

KAIST'S TOP 10 RESEARCH ACHIEVEMENTS OF 2020

KAIST ranked 12th in QS Asia University in 2021,
Ranked 2nd in domestic university rankings.

The professors and researchers of KAIST have been
consistently showing the world the full potential of
Korea's science and technology capabilities.

The followings are KAIST's top 10 research results
published and highlighted in world-renowned
scientific journals in 2020.



TOP 10 RESEARCH
ACHIEVEMENTS

Rare-earth-platinum alloy nanoparticles for catalysis

Department

Department of Chemistry

Principal Investigator

Ryong Ryoo

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Metal nanocatalysts are a vital component in chemical processes. Particularly, controlling the catalytic properties by alloying 2 or more metal components in the form of nanoparticles is highly important. However, rare-earth elements could not be formed in the form of metal nanoparticles due to their low chemical reduction potential. Prof. Ryoo and his group members established a route to disperse rare-earth elements in the form of single atomic species using the surface of mesoporous zeolite. This increased the chemical reduction potential of the rare earth elements, thereby allowing the formation of rare-earth-platinum alloy nanoparticles. The alloy nanoparticle catalysts exhibited an outstanding performance in a petrochemical reaction producing propylene. This result provides a new concept in the field of heterogeneous catalysis and will greatly contribute to the pioneering of basic research and application in this field.

1. Background

Professor Ryong Ryoo has performed research on the synthesis of mesoporous materials over the past two decades at KAIST. Prof. Ryoo published 5 papers in Nature and 1 paper in Science regarding the synthesis of various porous materials, including the CMK-series mesoporous carbons which was named after KAIST. In the last semester before his retirement, Prof. Ryoo published a paper in Nature as the first author and corresponding author, which is titled "rare-earth-platinum alloy nanoparticles in mesoporous zeolite for catalysis". Upon expansion of his research direction from the synthesis of mesoporous materials to the exploration of surface chemical properties, Prof. Ryoo has newly discovered a phenomenon (that is, dispersing rare-earth elements on the mesopore surface in a single atomic state) and explored the possibility of its application in the field of catalyst synthesis. This research has opened up the opportunity of applying the mesoporous zeolite pioneered by KAIST as a propane dehydrogenation catalyst. Propane dehydrogenation is a reaction that converts propane in shale gas and natural gas to propylene and is currently the most important research topic in the field of petrochemical industry.

2. Contents

Rare-earth elements are difficult to reduce into a metallic state due to their low chemical reaction potential, making them difficult to form into metal nanoparticles or alloy nanoparticles with other elements. Prof. Ryong Ryoo's research team succeeded in dispersing rare-earth elements on the surface of the zeolite as single atomic species by controlling the surface properties of the mesoporous zeolite.

The single atomically dispersed rare-earth elements exhibited higher chemical reduction potential compared to that of the conventional rare-earth oxides, allowing them to be easily reduced. Using this strategy, the research team could successfully generate intermetallic compound nanoparticles between rare-earth elements (La, Ce, Y) and platinum, which were previously considered impossible. The Pt-La, Pt-Y, and Pt-Ce nanoparticles obtained in this manner were intermetallic compounds having an L12 structure, as seen in the atomic-resolution STEM image of Fig. 1a. The rare-earth-platinum nanoparticles showed excellent catalytic activity and stability in the propane dehydrogenation reaction. The catalytic activity of rare-earth-platinum catalysts was maintained for as short as 7 days to as long as 20 days, as seen in Figure 1b and 1c. This is several times to tens of times longer than the catalytic lifetime of the commercial Pt-Sn catalyst supported on alumina.

3. Expected effect

The principle of the atomistic alloying process discovered in this study would be applicable for the formation alloys not only between platinum and rare-earths but also between platinum and other transition metals. It is expected that the synthesis strategy would be helpful for the design of other alloy catalysts for not only propane dehydrogenation but also other industrially important chemical reactions.

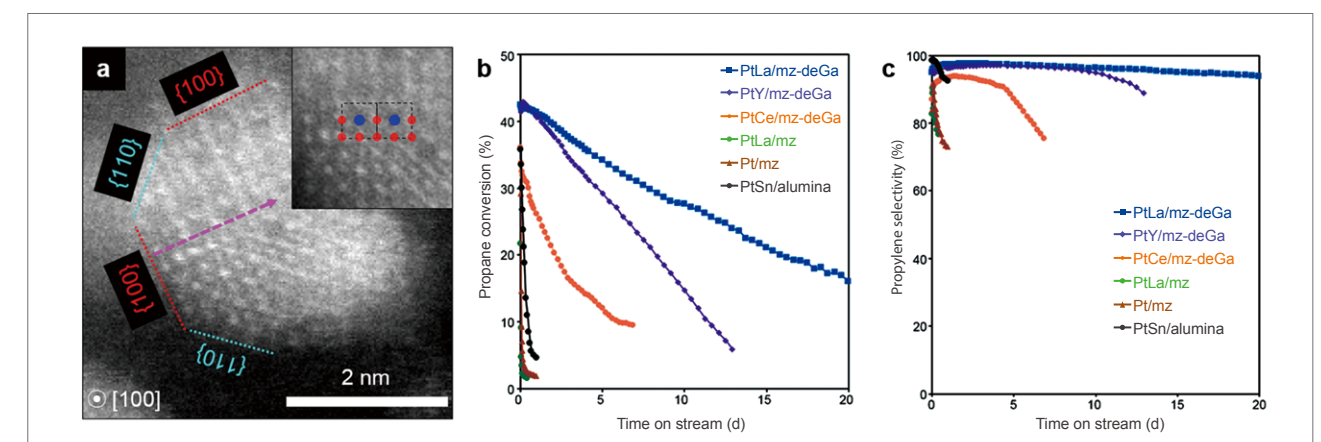


Figure 1. (a) Atomic resolution STEM photograph of Pt₃Y intermetallic compound alloy nanoparticles with L12 structure supported on mesoporous zeolite. (b) Propane conversion and (c) propylene selectivity over time of various platinum-based catalysts in propane dehydrogenation



Research outcomes

[Paper] R. Ryoo,* J. Kim, C. Jo, S. W. Han, J.-C. Kim, H. Park, J. Han, H. S. Shin, and J. W. Shin, "Rare-earth-platinum alloy nanoparticles in mesoporous zeolite for catalysis", Nature 585, 221–224 (2020) [2019 Impact Factor = 42.778].

[Patent] R. Ryoo, J. Kim, C. Jo, J.-C. Kim, in preparation

[Press release] Prof. Ryong Ryoo at KAIST develops Pt-REE alloy nanocatalysts, Yonhap News, September 10, 2020

KAIST develops propylene production technology from shale gas, Chosun Biz, September 10, 2020

Research funding

This research was funded by Institute for Basic Science (IBS-R004-D1-2020-a00)

TOP 10 RESEARCH
ACHIEVEMENTS

Tracking the movements of all atoms in a molecule

Department

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Fundamental studies of chemical reactions often consider the molecular dynamics along a reaction coordinate using a calculated or suggested potential energy surface. But fully mapping such dynamics experimentally, by following all nuclear motions is challenging and has not yet been realized even for simple triatomic molecules. In this work, we track the movements of all the gold atoms in the gold trimer complex during photoinduced bond formation using femtosecond X-ray liquidography. Tracking the atomic movements reveals that within the first 35 femtoseconds after photoexcitation, a covalent bond forms and the second covalent bond subsequently forms within 360 femtoseconds. Femtosecond X-ray liquidography offers a means of tracking the atomic motions involved in many chemical reactions.

1. Background

Targeted cancer drugs work by striking a tight bond between cancer cell and specific molecular targets that are involved in the growth and spread of cancer. Detailed images of such chemical bonding sites or pathways can provide key information necessary for maximizing the efficacy of oncogene treatments. In this regard, fundamental studies of chemical reactions often consider the molecular dynamics along a reaction coordinate using a calculated or suggested potential energy surface. However, atomic movements in a molecule have never been captured in the middle of the action, not even for an extremely simple molecule such as a triatomic molecule, made of only three atoms. In this work, we track the movements of all the gold atoms in the gold trimer complex during photoinduced bond formation using femtosecond X-ray liquidography.

2. Contents

We succeeded in observing the real-time positions of atoms in the molecule that forms chemical bonds and uncovering whether two chemical bonds are formed one by one or simultaneously. They also unveiled how quickly and how far the distance between atoms changes in the process of the chemical bond formation. In 2015, we reported in Nature the observation of the formation of two chemical bonds in a gold trimer (Nature, 2015, 518, 385 – 389). After 5 years, based on dramatically improved experimental and analytical methods, they succeeded in observing in real time the movements of the three gold atoms even before the chemical bonds are formed and revealing even the specific reaction mechanism in which two chemical bonds are formed sequentially rather than simultaneously (Nature, 2020, 582m 520-524).

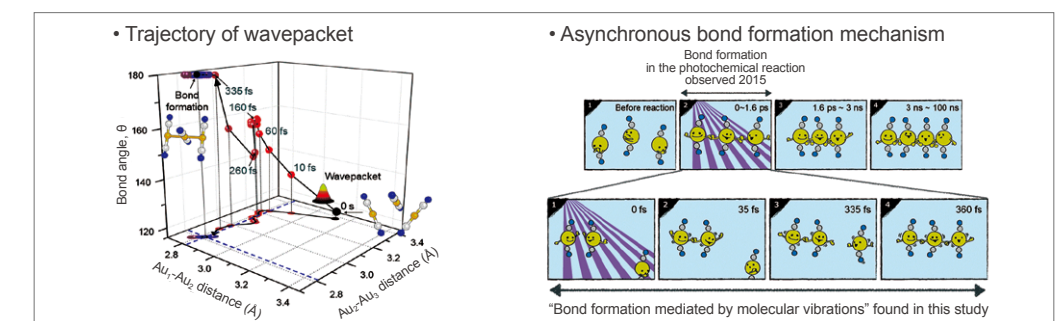
The basic unit that determines the properties of a matter is a molecule, and the basic unit that makes up a molecule is an atom. In other words, a molecule forms when these atoms are bound together through a chemical bond. For example, protein molecules are made up of thousands of atoms, but revealing how these atoms are actually moving has never been observed directly, even for an extremely simple molecule such as a triatomic molecule, made of only three atoms. To find the answer to this basic question, the research team used a gold trimer complex as a model system. In the gold trimer complex, three gold atoms are located in close proximity, and upon laser illumination, they react to form chemical bonds.

It is never easy to capture atomic movements in real time because the atomic movement is extremely fast, that is the femtosecond level in time, and the extent of the movement is minute, that is at the angstrom level in space. To solve this challenging task, we used an experimental technique called "femtosecond x-ray liquidography (solution scattering)", which combines laser photolysis and x-ray scattering techniques. A laser pulse was used to irradiate the sample, thereby initiating the chemical bond formation reaction in the gold trimer complex, and "femtosecond x-ray pulses" obtained from a special light source called x-ray free-electron laser were used to interrogate the bond-forming process. By analyzing time-resolved x-ray scattering images, real-time positions of the three gold atoms were tracked.

Tracking the atomic movements reveals that within the first 60 femtoseconds after photoexcitation, a covalent bond forms and the second covalent bond subsequently forms within 360 femtoseconds. In addition, it was observed that the atoms did not stay in the same position after the chemical bonds were formed, but the distance between the atoms increased and decreased periodically, exhibiting the molecular vibration. In this study, how fast and how much the molecule vibrates were observed in real time.

3. Expected effect

The research team plans to apply the method of 'real-time tracking of atomic positions in a molecule and molecular vibration using femtosecond x-ray scattering' realized through this study to reveal mechanisms of organic and inorganic catalytic reactions and reactions involving proteins in the human body. Through the applications, it is expected to maximize the efficiency of various catalytic reactions used industrially, and to provide basic information necessary for controlling protein reactions, treating diseases, and developing new drugs.



Research outcomes

[Paper] J. G. Kim, S. Nozawa, H. Kim, E. H. Choi, T. Sato, T. W. Kim, K. H. Kim, H. Ki, J. Kim, M. Choi, Y. Lee, J. Heo, K. Y. Oang, K. Ichyanagi, R. Fukaya, J. H. Lee, J. Park, I. Eom, S. H. Chun, S. Kim, M. Kim, T. Katayama, T. Togashi, S. Owada, M. Yabashi, S. J. Lee, S. Lee, C. W. Ahn, D. -S. Ahn, J. Moon, S. Choi, J. Kim, T. Joo, J. Kim, S. Adachi, and H. Ihee*, "Mapping the emergence of molecular vibrations mediating bond formation", Nature, 582, 520-524 (2020) [2019 Impact Factor = 42.778]

Research funding

This work was supported by the Institute of Basic Science (IBS-R004).



Astrocytes phagocytose adult hippocampal synapses for circuit homeostasis

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In the adult hippocampus, synapses undergo constant formation and elimination. However, the exact function and regulatory process of synapse elimination in the adult brain are largely unknown. Here, we reveal a significant role of astrocytic phagocytosis in maintaining proper hippocampal synaptic connectivity and plasticity. By utilizing mCherry-eGFP phagocytosis reporters, we find that excitatory as well as inhibitory synapses are eliminated by glial phagocytosis in the adult hippocampal CA1 region. Surprisingly, our data show that astrocytes play a major role in neuronal activity-dependent elimination of excitatory synapses. Furthermore, knocking-out the phagocytic receptor Megf10 in adult astrocytes reduces their ability to eliminate excitatory synapses, and as a result, induces the accumulation of excessive but functionally impaired synapses. Finally, we show that Megf10 knock-out mice exhibit defective long-term synaptic plasticity with impaired hippocampal memory formation. Taken together, our data provide strong evidence that astrocytes eliminate unnecessary excitatory synaptic connections in the adult hippocampus through Megf10, and that this astrocytic function is critical for homeostasis of circuit connectivity important for cognitive functions.

1. Background

Adult synapses continuously undergo formation and elimination, and these synapse turnover events are well represented during experience-dependent plasticity and cognitive functions. However, how synapses in the adult brain get eliminated and whether synapse elimination plays a direct role in circuit homeostasis are not well known. Previously, we have found a phagocytic function of astrocytes in eliminating synapses during postnatal development (Chung et al., 2013, Nature). By phagocytosing synapses through the MEGF10 and MERTK phagocytic receptors, astrocytes actively contribute to activity-dependent synapse pruning and developmental circuit refinement. Moreover, contrary to the previous notion that microglia are the sole mediator of synapse elimination, astrocytes were shown to play a major role in eliminating synapses in developing brains. Based on this finding, we hypothesized that synapses in the adult brains is also refined by astrocytic phagocytosis, and that such elimination is critical for maintaining circuit homeostasis.

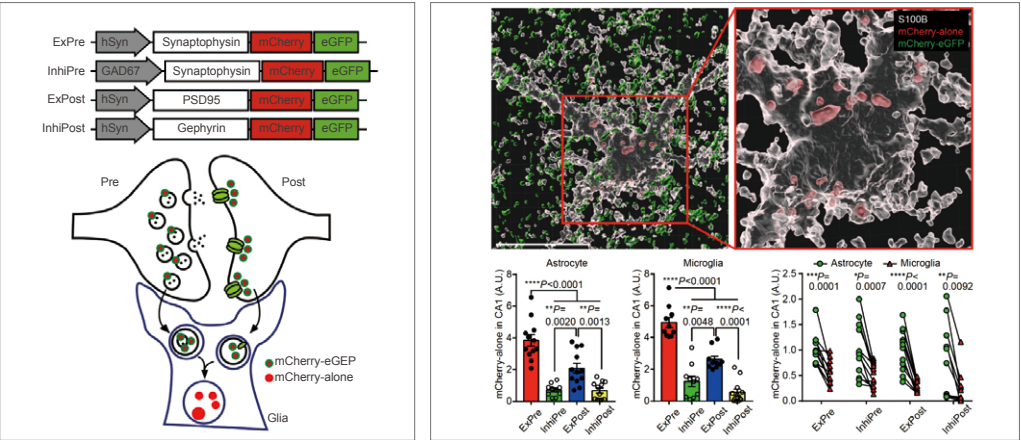
2. Contents

We first developed a novel sensor to detect synapse elimination by glial cells in the adult brains. We took advantage of an mCherry-eGFP reporter system that has been previously utilized to monitor autophagic acidification influx. Whereas both mCherry and eGFP maintain intact fluorescent intensities under neutral

pH conditions, only the mCherry but not eGFP signal is preserved in acidic environments, such as in the lysosome. By tagging an identical pH-indicator (i.e. mCherry-eGFP) to different synapse types, we show that our AAV-based synapse phagocytosis reporters accurately incorporate into excitatory and inhibitory synapses in vivo and produce mCherry-alone puncta when they are engulfed by glial cells (Fig 1). Next, to specifically block synapse elimination by astrocytes, we generated astrocyte-specific Megf10 knock-out animals where Megf10 deletion was achieved by tamoxifen-induced Cre activation. Using these animals, we were able to selectively and locally downregulate astrocytic synapse phagocytosis in the hippocampus. Using these novel tools, we show that, for the first time, it is astrocytes, but not microglia, that constantly eliminate excessive and unnecessary adult excitatory synaptic connections in response to neuronal activity. We further show that without this astrocytic function, precise re-patterning and homeostasis of hippocampal circuit connectivity cannot be maintained. As a result, the animal with defective astrocytic phagocytosis also showed impaired hippocampal learning and memory.

Figure 1.
A working model of mCherry-eGFP synapse phagocytosis reporter

Figure 2.
3D reconstruction showing astrocyte (White, S100B) with reporter-tagged synapses (green, mCherry-eGFP) and engulfed synapses (red, mCherry-alone). Detailed quantification revealed astrocytes play a major role in eliminating excitatory synapses than microglia in the adult hippocampus.



3. Expected effect

Our paper challenges the general consensus in this field that microglia are the primary synapse phagocytes that control synapse number in the brains. By utilizing unbiased synapse phagocytic reporters, we show that at least in the adult hippocampal CA1 region, astrocytes are the major player in eliminating synapses, and this astrocytic function is essential for controlling synapse number and plasticity. Secondly, our study shed light on the functional role of synapse elimination during learning processes: not only making new ones, memory learning and storing information also require eliminating unnecessary connections. We provide evidence that astrocytes play a major role in this process. We are just beginning to understand how astrocytic phagocytosis affects synapse maturation and homeostasis. In our preliminary data, each brain regions appears to have different rates of synapse elimination by astrocytes. Such differences can be originated from various internal or external factors. Elucidating how astrocytes integrate those factors and modulate each circuit would be our immediate next steps. Our long-term goal is understanding how astrocyte-mediated synapse turnover affects the initiation and progression of various neurological disorders.



Research outcomes
[Paper] Lee JH*, Kim JY*, Noh S, Lee H, Lee SY, Mun JY, Park HJ*, Chun WS*. Astrocytes phagocytose adult hippocampal synapses for circuit homeostasis, Nature (Article), 23 December 2020. (* Equally contributed).

Research funding
Samsung Science & Technology Foundation (SSTF-BA1701-18)
National Research Foundation of Korea (2016M3C7A190539)



Gold and Bronze Medalists in Cybathlon 2020: The Fastest and the Most Versatile Wearable Robot in the World

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The Cybathlon 2020, an international competition for innovative assistive robot technologies for people with disabilities, was held for Korean teams at KAIST on November 13. The teams Angel Robotics 1 and 2, both from the Robotic Systems Control Laboratory and a robotics startup company led by Professor Kyoungchul Kong of the Department of Mechanical Engineering, competed against twelve other teams and placed the first and the third.

1. Background

The development of medical and rehabilitation technology have increased the life expectancy of the spinal cord injury (SCI) patients. The robotic technologies for these people have an ample room for development in that the current ones are yet to be fully and naturally incorporated into the wearers' daily lives. The blueprint of those improvements should mainly be focused on accomplishing the agility and versatility, which are the essential prerequisites for carrying out the various tasks in our daily lives. Accordingly, a research team in KAIST sets a goal to create the most functional wearable robots for the people with disabilities and to evaluate the technical performance via the global competition in Cybathlon 2020.

2. Key features

The factors that make the WalkON Suit the fastest and the most versatile wearable robot in the world.

Highest walking speed among wearable robots

The exoskeletal walking had been too slow for the daily lives, not even being able to assist in crossing the crosswalk for the given period. The walking speed of WalkON Suit is now similar as the normal walking speed, i.e., 0.84m/s, which is the world record.

Faster task completion time than those of the powered wheelchairs

The wheelchairs have been widely used as an equipment for the movement of the people with disabilities. The results of Cybathlon 2020, however, verify that the agility of the WalkON Suit in completing the tasks match those of the powered wheelchairs, even superior for some tasks.

Descending stairs while facing forward, one stair per step

As walking down the stairs has been the most challenging task, other research teams had chosen a way to walk backward. This method, however, is dissimilar to the natural human motion nor is it practical for the daily lives of people. The team of KAIST successfully developed the technology of walking down one stair per step.

3. Summary of the global competition

The aim of benefiting more people with our technology

The assistive methodologies and hardware components are not intended for the usage of just one person; it rather has been directed toward a more widespread usage by the public. We have enriched our research by the help of six disabled participants in preparation for the competition.

Rank	Research Team	Race 1		Race 2		Race 3	
1	KAIST	100	4m 46s	100	3m 57s	100	3m 47s
2	Twice	100	5m 21s	100	4m 40s	100	4m 49s
3	KAIST	100	6m 11s	100	6m 39s	100	5m 51s
4	IHMC Robotics	85	6m 00s	100	6m 51s		

The results of the powered exoskeleton race in Cybathlon 2020 are given in the table. Our team won both the gold and bronze medal by carrying out all of the 6 tasks without any failure while accomplishing the best record among all the teams.

4. Expected effects

The competition in Cybathlon 2020 further accelerated the advancement of robotic technology. People with disabilities such as complete paraplegia, spinal cord injuries, etc., are expected to be more capable of utilizing the most advanced technologies in motion assistance. In the near future, the wearable robots may improve the quality of lives of our target users and assist in them achieving more in their lives. With the accomplishment in Cybathlon 2020, we have proved that this future is near us in KAIST, Korea.



Research outcomes

[Award] Gold medal in Powered Exoskeleton Race of Cybathlon 2020
Bronze medal in Powered Exoskeleton Race of Cybathlon 2020

Research funding

This work was supported by the Technology Innovation Program [or Industrial Strategic Technology Development Program (20003914)] funded by the Ministry of Trade, Industry and Energy (MOTIE, South Korea).

TOP 10 RESEARCH
ACHIEVEMENTS

Fair Machine Learning

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As machine learning (ML) becomes prevalent in our daily lives involving a widening array of applications such as medicine, finance, job hiring and criminal justice, one critical aspect in the design of ML algorithms is to ensure fairness: guaranteeing the irrelevancy of a prediction to sensitive attributes such as gender and race. There has been a proliferation of fair ML algorithms. One challenge that arises in the prior efforts is that they rely upon "proxies" for fairness measures, thereby suffering from achieving the optimal fairness-vs-accuracy tradeoff. In this work, we propose an information-theoretic approach based on mutual information (MI) that can faithfully respect fairness measures, thus obtaining the optimal tradeoff. We also develop a robust version of the method that can well protect against data poisoning. In addition, we develop an upgraded version based on kernel density estimation to address the training instability problem that most MI-based algorithms are faced with. This work was published in the top-tier AI conferences: ICML 2020 and NeurIPS 2020. We expect that our research enables fair ML systems to promote social welfare while embracing equity and inclusion for minority populations.

1. Background

The last decade has witnessed an unprecedented explosion of academic and popular interests in machine learning. Machine learning is now employed to make critical decisions that affect human lives, cultures, and rights, e.g., filtering job applicants, loan screening, and informing bail & parole decision. With a surge of such sensitive applications, there has been a growing concern in the design of trustworthy AI. One critical issue of recent interest is concerning discrimination against minor groups and underrepresented populations. See Fig. 1. Training data often contains biases and this may lead to unfair classifiers that make biased decisions against minority populations. This motivates the need for the design of fair classifiers



Figure1. (Upper) In 2016, ProPublica revealed that COMPAS tends to discriminate black criminals against whites. For instance, a white criminal in the above, named Fugett, was rated a low recidivism score, although he was later rearrested several times. (lower) U.S. Supreme Court has been employing machine learning software named COMPAS for the purpose of predicting the likelihood of recidivism of criminals. COMPAS outputs a recidivism score, ranging from 0 to 10 (the higher the more likelihood of recidivism).

that can guarantee the irrelevancy of a prediction to sensitive attributes such as gender and race.

There has been a proliferation of fair classifiers. One prominent approach in the prior algorithms is to introduce expressible "proxies" for fairness measures, instead of directly employing fairness measures that are known to be non-straightforward to compute. However, such a proxy-based approach may not ensure the best fairness performance.

2. Contents

During the past years, we have been pioneering this crucial and challenging topic. We made two major contributions. First, we proposed a computationally efficient fair classifier that faithfully respects fairness measures without relying upon their proxies [Paper 1]. The left plot in Fig. 2 demonstrates the accuracy-fairness tradeoff of our proposed algorithm in terms of a popular fairness measure called Disparate Impact (the higher the fairer). We see that ours offers a better tradeoff performance relative to the state of the art that relies upon a proxy of Disparate Impact. Our second contribution is to develop a unified framework that holistically satisfies the two crucial aspects in trustworthy AI: (i) achieving fairness; (ii) ensuring robustness against data poisoning [Paper 2]. As demonstrated in the right plot of Fig. 2, our unified approach can achieve the optimal accuracy-fairness tradeoff, while attaining minimal tradeoff degradation in the presence of data poisoning. In contrast, prior fair algorithms are vulnerable to data poisoning.

3. Expected effect

As machine learning is prevalent in a widening array of sensitive applications that require critical decisions, fair machine learning plays a crucial role to bring about healthy, fruitful, and fair societies that can nurture truly innovative and diverse ideas from a variety of different demographics. Applications are everywhere, including government agencies, financial institutions, companies, public institutions, medical institutions, to name a few. Our fair-robust classifier is a core technology that can equip them with two crucial capabilities: ensuring fairness and protecting against data poisoning, and it is expected to improve the lives of historically underrepresented populations as well as equally support all populations. We believe that our work can promote social welfare while embracing equity and inclusion for minority populations.

[Ref 1]
D. Dua and C. Graff, "UCI machine learning repository," 2017.

[Ref 2]
B. H. Zhang, B. Lemoine and M. Mitchell, "Mitigating unwanted biases with adversarial learning," AIES, 2018.

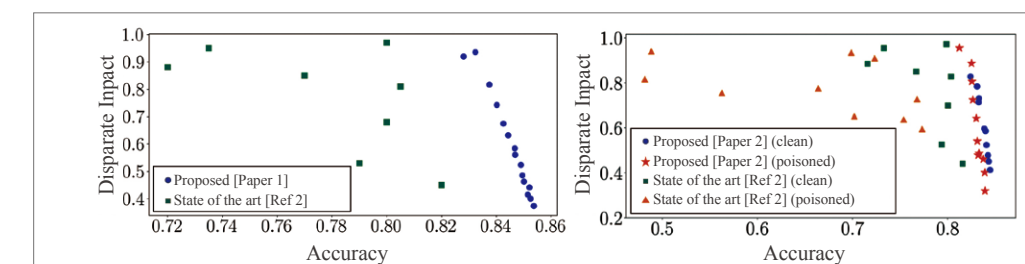


Figure 2. (Left) Accuracy-fairness tradeoff of our proposed algorithm evaluated on AdultCensus [Ref 1]; (Right) Accuracy-fairness tradeoff on clean and poisoned (10% of data) datasets. We observe that our proposed algorithms achieve better tradeoffs compared to Google's recent fair classifier: Adversarial Debiasing [Ref 2].



Research outcomes

[Paper] J. Cho, G. Hwang and C. Suh, "A fair classifier using kernel density estimation," NeurIPS, Dec. 2020 (top-tier AI conference).
Y. Roh, K. Lee, S. E. Whang and C. Suh, "FR-Train: A mutual information-based approach to fair and robust training," ICML, Aug. 2020 (top-tier AI conference).

[Award] A two-year grant from U.S. Air Force Office of Scientific Research (AFOSR)
Naver paper award, Aug. 2020.

Research funding

Air Force Office of Scientific Research (AFOSR) grant funded by the U.S. government (No. FA2386-19-1-4050, "Validating Simulator-based Learning via Interpretation")
Institute for Information & communications Technology Planning & Evaluation (IITP) grant funded by the Korea government (MSIT) (No. 2019-0-01396, "Development of framework for analyzing, detecting, mitigating of bias in AI model and training data")



GANPU: An On-Device Training Processor for Generative Adversarial Networks

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This research is regarding an energy-efficient AI processor for generative adversarial networks (GAN), targeting inference and training of the models on mobile platforms. GANs are highly praised for their ability to generative new data, but they not only require larger number of computations, but also consist of multiple networks, making it difficult to optimized the hardware architecture. This research proposed a reconfigurable processor architecture to efficiently handle multi-network and a method to accelerate sparse convolution. It achieved 4.8 times higher energy-efficiency compared to the previous state-of-the-art, enabling on-device AI on performance-limited and battery-limited mobile devices.

1. Background

Generative Adversarial Networks (GAN) can generate and recreate new images, so they are used in a wide range of applications, from image style transfer to synthetic voice generation. Deepfakes, which have become a big social issue by synthesizing other people's faces on top of the existing videos, is also a GAN-based technique. GANs can be used in various applications of mobile devices where a lot of video and photo contents are produced as well as consumed. Therefore, they have attracted great attention not only from academia but also from industry.

However, GANs have complex algorithmic architectures, incorporating multiple Deep Neural Networks (DNN) to be trained in a single model. Moreover, each individual DNNs in a GAN have different characteristics, making it difficult to optimize as a semiconductor accelerator. In addition, GANs require more computations than conventional AI models to generate high-resolution images due to the high video fidelity requirement of the recent displays and image sensors. Therefore, until this research, mobile devices were regarded unsuitable to implement GANs on due to limited speed and power. Moreover, there are even greater limitations to realize on-device training for advanced GAN operations.

2. Contents

Most of the previous DNN accelerators supported only inference. Although a few DNN training accelerators have been introduced, they only supported a single DNN. In this research, we proposed the world's first low-power GANPU (Generative Adversarial Networks Processor Unit) capable of not only inference but also training on mobile devices and supports multi-DNN such as advanced GAN.

More specifically, adaptive spatio-temporal workload multiplexing (ASTM) is proposed that variably rearranges the processor architecture according to types and numbers of independent DNNs to accelerate

multi-DNN such as GAN. ASTM enables efficient allocation of limited resources such as external memory bandwidth and computational resources. Also, there are lots of zeros in the data due to the nonlinear function of the DNN. By designing a processor architecture that skips input-output activation sparsity, the speed and energy efficiency in the inference and training are maximized. The proposed architecture achieved a 28.53x throughput increase when input-output activation sparsity is 90%.

The GANPU with the above technology achieved 4.8 times higher energy efficiency than the conventional DNN accelerators. Additionally, they showed an application that allows users to directly modify photos taken with a tablet camera on a tablet connected to GANPU. A face modification system is also implemented in which GANPU automatically completes and displays 17 features such as hair, glasses, and eyebrows on the face in the photo.

(Demonstration Video – <https://www.youtube.com/watch?v=HnNWsgqkEU0>)

3. Expected effects

The world's first low-power AI semiconductor that enables training as well as inference on a single chip and accelerates multi DNNs at the same time. It is significant in that it enables new applications of artificial intelligence such as face modification, synthetic voice generation, and video synthetic in mobile devices.

In addition, the proposed AI semiconductor in this study enables privacy protection by supporting on-device GAN training without sending data to the server. Moreover, its utilization is noted in that it is a processor that enables style transfer, image synthesis, and restoration of distorted images on mobile devices. From this, a new era of AI is opened in which mobile devices can draw natural pictures by themselves.



Fig 1. Demo System with GANPU

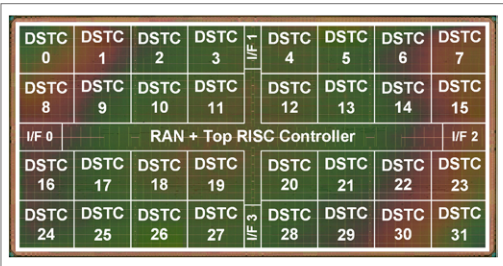


Fig 2. Chip Photo



Research outcomes

- [Paper] S. Kang, D. Han, J. Lee, D. Im, S. Kim, S. Kim, H-J. Yoo, "GANPU: A 135TFLOPS/W Multi-DNN Training Processor for GANs with Speculative Dual-Sparsity Exploitation," 2020 IEEE International Solid-State Circuits Conference (ISSCC 2020).
- S. Kang, D. Han, J. Lee, D. Im, S. Kim, S. Kim, J. Ryu, H-J. Yoo, "GANPU: A Versatile Many-Core Processor for Training GAN on Mobile Devices with Speculative Dual-Sparsity Exploitation," 2020 IEEE Hot Chips Symposium. Air Force Office of Scientific Research (AFOSR) Naver paper award, Aug. 2020.
- [Patent] Domestic patent · US patent application completed
- [Award] 26th Samsung Electronics Human Tech Thesis Award - Gold Prize Award
2020 Microsoft Research Asia Fellowship Award
- [Press release] YTN news report, "Development of self-drawing AI semiconductor chip"
https://www.ytn.co.kr/_ln/0115_202004070308303992
Reported on about 30 domestic media including Munhwa-Ilbo and Donga-Science
<http://www.munhwa.com/news/view.html?no=2020050401031805000002&mobile=false>

TOP 10 RESEARCH
ACHIEVEMENTS

Epigenetic Reprogramming of Cancer via Microenvironment Engineering

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In many cancers, tumour progression is associated with increased tissue stiffness. Yet the mechanisms associating tissue stiffness with tumorigenesis and malignant transformation are unclear. We show that the stiffness of the extracellular matrix of gastric cancer reversibly regulates the DNA methylation of the promoter region of the oncogenic Yes-associated protein (YAP). Our findings offer the insight into promising mechanotherapeutic strategies specifically targeting the mechanical properties of the ECM, to regulate epigenetic status and oncogenic transcription activity of malignant tumor cells.

1. Background

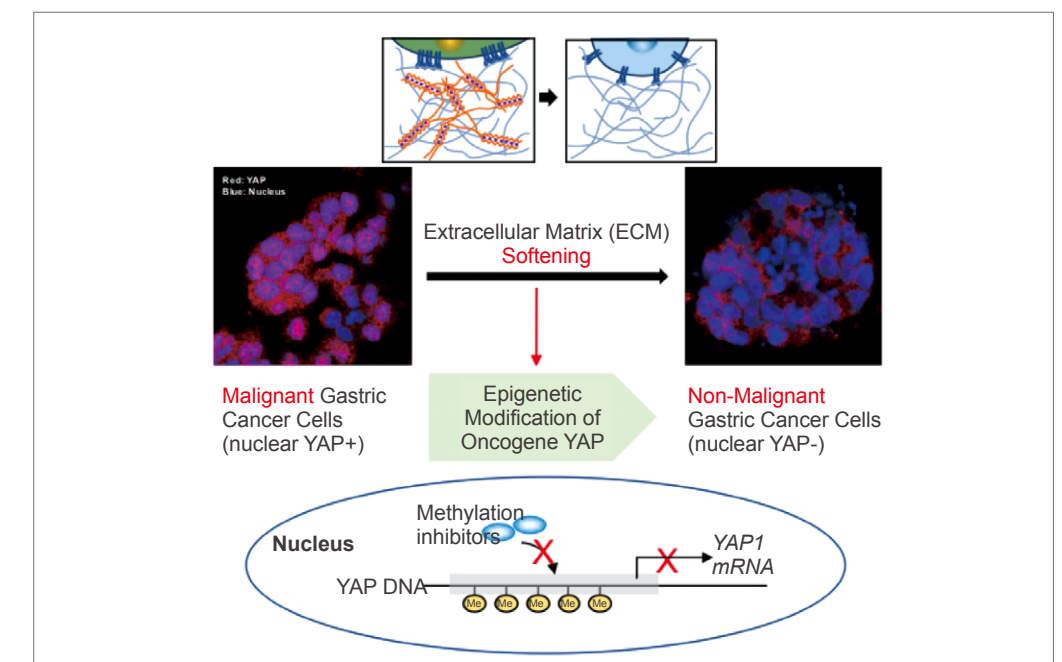
Extracellular cues are recognized as potent regulators of epigenetics in the development and progression of solid tumours. Among the extracellular signals, increased extracellular matrix (ECM) stiffness is closely associated with pathological states and is considered a critical factor that precedes tumorigenesis. While it remains unclear exactly how ECM stiffening causes the malignant phenotype of cancer cells, there is evidence that external biophysical cues can be mechanically transmitted via cytoskeletal tension into the nucleus, impacting gene expression through mechanosensors and intracellular mechanotransducers, such as Yes-associated protein (YAP). Although mechanical stimulus is recognized as a crucial determinant of cancer cell fate, hinting at the involvement of epigenetic regulation, it remains unclear whether YAP activation by matrix stiffness is accompanied by epigenetic changes, and whether any such effects are reversed by matrix stiffness alteration.

2. Contents

To investigate matrix stiffness-induced mechanotransduction at the epigenetic level, we studied gastric cancer cells. Gastric cancer (GC) is one of the leading causes of death in East Asia, and GC incidence is rising among younger generations of adults. Extracellular matrix (ECM) density is increased in GC, and it is widely known that a stiff cancer ECM helps cancer cells proliferate and invade into nearby tissues; consequently, stiff tumor microenvironments correlate to a worse prognosis and decreased life expectancy.

In order to confirm matrix stiffness-induced mechanotransduction, we constructed collagen and interpenetrating polymer network (IPN)-based 3D gel matrices, embedded with gastric cancer cells, to recapitulate the tumor microenvironment. The stiff matrix (IPN) induced YAP activation and promoted a mesenchymal phenotype of gastric cancer cells. The YAP expression increasingly deactivated with time after matrix softening (Figure 1). Total YAP expression was also reduced, indicating that lower

transcriptional activity may epigenetically reduce total YAP gene expression. DNA hypomethylation of YAP induced by a stiff matrix can be reversed by softening the matrix. The methylation index of YAP DNA recovered with time after matrix softening. Transcriptome analysis by bulk RNA sequencing and Chromatin Immunoprecipitation-Atlas analysis identified DNA methylation-modifying genes that were recovered by matrix softening by comparing control and YAP-depleted cells. siRNA treatments of 3 genes (GRHL2, TET2, and KMT2A) confirmed the recovery of YAP DNA methylation comparable to the soft control. Upon a proliferation and drug resistance analysis, GC cells in the softened matrix were less proliferative and less resistant to drugs than those in the stiff matrix, confirming that the softening was effective in suppressing malignancy. These findings suggest that mechanotherapy to soften tumor tissues and surrounding ECM may be an appropriate addition along with chemotherapy for better patient prognosis.



3. Expected effect

Clinically, it is important to identify potential therapeutic vulnerabilities in ECM-mediated tumour progression because tumours such as scirrhus gastric cancer harbour the poorest prognosis while few therapies are available. DNA methylation is known to be reversible, similar to other biochemical and physiological modifications, and is thus regarded as a promising target for therapeutic interventions. In this respect, our findings offer insight into promising mechanotherapeutic strategies specifically targeting the mechanical properties of the ECM, to regulate the epigenetic status and oncogenic transcription activity of malignant tumour cells.



Research outcomes

[Paper] M. Jang, J. An, S. W. Oh, J. Y. Lim, J. Kim, J. K. Choi*, J.-H. Cheong*, P. Kim*, "Matrix stiffness epigenetically regulates the oncogenic activation of the Yes-associated protein in gastric cancer", Nature Biomedical Engineering, (2020) [2020 IF: 18.952]

Research funding

This research was funded by the Basic Science Research Program through the National Research Foundation of Korea (NRF), funded by the Ministry of Education (NRF-2019R1A2C2084142), and the Korea Health Technology R&D Project through the Korea Health Industry Development Institute (KHIDI), funded by the Ministry of Health and Welfare, Republic of Korea (HI14C1324).



Fundamental Technology Development for Reverse Aging

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Our study showed that cellular senescence, previously considered an irreversible biological phenomenon, may represent a reversible state and it can be systematically controlled. To identify targets the inhibition of which would convert senescent cells into quiescent cells, we constructed a molecular regulatory network model of cellular senescence. From the model simulation, we identified PDK1 as a promising target that can revert the senescent state into a quiescent state. We validated this prediction in experiments with human dermal fibroblasts, which showed that PDK1 inhibition eradicates senescence hallmarks by suppressing both nuclear factor κ B and mTOR signaling through the inactivation of a positive feedback loop composed of PDK1, AKT, I κ B κ B, and PTEN, resulting in restored skin regeneration capacity. Our findings provide insight into a potential therapeutic strategy to treat aging and age-related diseases. Building on this discovery, the Amorepacific R&D center is developing cosmetics that can improve wrinkles on aged skin using PDK1 inhibiting ingredients extracted from camellia.

1. Background

Cellular senescence is known as an irreversible, stable and persistent exit from the cell cycle in response to stresses such as telomere shortening, oxidative stress, oncogene activation and DNA damage. Ordinarily, cellular senescence prevents proliferation of damaged cells, thereby preventing them from turning cancerous. However, during aging, senescent cells accumulate in tissues and secrete proinflammatory cytokines that can contribute to aging and age-related diseases, including cancer. Recent studies have shown the possibility that cellular senescence might be reversed. For instance, partial reprogramming by transient expression of OSKM(Oct4, Sox2, Klf4, and c-Myc) improved regenerative capacity of multiple organs including liver, heart and skeletal muscle and showed extended lifespan in mouse model of pre-mature aging. However, the attempts to revert cellular senescence in laboratory settings have shown limitations such as impaired tissue regeneration and tumorigenesis. Therefore, more sophisticated control engineering techniques are needed to be developed to discover new drug target(s) that can exclude such side effects and induce stable reverse aging.

2. Contents

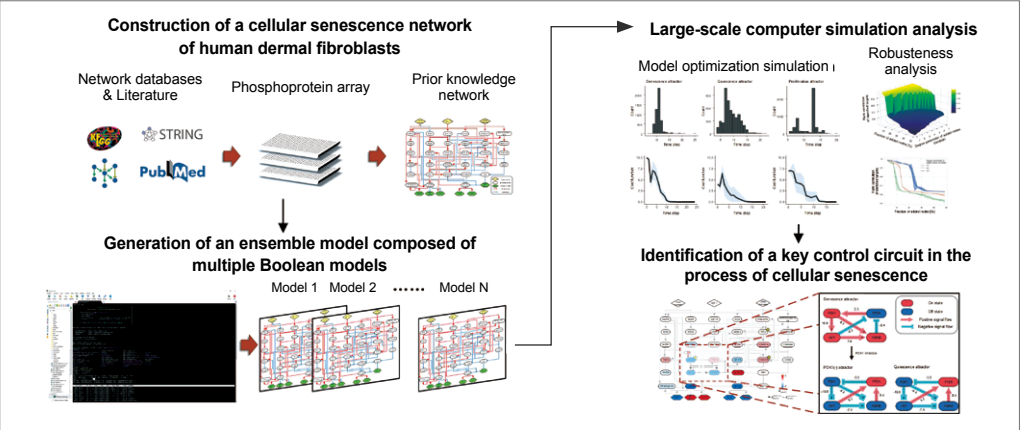
In this study, Professor Kwang-Hyun Cho and his team members constructed a network model of cellular senescence signaling in human dermal fibroblasts. By analyzing model simulation results through systems

biology approach, they identified a key molecule that is crucial in restoring aged dermal fibroblasts to young cells. From a large-scale computational dynamic analysis of the network model, they identified 3-phosphoinositide-dependent protein kinase 1 (PDK1) as a novel target that can reverse aged cells to young cells. PDK1 forms a positive feedback loop that is activated during senescence and up-regulates both mTOR and NF- κ B. Through collaboration with AMOREPACIFIC, Prof. Cho's team confirmed through wound healing assay and 3D reconstructed skin model experiments, that PDK1 inhibition in aged human dermal fibroblasts erases senescence markers and restores normal cell capacity that allow them to react and stably proliferate in response to environmental signals appropriately. These results showed that PDK1 activates mTOR and NF- κ B in aged human dermal fibroblasts to induce Senescence Associated Secretory Phenotype (SASP) and is associated with maintaining aging phenotypes. Prof. Cho's team became the first to report PDK1 inhibition as a novel single target that can safely revert aged cells to young cells.

3. Expected effect

This study has successfully demonstrated reversing aged cells to young cells using systems biology approach as a novel anti-aging strategy. This novel anti-aging strategy involving the development of novel drugs that can target the identified biomolecule and validation of its reverse aging capacities through preclinical studies provides new insight into a potential therapeutic strategy to treat aging and age-related diseases. Using the results from this study, AMOREPACIFIC R&D Center is currently developing cosmetics that can alleviate wrinkles on aged skin using PDK1 inhibitory agents from camellia extract.

Figure 1. Ensemble Boolean network model simulation analysis. Prof. Cho's team constructed a comprehensive mathematical model of senescence signaling network of human dermal fibroblasts by integrating all available information from literature, network databases and in-house protein array data and generated an ensemble model of Boolean networks (about 5,000 models) that best explain the experimental observations. By further analyzing the ensemble model, a core regulatory circuit of cell aging was identified.



Research outcomes

- [Paper] An, S., Cho, S.Y., Kang, J., Lee, S., Kim, H. S., Min, D. J., ... & Cho, K.-H.* (2020). Inhibition of 3-phosphoinositide-dependent protein kinase 1 (PDK1) can revert cellular senescence in human dermal fibroblasts. Proceedings of the National Academy of Sciences (PNAS).
- [Patent] K.-H. Cho*, S.B. Lee, S.G. An, J.S. Kang, S.Y. Cho, H.S. Kim (KAIST), Composition for reverse control of cellular senescence comprising PDK1 inhibitor, EP No. EP19204217.4 (Oct. 21, 2019)
- K.-H. Cho*, S.B. Lee, S.G. An, J.S. Kang, S.Y. Cho, H.S. Kim (KAIST), Composition for reverse control of cellular senescence comprising PDK1 inhibitor, PCT No. PCT/KR2019/012970 (Oct. 2, 2019).

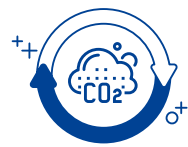
Research funding

National Research Foundation of Korea grant funded by the Korea government, the Ministry of Science and Information & Communication Technology [2020R1A2B5B03094920]

Electronics and Telecommunications Research Institute grant funded by the Korean government (20Z51100, Core Technology Research for Self-Improving Integrated Artificial Intelligence System)

Korea Advanced Institute of Science and Technology Grand Challenge 30 Project

Amorepacific R&D Center

TOP 10 RESEARCH
ACHIEVEMENTS

Heterogeneous Metal Atomic Catalysts for Gas-Phase Pollution Remediation

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Automobile emission contains toxic environmental pollutants, such as CO, hydrocarbon(C_3H_6 , C_3H_8) and NO_x , and they should be purified by heterogeneous catalysts. Typical automobile catalysts have showed insufficient performance for pollution remediation due to poor activity at low temperature($\leq 150^\circ C$) and low durability under hydrothermal aging($\geq 750^\circ C$, 25 h). In this research, metal(Pt, Pd, Rh) atomic catalysts were fabricated, and they showed superior low-temperature activity. Furthermore, they exhibited excellent durability under hydrothermal aging, long-term reaction and recycling test. Thus, this technology would lead the field of automobile catalysts, and have tremendous academic and industrial values.

1. Background

Carbon monoxide (CO), hydrocarbons (C_xH_y), and nitrogen oxides (NO_x) emitted from automobile exhaust gas are toxic molecules to the human respiratory system, and are representative atmospheric environmental pollutants that become precursors of fine dust and smog. These pollutants should be purified to nitrogen (N_2), water (H_2O), carbon dioxide (CO_2) through oxidation and reduction reactions using heterogeneous metal catalysts. However, conventional catalysts have showed poor activity at low temperatures (below $150^\circ C$) and poor durability at high temperatures (above $750^\circ C$, with humidity). Specifically, for gasoline hybrid vehicles, it is important to develop a highly active metal catalyst working at low temperatures because the temperature of the exhaust catalyst layer is lowered while the fuel efficiency is greatly enhanced. At the same time, high temperatures are accompanied during fuel combustion process in the engine, so the catalyst structure should have high durability even in high temperature condition.

2. Contents

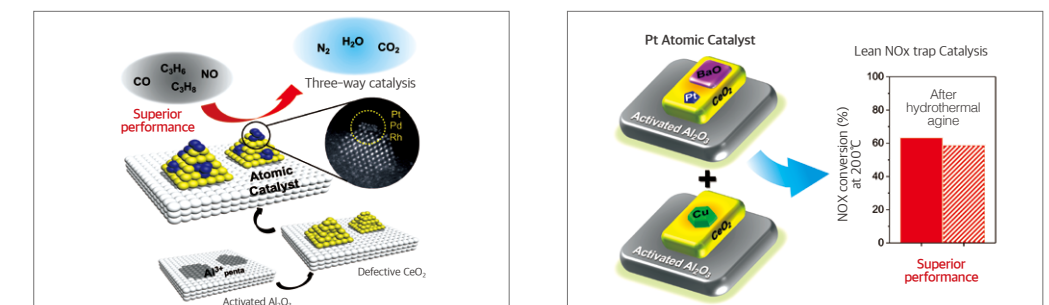
Support design is mostly important to fabricate the metal atomic catalysts, which are all the metal atoms are exposed on the surface (100% metal dispersion) with strong metal-support interaction. The structure of metal atom is determined as the characteristics of the support, and then the activity and durability of the metal catalyst would be changed. In this study, Prof. Hyunjoo Lee research group devised the highly defective reducible metal oxide supports to fully disperse and strongly anchor the metal atoms. The reducible metal oxide has a characteristic that the oxidation number of the metal is easily changed depending on the conditions, resulting in oxygen vacancy defect sites. In this study, a large amount of

coordinatively unsaturated Al^{3+}_{penta} species, which are strong anchoring sites, were created by pre-reducing the alumina ($\gamma-Al_2O_3$) support. Then, ceria (CeO_2) was impregnated to the Al^{3+}_{penta} sites, resulting in alumina-ceria dual structure support. Strong interaction of alumina-ceria produced the highly defective ceria with many Ce^{3+} sites. When the metals (Pt, Pd, Rh) were impregnated to the defective ceria, exceptionally strong interaction of metal-ceria effectively lowered the surface free energy of labile metal atoms. As a result, metal atomic catalysts (Pt, Pd, Rh/ CeO_2 - Al_2O_3) were designed with 100% metal atom dispersion.

Metal atomic catalysts were employed for gas-phase pollution remediation of three-way catalysis (TWC) and lean NO_x trap catalysis (LNT). TWC is a simultaneous surface reaction of oxidation of CO and C_xH_y , and reduction of NO_x . Metal atomic catalysts exhibited the world's best low-temperature activity, and showed higher activity and durability than commercial TWC catalyst. Specifically, all of CO, C_3H_6 , and NO were completely removed below $150^\circ C$, and conversion of C_3H_8 , which is difficult to remove, reached to 100% below $300^\circ C$. Furthermore, metal atomic catalysts showed excellent durability against hydrothermal aging ($900^\circ C$, 24h), long-term reaction ($150^\circ C$, 420h), recycle test without any degradation. In LNT, NO_x is trapped on the catalyst surface under fuel-lean condition, and then NO_x is catalytically reduced to N_2 under fuel-rich condition. Metal atomic catalysts showed 3 times higher performance than commercial LNT catalyst for low-temperature NO_x removal below $200^\circ C$. In addition, even after hydrothermal aging ($750^\circ C$, 25h), the structure of the metal atomic catalyst was unchanged, and 93% of the initial performance was achieved.

3. Expected effect

Prof. Hyunjoo Lee research group developed the novel concept of metal atomic catalysts with superior performance for gas-phase pollution remediation. Metal atomic catalysts, which have 100% dispersion by strong interaction with defect sites of defective support, showed the world's best activity and durability. Thus, this technology would lead the future in the automobile catalyst field, and present guidelines for the development of highly active and durable heterogeneous metal catalysts. This technology can be applied for modern gasoline hybrid vehicles as it can efficiently deal with continuously strengthened environmental regulations. Furthermore, it would be possible to apply this technology to all industries requiring exhaust gas purification such as ship, aviation, motorcycles, and power plants. The metal atomic catalysts have infinite academic and industrial values in heterogeneous catalysis, and would make great impacts on the future society.



Research outcomes

[Paper] H. Jeong, O. Kwon, B.-S. Kim, J. Bae, S. Shin, H.-E. Kim, J. Kim, H. Lee*, "Highly Durable Metal Ensemble Catalysts with Full Dispersion for Automotive Applications beyond Single-Atom Catalysts", Nature Catalysis 3, 368-375 (2020) [2020 Impact Factor = 30.471]
B.-S. Kim, H. Jeong, J. Bae, P. S. Kim, C. H. Kim, H. Lee*, "Lean NO_x Trap Catalysts with High Low-Temperature Activity and Hydrothermal Stability", Applied Catalysis B: Environmental 270, 118871 (2020) [2020 Impact Factor = 16.683]

Research funding

This research was supported by the National Research Foundation of Korea (grant numbers NRF-2016R1A5A1009592 and 2018R1A2A2A05018849) and Hyundai NGV (grant number R-183091.0001).



TOP 10 RESEARCH
ACHIEVEMENTS

Mobile and Extendable Negative Pressure Clinic Module For Contagious Disease Hospital Service

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Department of Industrial Design

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To solve the shortage problem of negative pressure wards in the pandemic situation, we developed Mobile Clinic Module (MCM), a modular negative pressure ward system that enables building, effectively transporting, and storing medical environments for moderate to severe patients in a short time. MCM enables stepwise negative pressure conversion and effective air circulation in the ward. MCM addresses the requirement of usability, emotional satisfaction as well as functionality, utility and cost. It can also be used for various mobile healthcare facilities.

1. Background

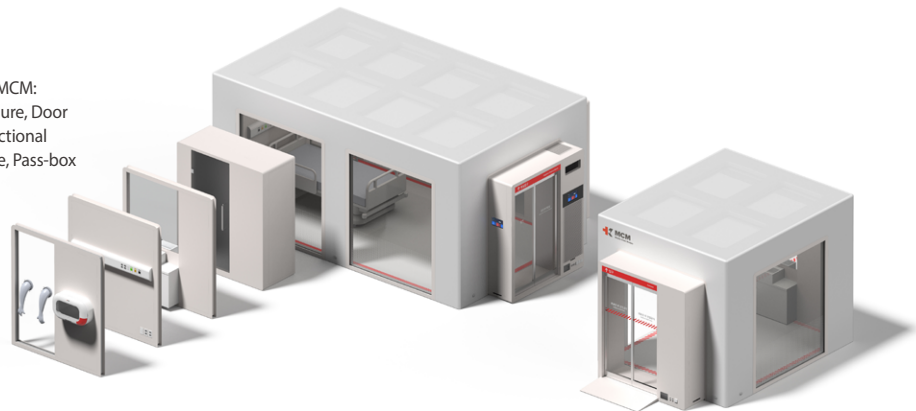
In a pandemic situation, such as COVID-19, the demand for negative pressure wards to treat infectious patients surges. Existing prefabricated buildings have been focused only on quarantine, which makes it difficult to support medical activities. We addressed this problem by design-centric approach considering the needs of various stakeholders such as medical staff, patients and administrators.

2. Contents

Key Features of Mobile Clinic Module (MCM)

MCM is a modular system for building negative pressure ward. It supports rapidly installation, effective transportation and storage. MCM considered usability and emotional satisfaction as well as the basic requirements of bio-safety, cost and efficiency.

Figure 1.
Main components of MCM:
Frame (Negative Pressure, Door etc.), Air tent, and Functional panel(Medical Console, Pass-box and Globe etc.)



MCM's main components are Frame, Air tent and Function panel. It is possible to build various medical facilities by assembly of three. The key component is the negative pressure frame which effectively makes differential pressure spaces. The air tent makes it easy and quick to install rooms. The air pressure is kept by the sensing system. The functional panel reinforces the structural stability of the tent while providing functional support. The medical panel supplies essential medical gas. The glove & pass box panel can be used to transfer objects without wearing protective clothing. The basic MCM unit consists of the anteroom and the patient room can be installed within about 15 minutes. Compared with the reconstruction method, it reduce costs by about 80%. When stored, the volume is reduced by about 75%, the weight by 60%. The whole ward can be transported by air.

Design Development and Evaluation

MCM was developed through user-centered design and iterative prototyping. We have understood the processes for hospitalization and treatment of infected patients through collaboration with medical staff. Within four months, user-research, design, prototyping and the ward construction have been completed. We received positive feedback from the clinical evaluation done at the Korea Institute of Radiological and Medical Sciences' outdoor parking lot space with 500-square-meter where the ward is installed.



Figure 2. A negative pressure ward in the Korea Institute of Radiological & Medical Science



Figure 3. Inside of the negative pressure ward

3. Expected effect

MCM will become an essential quarantine system in the infectious disease crisis situation that will be repeated periodically. It will prevent the collapse of medical system in emergency. During the normal period, it will minimize unnecessary ward extensions. It can be used as a variety of medical facilities such as mobile hospital, emergency beds in residential treatment centers and screening clinics as well as the isolation ward.



Research outcomes

The study aimed at practical use in the COVID-19 crisis situation, and the negative pressure isolation ward installed in the Korea Institute of Radiological & Medical Science is the main achievement.

[Patent] Assembled Modular System for Building Positive and Negative Pressure Facilities (2021. 1. 27. Korean Patent Registration confirmed)

Eight cases including the negative pressure frame for the mobile negative pressure ward construction, the mobile negative pressure ward unit including the anteroom, the mobile negative pressure ward unit for the intensive care unit negative pressure, the medical equipment panel for the mobile negative pressure ward construction, the mobile negative pressure ward construction globe and pass box panel. (2020. 12. 10. Application)

[Award] iF Design Award entry (2020. 12. 03.)