

Biography: Dr. Yong-Ki Park

Name: Yong-Ki Park

Title: Research fellow

Affiliation: Korea Research Institute of Chemical Technology (KRICT)

Address: 141 Gajeongro, Yuseong, Daejeon 34114, South Korea

Tel. +82-42-860-7672, E-mail. ykpark@kRICT.re.kr



Professional Activity

1994. 4 – 1995. 2	Research Associate, KAIST, Korea
1995. 7 – 1996. 6	Post Doctoral Researcher, University of California, Berkeley, USA
1996. 7 – 2002.8	Senior Researcher, KRICT, Korea
2002. 9 – Present	Principal Researcher, KRICT, Korea
2022. 5 – Present	Director, Center for Low-carbon Chemical Process (LCP)

International Academic Activity

2018. – Present	Committee member of Asian Pacific Association of Catalysis Societies (APACS)
2019. – Present	Board member of International Zeolite Association (IZA)

Honors and Awards

2015. 5	Seokmyung Outstanding Chemical Engineers, KICChE
2022. 4	Yeosan Catalytic Science Award, KICChE

Current Research Topics

- Catalytic naphtha cracking
- Hybridization of catalytic naphtha cracking and MTO
- Propane dehydrogenation in fluidized-moving bed (FPDH)
- CO₂ capturing process by dry sorbent

Catalyst & Adsorbent Engineering for Fluidized bed-based Low-carbon Chemical Processes

Yong-Ki Park, Ki Woong Kim, Na Young Kang, Jae Deuk Park, Dae Sung Park, Ji Ho Shin, Do Kyoung Kim, Ji Woong Woon, You In Park

¹Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea

*E-mail: ykpark@kriict.re.kr

In order to meet stringent carbon emission regulations in light olefin production and realize Future Net-zero in petrochemicals, minimizing carbon emissions in chemical production is a top priority. This requires not only a microscopic approach to reduce energy consumption during reactions, but also a macroscopic approach that integrates chemical processes such as reaction and separation processes and integrates different industrial sectors.

Since the petrochemical industry has a long history and most processes are already optimized to minimize energy consumption and carbon emissions, it is very difficult to achieve further efficiency on its own. Therefore, new approaches have been attempted to utilize low value chemicals produced in other industries in the short term and renewable resources in the long term. The Carbon2Chem® program proposed by Thyssenkrupp Co. in Germany is one of the leading examples of reducing carbon emissions in the steel and petrochemical industries by utilizing steel by-product gases and renewable electricity to make energy-intensive chemicals such as MeOH and ammonia.

To make chemicals from low value chemicals and/or renewable resources, new concepts of reaction and separation technology are required as follows.

1. Reaction: Catalytic materials and systems for managing large-scale energy intensive reactions
2. Separation: Adsorption and membrane materials and processes capable of

operating under mild operation condition to replace conventional energy intensive distillation process

For over 10 years, in order to minimize CO₂ emissions from chemical processes, we have been developing novel chemical processes such as hybridization of MTO and catalytic naphtha cracking in fluidized bed reactors, olefin/paraffin separations using adsorbents and membranes, and CO₂ separation using membrane contactors. In this talk, we would like to introduce these new approaches, discuss their challenges, and share our experience in developing materials from the laboratory to commercial scale.

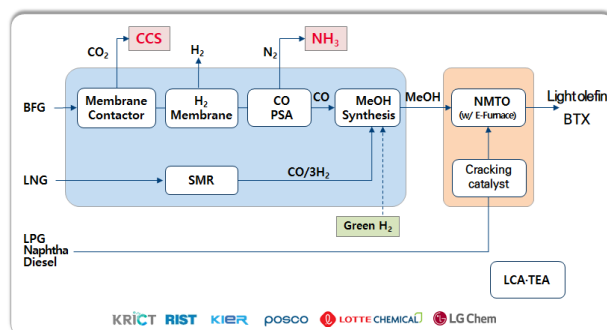


Fig. 1. Convergence of steel and petrochemical industries: Suggested scheme for production of light olefins using steel by-product gas

REFERENCES

- [1] KR10-2022-0138032
- [2] KR10-2021-0066737, KR 10-1759101
- [3] KR10-2021-012073

Name: Hiromi Yamashita

Title: Professor

Affiliation: Graduate School of Engineering, Osaka University

Address: 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Tel. +81-6-6879-7457, E-mail. yamashita@mat.eng.osaka-u.ac.jp



Education Activity

1978. 4 – 1987. 3 Kyoto University (BC, MC, DC), PhD

Professional Activity

1987. 4 – 1992. 9 Assistant Professor, Tohoku University
1992. 7 – 1992. 8 Visiting Researcher, The Pennsylvania State University
1992. 9 – 1995. 3 Assistant Professor, Osaka Prefecture University
1993. 6 – 1993. 10 Visiting Researcher, The University of Texas at Austin
1995. 4 – 2003. 12 Associate Professor, Osaka Prefecture University
1998. 6 – 1999. 18 Visiting Researcher, California Institute of Technology
2004. 1 – Present Professor, Osaka University
2010. 3 – 2010. 4 Invited Professor, University of Pierre and Marie Curie

International Academic Activity

2012. 1 – Present Editor of Applied Catalysis B: Environmental
2016. 8 – Present International Advisory Board of International Association of Catalysis Societies
2019. 5 – 2000. 5 President of Catalysis Society of Japan
2019. 8 – Present President of Asia and Pacific Association of Catalysis Societies
2019. 1 – Present Member of Academia Europea
2021. 1 – Present Editorial Board of ChemCatChem
2023. 1 – Present Editorial Council of Microporous and Mesoporous Materials

Honors and Awards)

1998. 3 Promotion Award, Catalysis Society of Japan
2005. 3 Distinguished Service Award, Japan Institute of Metals & Materials
2009. 9 Award, Japanese Photochemistry Association
2015. 3 Award, Catalysis Society of Japan
2016. 9 Achievement Award, Japan Society of Coordination Chemistry
2020. 5 Award, the Japan Petroleum Institute
2023. 5 Award, Japan Society of Vacuum and Surface Science

Current Research Topics

- Design of nanostructured catalysts and photocatalysts for renewable energy and environmental uses

Design of Nanostructured Catalysts and Photocatalysts in Nano-Porous Materials for Renewable Energy and Environmental Uses

Hiromi Yamashita

Graduate School of Engineering,

Osaka University, Osaka 565-0871, Japan

*E-mail: yamashita@mat.eng.osaka-u.ac.jp

Designs of “active sites”, “reaction fields” and “energy injection” are important for catalyst development. In the nanospace of zeolite, mesoporous silica and MOF, it is possible to control the structure of catalytic active sites in forms of fine particles, clusters, molecules, and atomic moieties, and also possible to control the reaction fields with unique properties such as hydrophobicity and electrostatic fields. Ultrafine semiconductor photocatalysts, single-site photocatalysts, plasmonic catalysts, nano-alloy catalysts, Yolk-shell catalysts, and MOF photocatalysts, can be designed for H₂ production, CO₂ fixation, H₂O₂ synthesis, and various selective reactions.

Single-site photocatalysts: The tetrahedrally coordinated metal oxide (Ti, Cr, V, Mo oxide) moieties isolated in the silica matrixes of zeolite and mesoporous silica are named “single-site photocatalysts” which can promote attractive photocatalytic reactions.

Plasmonic catalysts: As plasmonic catalysts that can strongly absorb visible light due to localized surface plasmon resonance, Ag nanoparticles (NPs) with color depending on the particle size and morphology can be synthesized with microwave heating in meso-cavities. Hybrid with Pd significantly enhanced the catalytic H₂ production from ammonia borane (AB). As plasmonic materials based on earth abundant elements, reduced molybdenum oxide with oxygen defects and doped hydrogen displayed efficient H₂ production from AB and CO₂ reduction to CO/CH₃OH under visible light irradiation.

Nano-alloy catalysts: Formic acid (FA) is widely recognized as a convenient hydrogen carrier realizing a CO₂-mediated hydrogen storage energy cycle. The nano-alloy catalysts such as PdAg, PdAu, PdCuCr having electronic rich active sites with surface basic amino groups were developed for the efficient H₂ production from FA. On the contrary, PdAg catalysts have been designed for the hydrogenation of CO₂ to FA.

Yolk-shell catalysts: A synthesis of hollow silica spheres encapsulating PdAg NPs together

with aminopolymer, poly(ethyleneimine) (PEI) can be made (PdAg+PEI@HSS) using PEI as a self-template. Owing to the CO₂ capturing ability of PEI, (PdAg+PEI@HSS) showed excellent catalytic activity for CO₂ hydrogenation.

MOF photocatalysts: H₂O₂ has attracted much attention as an environmentally friendly oxidant as well as a promising liquid fuel. Application of MOF materials for photocatalytic H₂O₂ production via oxygen reduction is attractive. The linker functionalization, the missing-linker in the MOF frameworks, and the utilization of a noble two-phase reaction system using hydrophobic MOFs are effective to improve the photocatalytic activity for H₂O₂ production.

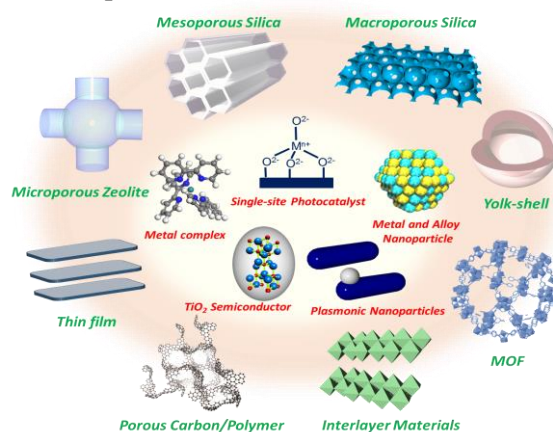


Fig. 1. Design of nanostructured catalysts and photocatalysts using nanoporous materials.

REFERENCES

- [1] Y. Kondo, et al., *Chem*, 8 (2022) 2924.
- [2] K. Shun, et al., *Chem. Sci.*, 13, (2022) 8137.
- [3] Y. Wen, et al., *Angew. Chem. Int. Ed.*, 61 (2022) e2022059.
- [4] H. Yin, et al., *Angew. Chem. Int. Ed.*, 61 (2022) e202114242.
- [5] Y. Kuwahara, et al., *Chem. Sci.*, 12 (2021) 9902.
- [6] K. Mori, et al., *Nature Comm*, 12 (2021) 3884
- [7] S. Masuda, et al., *Chem. Sci.*, 11 (2020) 4194.
- [8] K. Mori, et al., *Nature Comm*, 10 (2019) 4094.
- [9] Y. Isaka, et al., *Angew. Chem. Int. Ed.*, 58 (2019) 5402.
- [10] H. Yamashita, et al., *Chem. Soc. Rev.*, 47 (2018) 8072.
- [11] Y. Kuwahara, et al., *JACS.*, 140 (2018) 9203.
- [12] K. Mori, et al., *JACS.*, 140 (2018) 8902.
- [13] M. Wen, et al., *ACS Energy Lett.*, 2 (2017) .
- [14] H. Cheng, et al., *JACS.*, 138 (2016) 9316.
- [15] H. Cheng, et al., *Angew. Chem. Int. Ed.*, 53 (2014) 2910.
- [16] K. Fuku, et al., *Angew. Chem. Int. Ed.*, 52 (2013) 7446.
- [17] T. Kamegawa, et al., *Angew. Chem. Int. Ed.*, 52 (2013) 916.
- [18] Y. Kuwahara, et al., *JACS.*, 134 (2012) 10757.
- [19] T. Kamegawa, et al., *Adv. Mat.*, 24 (2012) 3697.

Name: Kiyotaka Asakura

Title: Professor

Affiliation: Institute for Catalysis, Hokkaido University

Address: Kita21-10, Kita-ku Sapporo 001-0021, Japan

Tel. +81-11-706-9113 E-mail. askr@cat.hokudai.ac.jp



Professional Activity

- 1984.10 – 1992. 9 Research Associate, Dept. of Chemistry, The University of Tokyo (Supervisor: Prof. Yasuhiro Iwasawa)
1992. 10 – 1993. 2 Lecturer, Dept. of Chemistry, The University of Tokyo
1993. 3 – 1994. 4 A.v Humboldt Fellow, Fritz-Haber Institute, Max Planck Society, Berlin
Germany. (Host: Professor Gerhard Ertl)
1994. 5 – 1999.3 Associate Professor, Research Center for Spectrochemistry, The University of Tokyo
1999. 4 – 2015.9 Professor, Catalysis Research Center, Hokkaido University
2014. 4 – 2018. 3 Director of Catalysis Research Center (Institute for Catalysis),
Hokkaido University
2015. 10 – Present Professor, Institute for Catalysis, Hokkaido University

International Academic Activity

2016. 8 – 2022.8 Associate Editor of PCCP, RCS
2008. 4 – Present Board member of Topics in Catalysis and Catalysis Letters.
- 2018-8 – 2022.7 Vice Chair of International XAFS Society
- 2022.8 – Present Chair of International XAFS Society

Honors and Awards (Max. 7)

- 1993.3 Young scientist award from Catalysis Society of Japan
- 2015.3 Academic Award from Japan Society of Surface Science
- 2016.3 Academic Award from Catalysis Society of Japan
- 2020.3 Academic Prize from Chemical Society of Japan

Current Research Topics (Max. 5)

- Operando X-ray absorption spectroscopy to catalysis, surface science, and electrochemistry
- Photoemission electron microscopy
- Synchrotron applications to Chemistry

The Structure and Catalysis of Single Crystal Metal Oxides and Other Compounds: How Can We Understand Its Complexity?

Kiyotaka Asakura,

¹*Institute for Catalysis, Hokkaido*

University, Sapporo, Japan

*E-mail: askr@cat.hokudai.ac.jp

The heterogeneous catalysts play a decisive role to reach the SDG though their surface structures are so complicated that we need studies on the model systems with a well-defined system such as single crystal surfaces.

In 1970's pioneering works were performed by Prof. G.Ertl and Prof. G. Somorjai on the metal single crystal surfaces. They revealed the mechanisms of CO oxidation reaction, NH₃ synthesis reactions, and the reaction-structure relationship.[1,2]

Metal oxides are the other target catalyst materials. They are used as oxidation catalysts, acid-base catalysts and photocatalysts. They are also used as catalyst supports. In 1990s the studies on the single-crystal oxide surfaces were started. However, single crystal oxide surfaces have two difficulties. One is that many oxides are insulator which hinders application of the surface sensitive electron methods. The other is the surface instability and easy reconstruction.

TiO₂(110) is the most stable semiconductor surface so that many works including STM, HREELS, LEED and SXRD have been carried out.[3] The stable TiO₂ (110) shows the reconstruction to the (1x2) structure whose atomic level surface structure has been recently revealed.[4]

X-ray technique is rarely used for the surface science studies because X-ray can deeply penetrate the bulk. The total reflection X-ray technique enhances the surface sensitivity. Polarization dependent total reflection fluorescence x-ray absorption fine structure (PTRF-XAFS) provides the 3-dimensional structures of single metal and metal nanoparticles on single crystal oxide surfaces such as TiO₂(110) and Al₂O₃(0001). It has revealed that the surface metal species

has a strong interaction with surface anion and less interaction of the anion defect. Surface premodifications of functional organic metals attained the atomical dispersion of metal species.[5,6] The other technique to investigate the oxide surface is AFM which does not require conductivity. Atomic image of MoO₃(010) was obtained.[7] Surface oxide films on a metal surface are the other choice to obtain the surface structure of insulator oxides. The oxidation of NiAl provides the Al₂O₃ single crystal film and physical vapor deposition of Si under the O₂ atmosphere on the Ru(0001) surface gives crystalline and amorphous SiO₂ film.[8,9]

In 2000, the metal compound catalysts draw much attention as a new class of catalyst such as Ni₂P, Pt₃Sn, Pd₂Ga and so on. However, the surface structure of metal compounds are further complicated due to their easier loss of light elements and reconstructions as shown in the single crystal surface of the Ni₂P(0001) and (101b0).[10]

REFERENCES

- [1] G. A. Somorjai, Y. Li, *Introduction to surface chemistry and catalysis*. Editor, John Wiley & Sons, **2010**.
- [2] G. Ertl, *Catalysis Reviews* **1980**, *21*, 201.
- [3] U. Diebold, *Surf. Sci. Reports* **2003**, *48*, 53
- [4] I. Mochizuki, H. Ariga, Y. Fukaya, K. Wada, M. Maekawa, A. Kawasuso, T. Shidara, K. Asakura, T. Hyodo, *Phys. Chem. Chem. Phys.*, **2016**, *18*, 7085
- [5] S. Takakusagi, W.-J. Chun, H. Uehara, K. Asakura, Y. Iwasawa, *Top. Catal.* **2013**, *56*, 1477.
- [6] S. Takakusagi, Y. Iwasawa, K. Asakura, *The Chemical Record* **2019**, *19*, 1244
- [7] S. Suzuki, Y. Ohminami, T. Tsutsumi, M. M. Shoib, M. Ichikawa, K. Asakura, *Chemistry Letters* **2003**, *32*, 1098
- [8] M. Bäumer, H.-J. Freund, *Progr. Surf. Sci.*, **1999**, *61*, 127
- [9] H.-J. Freund, *Acc.Chem.* **2017**, *50*, 446.
- [10] Q. Yuan, H. Ariga, K. Asakura, *Top Catal.* **2015**, *58*, 194.

Name: Kwang-Deog Jung

Title: Principal Researcher

Affiliation: Clean Energy Research Center, Korea Institute of Science and Technology

Address: 5, Hwarang-ro 14-gil Sungbuk-gu, Seoul 02792, South Korea

Tel. +82-2-958-5218, E-mail.jkdc@kist.re.kr



Professional Activity

1986. 3 – Present	Researcher in KIST (Korea Institute of Science and Technology)
1997. 5 – 1998. 5	Visiting Faculty, UC at Berkeley, USA
2003. 1 – 2003.12	Chair, Korea Energy Agency R&D CO ₂ committee
2008.1 – 2009.12	Financial Affair, KSCT (The Korean Society of Clean Technology)
2009. 1 – 2009.12	General Affair, KICChE (The Korean Institute of Chemical Engineers)
2020. 7 – Present	Director of CtX project, National Research Foundation of Korea

Honors and Awards (Max. 7)

2009. 3	Outstanding Research Team, KIST
2011. 4	Outstanding KIST researcher Award, KIST
2012. 2	Outstanding Research Team, KIST
2020. 9	Intellectual Presidential Award, Presidential Council on the Intellectual Property
2021. 2	Outstanding Research Team Award, KIST
2021. 4	Presidential Commendation, MISIT (Ministry of Science and ICT)

Current Research Topics (Max. 5)

- CO₂ hydrogenation: Methanol/DME Synthesis, Formic Acid Production
- Alkane dehydrogenation: Alkene production
- CO carbonylation/Ester hydrogenation: Acetic Acid and Methyl acetate/Ethanol synthesis
- Hydrogen production by thermo-chemical cycle (metal oxide cycle, IS cycle using VHTR)
- Artificial photosynthesis through mimetic engineering

Recent Progress in CO₂ Hydrogenation to Produce Formic Acid

Kwang-Deog Jung^{1*}, YoonLee² and Sungho Yoon³

^{1,2}Clean Energy Research Center, Seoul, South Korea

³Department of Chemistry, ChungAng University Seoul, South Korea

*E-mail: jkdc@kist.re.kr

The production of formic acid (FA) via CO₂ hydrogenation is considered a highly favorable option for the generation of value-added chemicals among CO₂ hydrogenation products. This is attributed to the fact that FA can be synthesized with the lowest H₂/CO₂ molar ratio, making it an efficient and cost-effective process. In that point of view, homogeneous catalytic system for FA production from CO₂ has been studied for replacing the conventional FA process for last decades and achieved the very high activity up to a TOF of 150,000 h⁻¹ [1]. Nonetheless, the difficulty of the homogeneous catalyst separation failed to success the development of FA processes, because the remaining catalysts in the product stream acted as a decomposition catalyst of formic acid during purification [2].

To overcome the problem, the heterogenized catalytic system was developed using triazine moiety to stabilize homogeneous Ir and Ru catalysts in our project team [3]. It was observed that the cheapest RuCl₃ precursor exhibited the activity and stability high enough even in a fixed bed reactor of three phases [4]. Recently, a FA process in a bench scale (10 kg/d) was successfully operated using triazine based Ru catalysts, although a few engineering problems are needed to be solved. The TEA/LCA analysis based on the experimental results showed the promising results on both CO₂ emission and economic view.

Nonetheless, there are a few issues to be solved in the catalytic systems as well as in the process engineering. The Ru loss is still observed in the long-run test and the difficulty of fabrication of expensive triazine based supports is another issue for developing the process. For the improvement of both

problematic catalytic issues, we studied on the n-doped carbon supports to immobilize Ru species. The effects of the carbon structures on the catalytic stability and activity were investigated. On the other hand, the N-doped TiO₂ system to immobilize Ru was studied as well. Firstly, the carbon structure of N-doped carbon will be discussed using various carbon precursors. Secondly, the importance of the pore structure on the activity will be presented. Because the catalytic system uses the viscous amine media, the pore structure should be examined to choose the catalysts. Thirdly, the importance of amine selection as reaction media to overcome thermodynamic equilibrium will be discussed. Practically, the amine for reaction media has a great influence on the energy efficiency as well as the catalytic activity. Finally, the TiO₂ supported catalytic system will be discussed to solve the fabrication problems of very hydrophobic supports. In parallel with the development of catalysts, we are planning to construct and operate the FA process of 100 kg/d scale in early 2025 and expects.

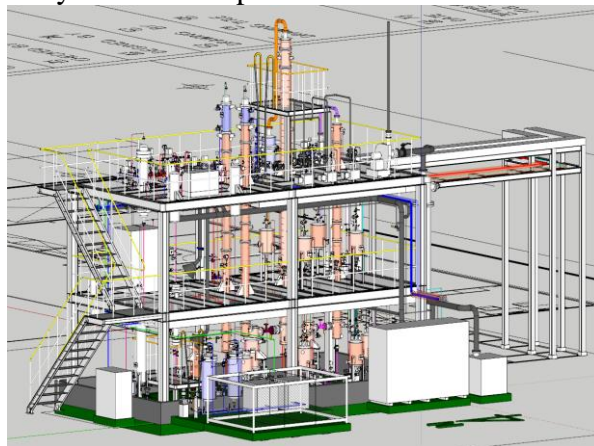


Fig. 1. The projected drawing of FA process of 100 kg/d scale

REFERENCES

- [1] R. Tanaka, M. Yamashita, K. Nozaki, J. Am. Chem. Soc., 131(40) (2009) 14168.
- [2] T. Schaub, R.A. Paciello, M. Limbach, Applied Homogeneous Catalysis with Organometallic Compounds, 3rd Ed., Wiley-VCH Verlag GmbH & Co, 2018, Chap. 35, p1601-p1614.
- [3] G.H. Gunasekar, K. Park, V. Ganesan, K. Lee, NK Kim, K.D. Jung, S. Yoon., ACS Catalysis 8(5) (2018) 73.
- [5] K.Park, G.H. Gunasekar, S.H. Kim, H. Park, S. Kim, K. Park, K.D. Jung, S. Yoon. Green Chem. 22(5) (2020) 1639.