA   |
| 2016. 01 – 2019. 01 | Head, Center for Green Carbon Catalysts, KRICT   |
| 2019. 02 – 2020. 02 | Director, Carbon Resource Institute (CRI), KRICT   |
| 2008.03 – Present   | Professor, University of Science and Technology (UST), Korea   |
| 2020. 03 – Present  | Director-General, Chemical & Process Technology Division, KRICT  |
| 2020. 12 – 2021.06  | Committee member of CCU Technology Innovation Roadmap (2021),<br>Government Ministries                       |
| 2020. 12 – Present  | Member, Climate & Environment Development Project Promotion Committee,<br>Ministry of Science and ICT, Korea |
| 2022. 12 – Present  | Member, Presidential Commission on Carbon Neutrality and Green Growth of<br>Korea                            |
| 2023. 01 – Present  | President of the CCUS Expert Committee, Sub-Commission on Carbon Neutrality and<br>Green Growth of Korea     |
| 2023. 01 – Present  | Vice President, Korea Zeolite Association (KZA)  |

Honors and Awards (Max. 7)

- |          |  |
|----------|--|
| 2018. 04 | Best Education Award of UST, Korea                         |
| 2008. 05 | Minister's Commendation, Ministry of Education and Science |

Current Research Topics (Max. 5)

- Biomass conversion
- CO<sub>2</sub> conversion
- Metal-organic framework materials as catalysts and adsorbents
- Inorganic Clusters and functional materials for catalysis

## Metal-Organic Frameworks as a Platform Catalyst for Biomass and CO<sub>2</sub> Conversion

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Carbon dioxide and biomass valorizations are the most important techniques in chemical and environmental society for mitigation of global warming in 21st century. For this purpose, developing efficient and noble catalysts with multifunctional properties is essential for solving raised global issues.

Metal-organic frameworks (MOFs) are porous crystalline solids with high surface area and tunable porosity having a multitude of applications in the realm of gas storage, adsorption, separation, and heterogeneous catalysis.[1] However, the saturated coordination environments of the metal ions or node clusters which comprise the framework of MOFs, limits its catalytic applicability in cases where the undercoordinated metal ions are primarily responsible for the catalytic activity. Therefore, post-synthetic immobilization or incorporation of secondary functional objectives on ligand or metal sites paves the way for imparting catalytic functionalities onto the MOF scaffold and has been researched extensively during the last decade. [2-5]

Here, we will present the catalytic results of biomass conversion, CO<sub>2</sub> hydrogenation, and simultaneous transformation of biomass and CO<sub>2</sub> over a various kinds of MOFs with different functionalities. First, a series of Zr-based metal organic frameworks (Zr-MOFs) containing various types of metal node to ligand coordination were synthesized and tested for catalytic transfer hydrogenation (CTH) reaction of furfural (FUR) to furfuryl alcohol (FOL). It was found that metal node

coordination plays a more important role than porosity in Zr-MOFs. Second, the facile methods for preparing single atom catalysts (SACs) by incorporating an Ir complex into a zeolitic imidazolate framework (so called ZIF) support will be discussed. The organometallic Ir complex was introduced at different stages of the porous coordination polymer synthesis, resulting in different immobilization efficiencies, particle shapes, and catalytic activities.

Third, for base-free hydrogenation of CO<sub>2</sub> the Mo<sub>132</sub> cluster was immobilized in porous MIL-101(Fe) by in situ encapsulation method to be used as a heterogeneous catalyst. The resulting Mo<sub>132</sub>@MIL-100(Fe) not only maintained its structural integrity and activity during three consecutive recycling reactions but also exhibited increased TON (1257) compared to Mo<sub>132</sub> cluster (TON = 452) at the same reaction condition. This study provides the first instance of incorporation Mo<sub>132</sub> cluster as a CO<sub>2</sub> hydration catalyst to enhance the yield of formic acid (FA), and the similar strategy can be applicable to various aqueous-phase CO<sub>2</sub> conversion.

Finally, I will briefly touch the synthesis of porous bimetallic ZIF with incorporation of square planar Pd and its catalytic application for CO<sub>2</sub> utilization.

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- [3] K. -R. Oh, Y. Han, G.-Y. Cha, A. H. Valekar, M. Lee, S. E. Sivan, Y. -U. Kwon, Y. K. Hwang, *ACS Sustain. Chem. Eng.* 9 (2021) 14051
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- [5] K. -R. Oh, H. Lee, G. -N. Yun, C. Yoo, J. W. Yoon, A. Awad, H. -W. Jeong, and Y. K. Hwang, *ACS Appl. Mater. Inter. in pressed* (<https://doi.org/10.1021/acsami.2c20240>)