



The First Mover in Environmental Sustainability

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2020 ANNUAL REPORT

KIST Europe

2020 ANNUAL REPORT





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KIST Europe Forschungsgesellschaft mbH



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K I S T
E U R O P E
A N N U A L
R E P O R T

PREFACE

Director's Greeting

"One must live the way one thinks or end up thinking the way one has lived." — Paul Bourget

Dear Readers,

KIST Europe was established in Saarbrücken, Germany in 1996. With the support of the Korean government, KIST Europe has enjoyed nearly 25 years of successful operations, accomplishing many great achievements and is performing its mission of facilitating joint research among high-tech R&D institutes throughout Korea and the EU. Such an outcome was possible because of our researchers and supporting staff - while they may hail from different cultural and ethnic backgrounds, they are united in their pursuit of excellence and their commitment to further enhancing their capabilities and expertise.

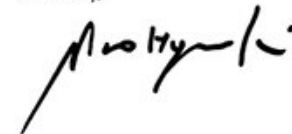
With this in mind, we are very pleased to present to you this annual report, summarizing our research activities and notable achievements for 2020. In this report, you will find affirmation of our specialized expertise in conducting open and innovative research, as well as detailed descriptions of the diverse forms of collaboration in which we participate.

Despite these past achievements, KIST Europe remains deeply committed to exploring potential new opportunities for cooperation. For research institutes seeking an experienced collaboration partner for joint research projects, or industry organizations wishing to expand into the Korean or European markets, KIST Europe, which plays a key role in facilitating S&T cooperation between Korea and the EU, could be the ideal partner to realize that.

I wish to thank everyone who has consistently supported the work we do at KIST Europe. It is only through your efforts that our success has been possible. My particular gratitude goes out to the Saarland Government and Saarland University for always standing by our side. I hope that our partnership will only continue to strengthen over the years to come.

Lastly, I wish to express my heartfelt appreciation to the staff at KIST Europe for their hard work and valuable contributions. Their dedication is truly unparalleled. As KIST Europe turns 25, we look forward to the journey ahead, and to strengthening KIST Europe's solidarity as the only Korean government R&D institute in Europe.

Sincerely,



Dr. Soo Hyun Kim
Director, KIST Europe



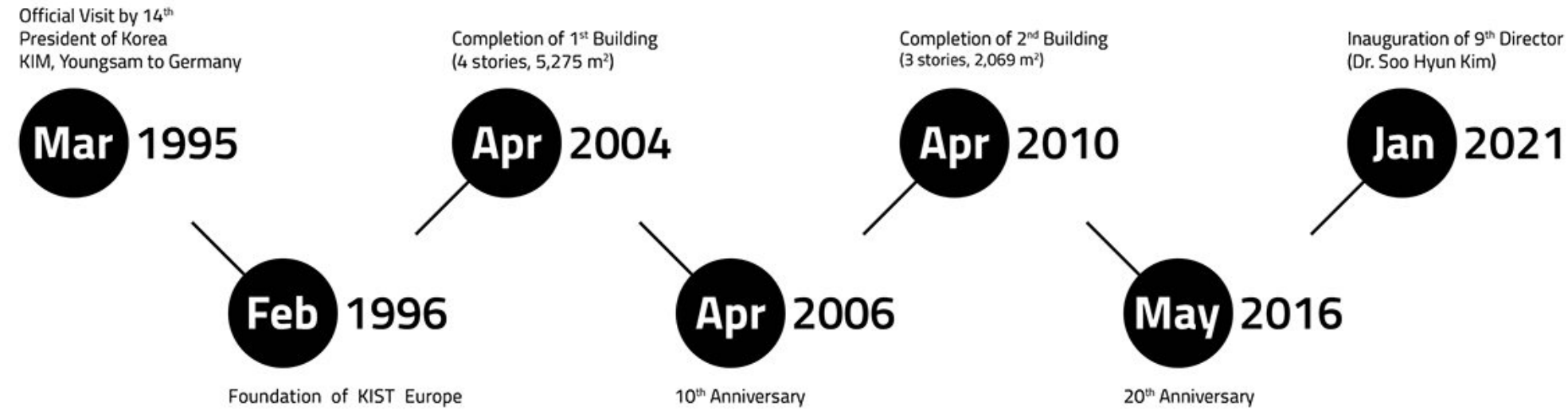
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OUR PROFILE



HISTORY OF KIST EUROPE

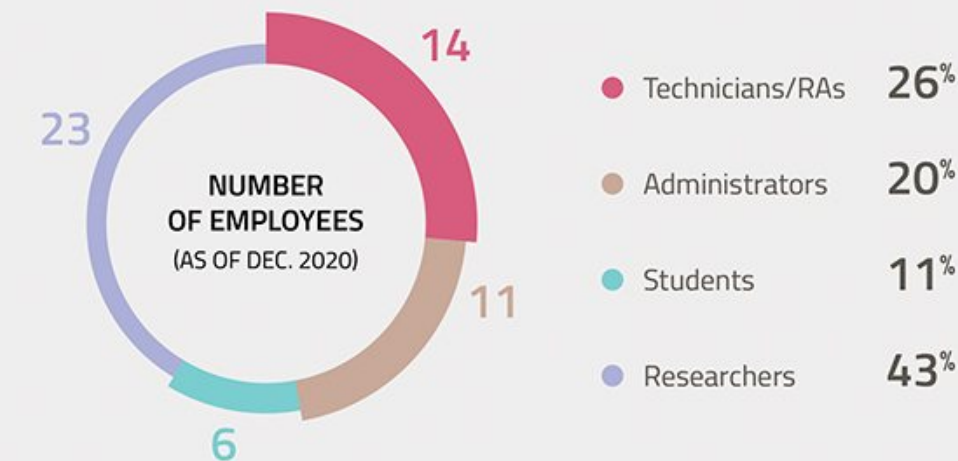
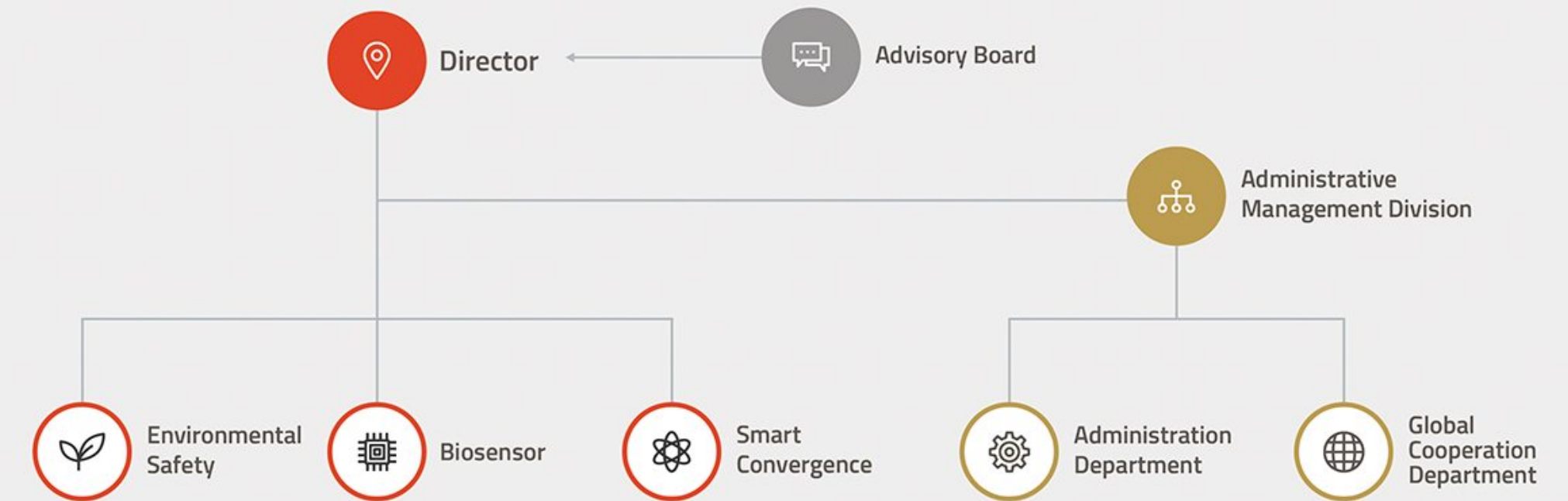


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Administrative Management Division

ORGANIZATION & PEOPLE



STRATEGIES

Capacity

- **Concentration on core research themes**
Development of core research themes based on internal research capacity and concentrations
- **Expansion of research infrastructure to strengthen core research capacities**



Open R&D

- **Launch of a global test-bed platform to stimulate R&D cooperation**
Establishment of an on-site Open Lab, the so-called Global Test-Bed, which provides the opportunity for feasibility studies in the area of technology convergence from both countries
- **Expansion of cooperation with EU**
Promotion of joint R&D between excellent research institutes in Korea and EU



Industry Support

- **Support for improved sustainability and industrial competitiveness**
Support for Korean and EU industries in complying with chemical regulations such as the EU – and Korean REACH



- **The First Mover in Environmental Sustainability**
 - Research on animal-free risk assessment
 - Platform-based global cooperation

ADVISORY BOARD



Korean Members (as of December 2020)



Dr. Seok-Jin Yoon
(Chairman)
President,
Korea Institute of Science and
Technology



Mr. Heekwon Jung
Director General of the International
Cooperation Bureau,
Korean Ministry of Science and ICT



Dr. You Seung Kim
Former President,
Korea Institute of Science and
Technology



Dr. Myung Soo Kim
Vice Mayor for Science,
Daejeon Metropolitan City



German Members (as of December 2020)



Mr. Henrik Eitel
Head of Saarland State Chancellery,
Saarland State Government



Prof. Dr. Manfred Schmitt
President,
University of Saarland



Prof. Dr. Andreas Schäffer
Director of Institute for Environmental
Research,
RWTH Aachen



Dr. Wolfgang Wahlster
Chief Executive Advisor,
German Research Centre for Artificial
Intelligence (DFKI)



Prof. Dr. Rolf Müller
Managing Director,
Helmholtz Institute for Pharmaceutical
Research Saarland (HIPS)

GUESTHOUSE FACILITIES

View



- 1 1st Building
- 2 2nd Building (Korea-EU Cooperation Center)
- 3 Guest House
- 4 Technical Center



- Accommodation for guest researchers, cooperation partners, research assistants, students & interns available
- Jointly used with neighbouring research institutes

GUESTHOUSE FACILITIES

Facilities



Single room

1 bed, drawers, closet with hangers, desk, kitchen with induction range, shower



Family room

2 beds, drawers, closet with hangers, desk, kitchen with induction range, shower, dining table, TV, sofa, balcony table, dishwasher, microwave



Rooms	15 single rooms (16m ²)	12 single rooms (24m ²)	2 family rooms (40m ²)	2 family rooms (60m ²)
Floor				
Capacity	Max : 1	Max : 1-2	Max : 2-3	Max : 3-4

Common Facilities



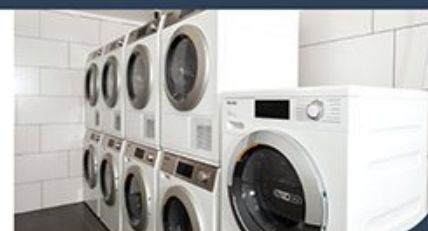
Lobby



Elevator



Laundry Room



Parking Area



OVERVIEW OF KIST HEADQUARTERS

History

The Leading Contributor in Science and Technology in Korea

1960 ~ 1980s

- February 1966 KIST is founded
- January 1981 KIST and the Korea Advanced Institute of Science (KAIS) combine to form the Korea Advanced Institute of Science and Technology (KAIST)
- June 1989 KIST separates from KAIST and is reestablished

1990s

- February 1996 KIST Europe is established
- March 1999 KIST becomes affiliated with the Korea Research Council of Fundamental Science & Technology under the Office of the Prime Minister

2000s ~ Present

- May 2003 KIST Gangneung is established
- January 2008 KIST Jeonbuk is established
- July 2017 KIST becomes affiliated with the National Research Council of Science and Technology under the Ministry of Science and ICT
- July 2020 Dr. Yoon Seok-Jin is appointed President of KIST

R&D History



- From Playing Catch-up
- To Innovation



- KIST Progressed Rapidly
- To Claim Technology
- Leadership

1966~

Developed key industrial technologies

1980~

Adopted and modified imported advanced technologies

1990~

Conducted original research in advanced technologies

2000~

Researching innovative, cutting-edge technologies

No. of Staff

Total Staff
(including temporary staff)
(as of 2020)

3,708

Regular Staff

Temporary Staff

Researchers

Specialists & Technicians

Administrative Staff

Students / Researchers

Post-docs & Interns 478 625

594

218

127

939

1,205

OVERVIEW OF KIST HEADQUARTERS

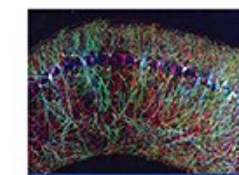
Location of Headquarters and Research Areas

Headquarters – KIST Seoul

KIST was established in 1966 with the primary goals of developing creative, original, and cutting edge technologies; improving Korea's scientific and technological capacities, and participating in the active transfer of these technologies. Initially, KIST focused on developing technologies suitable for industrialization, and these technologies contributed greatly to the modernization of Korea and fostered remarkable economic growth throughout the nation. Over the course of time, KIST has produced premier S&T talents and spun-off numerous specialized research institutes. Such achievements cemented KIST's status as Korea's leading S&T institute. By applying its accumulated R&R expertise, KIST is now expanding its role and taking on large-scale, long-term interdisciplinary R&D projects which are typically considered too challenging for universities or private entities. KIST is continually striving to advance the field of science and technology, both domestically and internationally.



Research Divisions



The Brain Science Institute

A hub for brain science research, unraveling the mysteries of the brain



The Clean Energy Institute

Leading a clean-technology society and new energy paradigm



The Post-Silicon Semiconductor Institute

Driving technology development in the Fourth Industrial Revolution through new semiconductor materials & devices



The Artificial Intelligence & Robotics Institute

At the heart of robot, media, and ICT convergence research, paving the way toward the future



The Bio & Medical Research Division

Exploring ways for humankind to enjoy longer, healthier lives

GRAND KIST



The Advanced Materials Research Division

Creating a new future with breakthrough materials



The National Agenda Research Division

Elevating Korea's status as a science and technology leader



The KIST Gangneung Institute of Natural Products

Bringing the world happiness through natural products!



The KIST Jeonbuk Institute of Advanced Composite Materials

Serving as a key player for composite materials technology in Korea

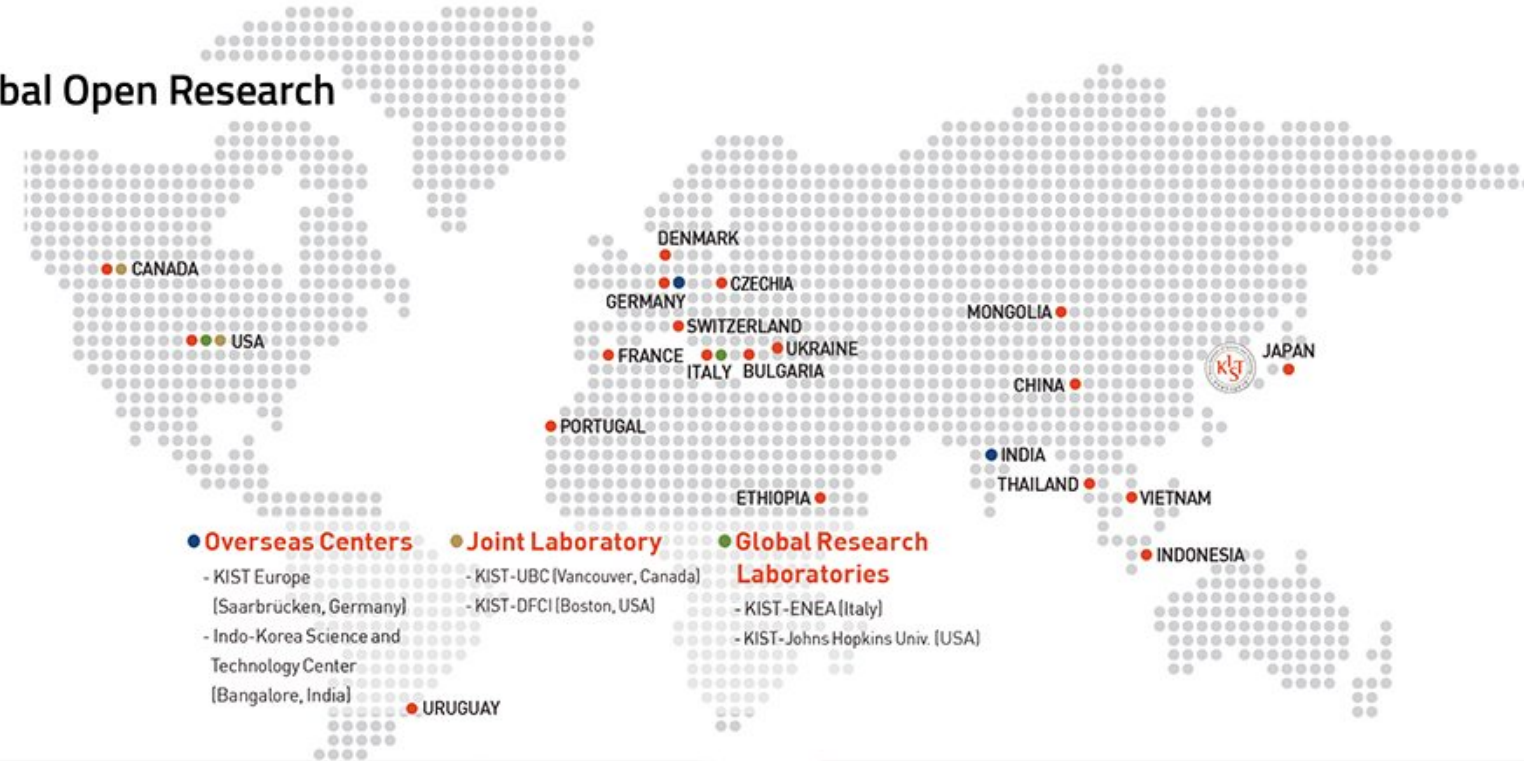


The Research Resources Division

A business innovation hub for national R&D in science and technology

KIST'S INTERNATIONAL COOPERATION ACTIVITIES

Global Open Research



KIST Europe



Founded in Saarbrücken, Germany in 1996, KIST Europe is Korea's only government R&D institute in Europe. Since its inception, KIST Europe has exhibited sustainable growth as it pursues its goal of establishing a bridgehead for Korean R&D institutes and industries seeking opportunities to collaborate and make advances into Europe.



In GERMANY

Indo-Korea Science and Technology Center



The Indo-Korea Science & Technology Center was established in Bangalore, India in 2020. Because India has emerged as an important world market, the center has contributed to building Korea's trade relations with India and has performed ICT convergence research (focusing on computational science) that takes advantage of India's rich potential in the science and technology field. The center has become the focal point in promoting scientific and technological exchanges between the two countries.



In INDIA

KIST'S INTERNATIONAL COOPERATION ACTIVITIES

Institutions in Partnership with KIST

Bulgaria

- Bulgarian Academy of Sciences (BAS)

Canada

- University of Waterloo
- University of British Columbia (UBC)

China

- Shanghai Academy of Science and Technology/Shanghai Industrial Technology Institute (SAST/SITI)
- Science and Technology Department of Sichuan Province

Czechia

- Charles University in Prague
- Czech Technical University in Prague

Denmark

- DHI Group

Ethiopia

- Adama Science and Technology University (ASTU)

France

- French National Centre for Scientific Research (CNRS)
- University of Grenoble Alpes (UGA)
- Laboratoire d'Electronique et de Technologies de l'Information (CEA-Leti)

Germany

- Technische Universität Berlin
- Forschungszentrum Karlsruhe GmbH
- Fraunhofer-Gesellschaft (FhG)
- Helmholtz Centre for Infection Research (HZI)
- Saarland University

Indonesia

- Universitas Indonesia (UI)

Italy

- Institute for Advanced Energy Technologies (ITAE)

Japan

- Institute of Physical and Chemical Research (RIKEN)
- Tohoku University
- Tokyo Institute of Technology

Mongolia

- Mongolia Academy of Sciences (MAS)
- Institute of Chemistry and Chemical Technology (ICCT)
- Mongolian National Olympic Committee (MNOC)

Portugal

- University of Minho

Switzerland

- Swiss Federal Laboratories for Materials Science and Technology (EMPA)

Thailand

- Asian Institute of Technology (AIT)

Ukraine

- V.N. Karazin Khrkiv National University
- National Technical University of Ukraine Kyiv Polytechnic Institute (NTUU KPI)

Uruguay

- National Agency for Research and Innovation (ANII)

USA

- National Institute of Biomedical Imaging & Bioengineering (NIBIB)
- Stony Brook University (SBU)
- Dana-Farber Cancer Institute
- National Cancer Institute (NCI)

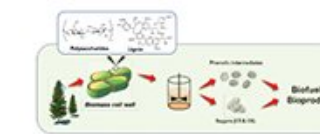
Vietnam

- The Ministry of Science and Technology of the Socialist Republic of Vietnam (MOST)

World Bank

- PASET (Partnership for skills in Applied Sciences, Engineering and Technology)

KIST-UBC On-Site-Lab



The KIST-UBC Biorefinery On-Site-Lab is a satellite laboratory supported by the Korea Institute of Science and Technology (KIST) which began operations on May 17, 2012. With the University of British Columbia and other research partners, the UBC's on-site laboratory is developing sustainable technologies to convert lignocellulosic biomass into biofuels and renewable materials. This laboratory is dedicated to developing next-generation biofuel and renewable chemicals from lignocellulosic biomass that can replace fossil-fuel derivatives.



In CANADA

KIST-DFCI On-Site-Lab

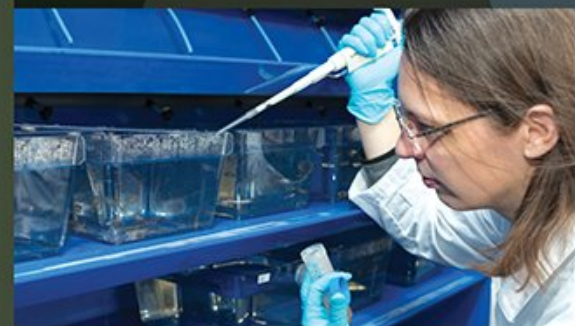


To create a synergistic effect by mutually cooperating in the area of cancer biology, The Korea Institute of Science and Technology (KIST) and Dana-Farber Cancer Institute, a major affiliation of Harvard Medical School, signed a MOU that will allow joint research in cancer biology. In 2013, in accordance with this agreement, subsequent measures have included various joint cancer research projects and the establishment of a lab at Dana-Farber Cancer Institute operated by KIST.



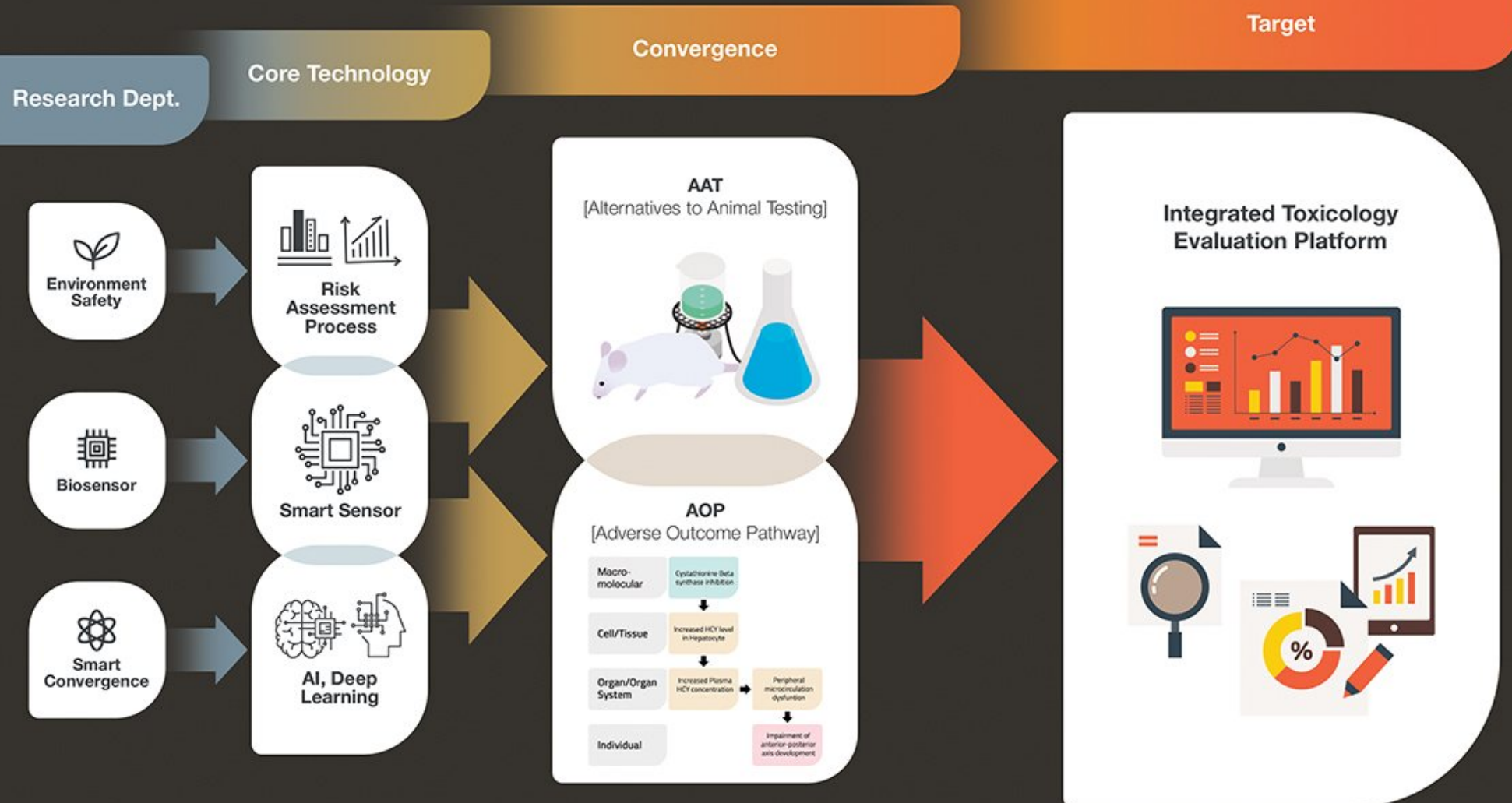
In AMERICA

RESEARCH
WITH PASSION



SIGNATURE RESEARCH

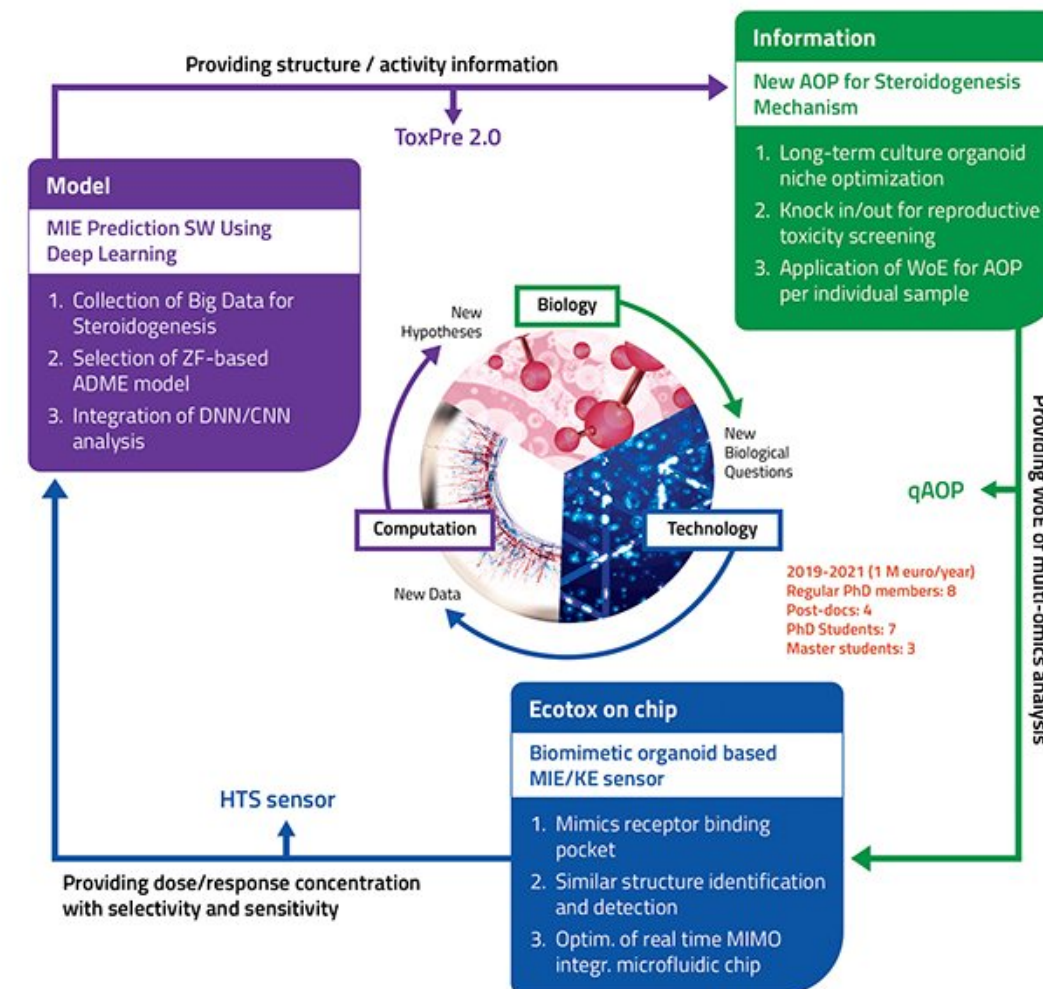
Integration of all possible capacities among KIST Europe researchers



SIGNATURE RESEARCH

Theme

- Development of Environmental Steroidogenesis AOP Framework



What is Adverse Outcome Pathway (AOP)?

- AOP is associated with toxicity pathways and regulatory applications
- AOP network is the functional unit of endpoint prediction
- A Molecular initiating event or early key event is essential for alternatives to animal testing
- AOP facilitates the multidisciplinary studies through the need for network building

Status of AOP Development

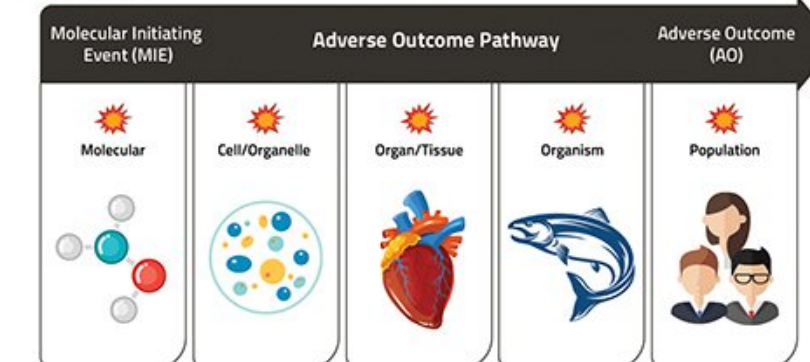
- OECD AOP network developed to date

- 270 AOPs (user defined)
- 750 Key Events
- 1000 Key Event Relationships

Definition of AOP

- Relationship of adverse outcomes from molecular to population level

Key Event (KE)



SIGNATURE RESEARCH

AOPs included in OECD* Workplan (*Organization for Economic Cooperation and Development)



Graphic representation for 3 applied AOPs

Reg. No.	AOP 271	AOP 289	AOP 292	AOP 297
Title	Inhibition of thyroid peroxidase leading to impaired fertility in fish	Inhibition of 5α-reductase leading to impaired fertility in female fish	Inhibition of tyrosinase leading to decreased population in fish	Inhibition of retinaldehyde dehydrogenase leading to population decline
PJT. ID in OECD Workplan	1.59	1.81	1.78	1.77
Pathway				
Macro-molecular	Thyropoxidase inhibition	5 alpha reductase inhibition	Tyrosinase inhibition	Retinaldehyde dehydrogenase inhibition
Cell/Tissue	Thyroid hormone synthesis, decreased	DHT level, decreased	L-Dopaquinone decreased	Retinoic acid (RA) synthesis decreased
Organ/Organ System	Plasma E2 concentrations, reduction	Plasma E2 concentration, reduction	Melanin decreased	Plasma RA level decreased
Individual	Cumulative fecundity and spawning, reduction	Decreased spawning and egg production	Pigmentation pattern decreased	Optical elements of the eye decreased
Population			Trajectory decreased	Visual impairment increased

Expected effect and Applicability

- Apply to OECD Test Guidelines
- Apply to Integrated models for toxicity prediction
- Apply to (Q)SAR Toolbox for environmental regulation

MAJOR ACHIEVEMENTS

Development of 10 AOP Title

- Expansion of own research capacities including COVID-19 research themes
- 2020 (4) : Own capacities
- 2019 (5) : Own capacities
- 2018 (1) : Joint development with Korea Institute of Toxicology

AOP No.	OECD PJT ID	AOP Title	Status	Ref.	Reg.Year
271	1.59	TPO inhibition leading to impaired fertility in fish --> Inhibition of thyroid peroxidase leading to impaired fertility in fish	Coaching	Co-Reg. with KIT	2018
289	1.81	Inhibition of 5α-reductase leading to impaired fertility in female fish	Coaching	Single Reg.	2019
292	1.78	Inhibition of tyrosinase leads to decreased population in fish	Coaching	Single Reg.	2019
297	1.77	Inhibition of retinaldehyde dehydrogenase leads to population decline	Coaching	Single Reg.	2019
301	-	Inhibition of Cystathionine Beta synthase leading to impaired the early development of anterior-posterior axis	Under Development	Single Reg.	2019
309	-	Luteinizing hormone receptor antagonism leading to reproductive dysfunction	Under Development	Single Reg.	2019
319	-	ACE2 antagonism leading to lung fibrosis	Coaching	Single Reg. [COVID-19]	2020
320	-	Binding of viral S-glycoprotein to ACE2 receptor leading to acute respiratory distress associated mortality	Coaching	Single Reg. [COVID-19]	2020
348	-	Inhibition of 11β-HSD leading to impaired spermatogenesis in fish	Under Development	Single Reg.	2020
349	-	Inhibition of 11β-hydroxylase leading to infertility in male fish	Under Development	Single Reg.	2020

SIGNATURE RESEARCH



Characterizing the potential estrogenic and androgenic activities of two disinfection byproducts, mono-haloacetic acids and haloacetamides, using in vitro bioassays

Da-Hye Kim, Chang Gyun Park, Young Jun Kim*

Environmental Safety Group, Korea Institute of Science and Technology (KIST) Europe, Saarbrücken, 66123, Germany

Abstract

Exposure to disinfection byproducts (DBPs) is potentially related to cytotoxic, genotoxic, mutagenic, and tumorigenic effects in humans, in addition to their adverse effects on the environment. However, their impacts on endocrine disruption, especially reproductive toxicity, remain largely unknown. In this study, the estrogenic and androgenic activities of DBPs and corresponding antagonistic activities were investigated using a yeast-based reporter assay, focusing on haloacetic acids and haloacetamides. We also examined the cytotoxicity of DBPs and mechanisms of antagonistic activities. Of the DBPs assayed, iodoacetamide (IAM) and bromoacetamide (BAM) were the most cytotoxic, with LC50 values of 0.0462 and 0.0537 mM, respectively, followed by chloroacetic acid (CAA; LC50 = 4.87 mM) and chloroacetamide (CAM; LC50 = 5.28 mM). Iodoacetic acid (IAA) and bromoacetic acid (BAA) were the least cytotoxic, with LC50 values of 5.52 and 6.35 mM, respectively. IAA (EC10 = 0.00573 mM; EC50 = 0.0215 mM) exhibited most potent estrogenic activity, and CAA (EC10 = 0.0434 mM) and BAM (EC10 = 0.0150 mM) showed weak estrogenic and androgenic activities, respectively. By contrast, IAM exhibited anti-estrogenic effects. These results suggest that DBPs interact with hormone receptors.

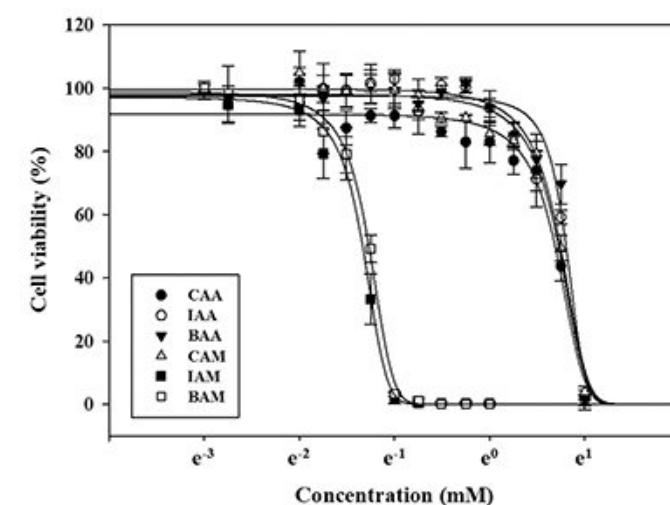
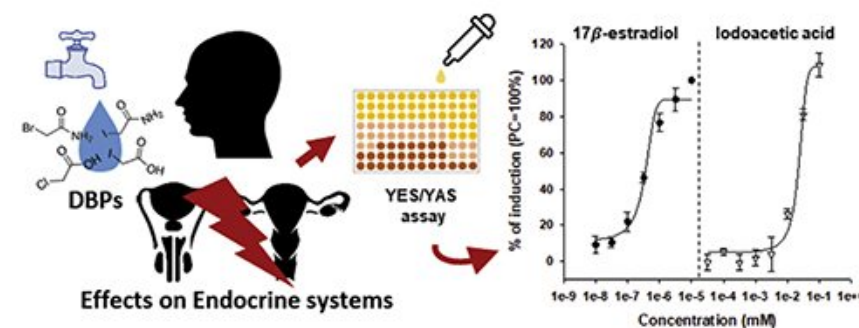


Fig. 1. Cell viability of target disinfection byproducts (DBPs). The results were shown as means \pm SD (n = 4).

*Reprinted from Characterizing the potential estrogenic and androgenic activities of two disinfection byproducts, mono-haloacetic acids and haloacetamides, using in vitro bioassays, Da-Hye Kim, Chang Gyun Park, Young Jun Kim, Volume 242, Chemosphere, 125198, Copyright (2021), with permission from Elsevier

MAJOR ACHIEVEMENTS



Matrix softness-mediated 3D zebrafish hepatocyte modulates response to endocrine disrupting chemicals

Kathryn M Sullivan ^{1,2}, Chang Gyun Park ³, John D Ito ⁴, Mikhail Kandel ^{5,6}, Gabriel Popescu ^{1,5,6}, Young Jun Kim ³, Hyunjoon Kong ^{1,2,4,6}

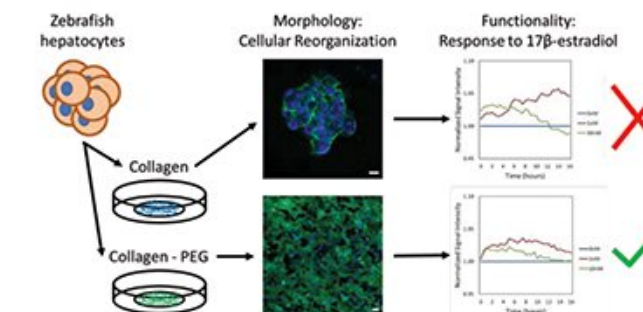
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Abstract

Endocrine disrupting chemicals (EDC) include synthetic compounds that mimic the structure or function of natural hormones. While most studies utilize live embryos or primary cells from adult fish, these cells rapidly lose functionality when cultured on plastic or glass substrates coated with extracellular matrix proteins. This study hypothesizes that the softness of a matrix with adhered fish cells can regulate the intercellular organization and physiological function of engineered hepatoids during EDC exposure. We scrutinized this hypothesis by culturing zebrafish hepatocytes (ZF-L) on collagen-based hydrogels with controlled elastic moduli by examining morphology, urea production, and intracellular oxidative stress of hepatoids exposed to 17 β -estradiol. Interestingly, the softer gel drove cells to form a cell sheet with a canaliculi-like structure compared to its stiffer gel counterpart. The hepatoids cultured on the softer gel exhibited more active urea production upon exposure to 17 β -estradiol and displayed faster recovery of intracellular reactive oxygen species level confirmed by gradient light interference microscopy (GLIM), a live-cell imaging technique. These results are broadly useful to improve screening and understanding of potential EDC impacts on aquatic organisms and human health.

*Reprinted (adapted) with permission from (Matrix Softness-Mediated 3D Zebrafish Hepatocyte Modulates Response to Endocrine Disrupting Chemicals, 2020 Nov 3;54(21):13797-13806, Kathryn M Sullivan, Chang Gyun Park, John D Ito, Mikhail Kandel, Gabriel Popescu, Young Jun Kim, Hyunjoon Kong, Copyright (2021) American Chemical Society.



14 Pa

256 Pa

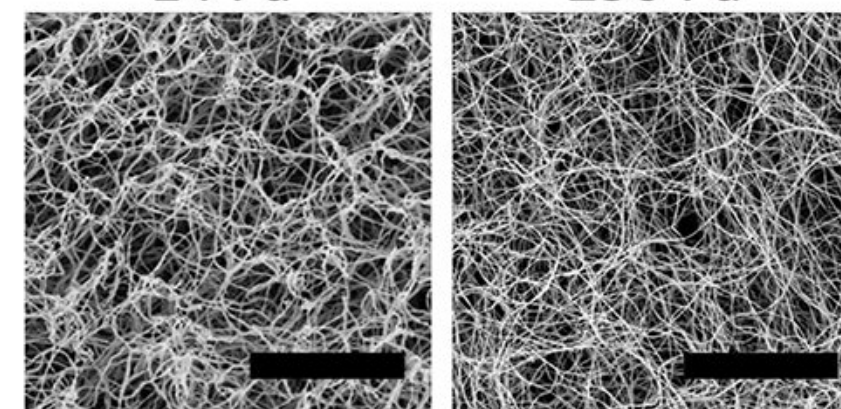


Fig. 3. Example images of each dataset, (a) MNIST, (b) EMNIST, (c) fashion-MNIST, (d) CIFAR-10, (e) CINIC-10. (PEG) and imaged with scanning electron microscopy. The black scale bars represent 5 μ m.



Mathematical modeling of a temperature-sensitive and tissue-mimicking gel matrix: Solving the Flory–Huggins equation for an elastic ternary mixture system

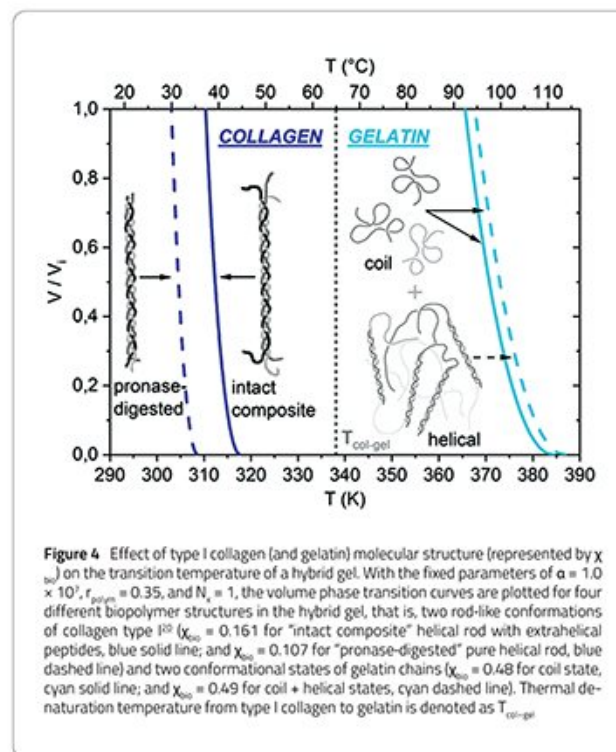
Baeckkyoung Sung

Environmental Safety Group, Korea Institute of Science and Technology (KIST) Europe, Saarbrücken, 66123, Germany

Abstract

Programmed to retain active responsivity to environmental stimuli, diverse types of synthetic gels have been attracting interests regarding various applications, such as elastomer biodevices. In a different approach, when the gels are made of tissue-derived biopolymers, they can act as an artificial extracellular matrix (ECM) for use as soft implants in medicine. To explore the physical properties of hydrogels in terms of statistical thermodynamics, the mean-field Flory–Huggins–Rehner theory has long been used with various analytical and numerical modifications. Here, we suggest a novel mathematical model on the phase transition of a biological hybrid gel that is sensitive to ambient temperature. To mimic acellular soft tissues, the ECM-like hydrogel is modeled as a network of biopolymers, such as type I collagen and gelatin, which are covalently crosslinked and swollen in aqueous solvents.

Within the network, thermoresponsive synthetic polymer chains are doped by chemical conjugation. Based on the Flory–Huggins–Rehner framework, our analytical model phenomenologically illustrates a well-characterized volume phase behavior of engineered tissue mimics as a function of temperature by formulating the ternary mixing free energy of the polymer–solvent system and by generalizing the elastic free energy term. With this formalism, the decoupling of the Flory–Huggins interaction parameter between the thermoresponsive polymer and ECM biopolymer enables deriving a simple steady-state formula for the volume phase transition as a function of the structural and compositional parameters. We show that the doping ratio of thermoresponsive polymers and the Flory–Huggins interaction parameter between biopolymer and water affect the phase transition temperature of the ECM-like gels.



Reprinted, by permission, from Baeckkyoung Sung, "Mathematical modeling of a temperature-sensitive and tissue-mimicking gel matrix: Solving the Flory–Huggins equation for an elastic ternary mixture system", *Mathematical Methods in the Applied Sciences*, 43, 18, 10637–10645. Copyright © 2020 by John Wiley & Sons, Inc.



Biosensors and Bioelectronics

Volume 160, 15 July 2020, 112216

Advanced molecular recognition of 3-nitro-L-tyrosine: The use of zwitterion embedded molecularly imprinted mesoporous organosilica with sub-nanomolar sensitivity

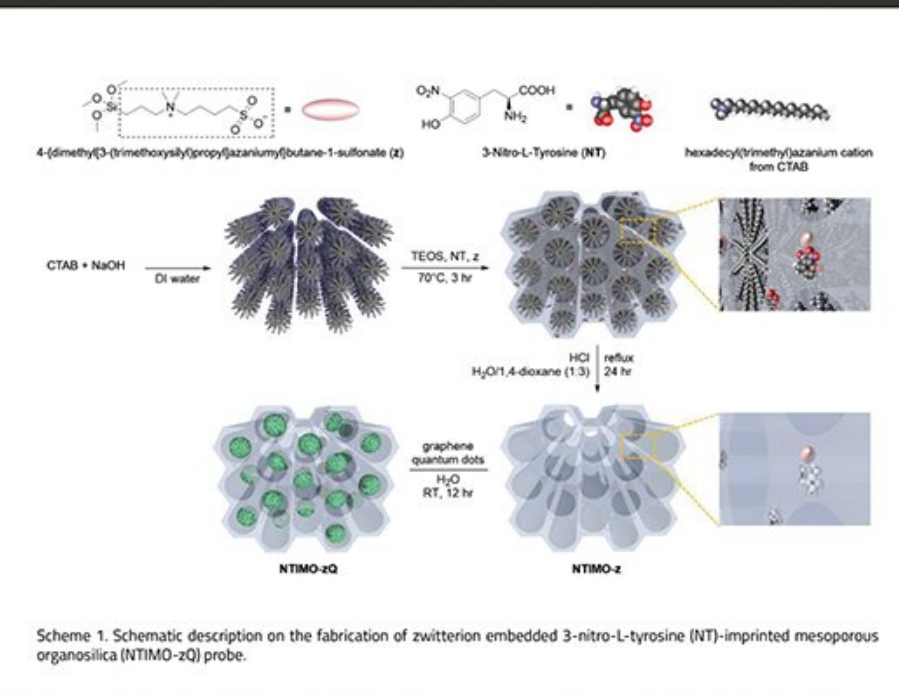
Youngdo Kim, Jaeho Lee

Biosensor Group, Korea Institute of Science and Technology Europe, Campus E7-1, 66123, Saarbrücken, Germany

Abstract

Fabricating a state-of-the-art system capable of probing any chosen target molecule with a high degree of selectivity is the foremost objective of molecular recognition materials. In this paper, we developed a versatile target-probe utilizing zwitterion embedded molecularly imprinted mesoporous organosilica to fill the gap in our current capabilities. Graphene quantum dots were encapsulated as a signal transducer to prepare the fluorescent probe (NTIMO-zQ), and the concentration-dependent emission change was analyzed by adding 3-nitro-L-tyrosine (NT). The NTIMO-zQ showed an unprecedented degree of fluorescence quenching which also exhibited a sub-nanomolar sensitivity for NT; proving itself to be the most sensitive NT probe reported to date. By investigating the sigmoidal fitting of this quenching behavior, the selectivity performance can be quantitatively analyzed; and the resulting measurements are taken to determine the effective concentration (EC50) values with respect to NT. The NTIMO-zQ probe presents an extremely low EC50 with NT (9.7 nM) compared to several other NT analogues. The probe we have developed is both reproducible and repeatable with a satisfactory recovery rate (97–102%), and moreover, it exhibits suitably low detection limit (0.0129 nM).

Reprinted from Advanced molecular recognition of 3-nitro-L-tyrosine: The use of zwitterion embedded molecularly imprinted mesoporous organosilica with sub-nanomolar sensitivity, Volume 160, Youngdo Kim, Jaeho Lee, *Biosensors and Bioelectronics*, 112216, Publication title, Vol / edition number, Author(s), Title of article / title of chapter, Pages No., Copyright (2020), with permission from Elsevier





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Objectives

The Environmental Safety Group contributes to the protection of human health and the environment from hazardous chemicals and mixtures containing these chemicals.

This group also contributes to enhancing the national competitiveness of the chemical industry by ensuring high safety standards for products.

R&D Areas

Alternative Toxicity & Ecotoxicity Assessments

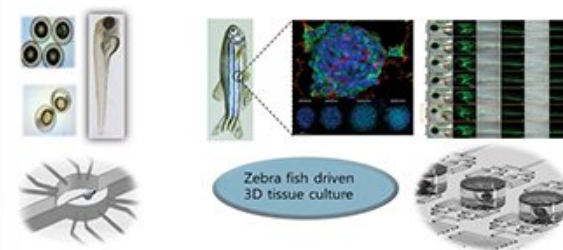
- 3D tissue mimicry for high-throughput toxicity screening
- Development of Alternatives to Animal Testing (AAT) systems for chronic toxicity screening
- Development of environmental risk assessment tools and modelling methodologies

Mathematical Biology & Computational Toxicology

- Development of analytical models for mechanism-based toxicity prediction
- Quantitative in silico approach for ecotoxicity screening
- ADMET/QSAR modelling and industrial applications

Development of Metabolomics and their Application to Biomarker Discovery

- Targeted/pseudo-targeted metabolomics of chemicals
- Metabolite identification and reaction phenotypes



3D tissue culture and ecotox on a chip fabrication



Food chain metabolomics monitoring and analysis

Journals

Min Jeong Baek, Jino Son, Jayoung Park, Yohan Seol, Baekkyoung Sung, and Young Jun Kim. 'Quantitative prediction of mixture toxicity of AgNO₃ and ZnO nanoparticles on *Daphnia magna*.' *Science and technology of advanced materials* 21.1 (2020): 333-345. Web of Science Core Collection: SCIE

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Biodegradable Magnesium Alloys Promote Angio-Osteogenesis to Enhance Bone Repair

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Abstract

Biodegradable metallic materials represent a potential step-change technology that may revolutionize the treatment of broken bones. Implants made with biodegradable metals are significantly stronger than their polymer counterparts and fully biodegradable in vivo, removing the need for secondary surgery or long-term complications. Here, it is shown how clinically approved Mg alloy promotes improved bone repair using an integrated state of the art fetal mouse metatarsal assay coupled with in vivo preclinical studies, second harmonic generation, secretome array analysis, perfusion bioreactor, and high-resolution 3D confocal imaging of vasculature within skeletal tissue, to reveal a vascular-mediated pro-osteogenic mechanism controlling enhanced tissue regeneration. The optimized mechanical properties and corrosion rate of the Mg alloy lead to a controlled release of metallic Mg, Ca, and Zn ions at a rate that facilitates both angiogenesis and coupled osteogenesis for better bone healing, without causing adverse effects at the implantation site. The findings from this study support ongoing development and refinement of biodegradable metal systems to act as crucial portal technologies with significant potential to improve many clinical applications.

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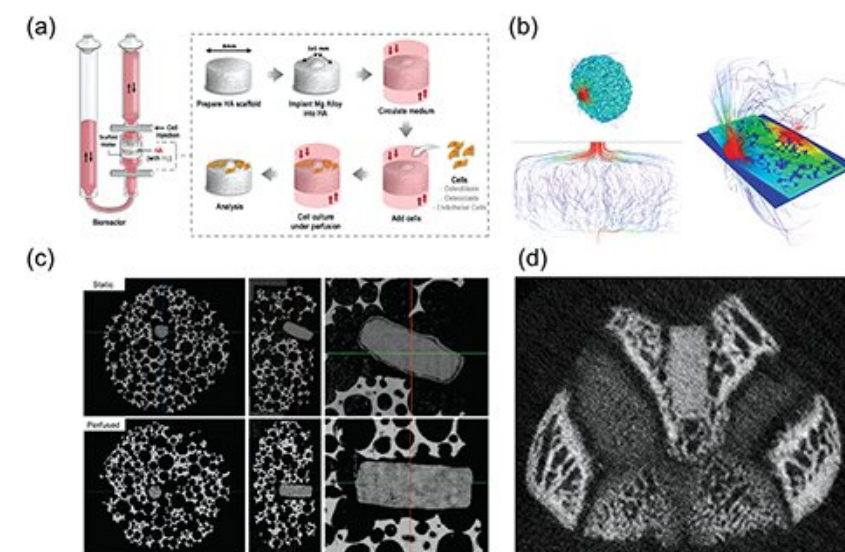


Figure 3. a) Schematic illustration of perfusion bioreactor and Mg sample implanted on HA scaffold b) Water molecular diffusivity simulation showing the flow of media through the open porous structure of hydroxyapatite scaffold. c) μ CT comparison of Mg5Ca12Zn samples immersed in static conditions with a thick layer of corrosion by-product on the surface of Mg and perfusion condition without accumulation of corrosion by-product on the surface after 4 weeks. d) 4 weeks postoperation in vivo CT of femoral condyle of SD rat implanted with Mg5Ca12Zn.



Quantitative prediction of mixture toxicity of AgNO₃ and ZnO nanoparticles on Daphnia magna

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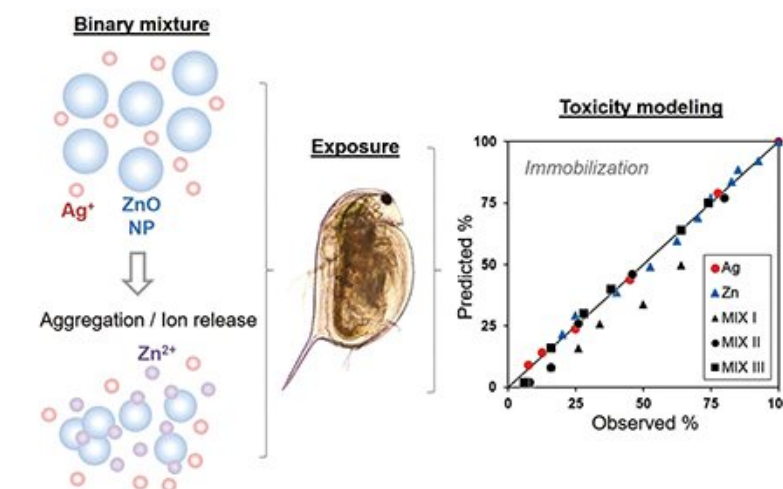
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Abstract

Once metal-based engineered nanoparticles (NPs) are released into the aquatic environment, they are expected to interact with other existing co-contaminants. A knowledge gap exists as to how the interaction of NPs with other co-contaminants occurs. Here we selected ZnO NPs among various NPs, with Ag ion existing as a contaminant in the aquatic environment by AgNPs widely used. A novel modeling strategy was demonstrated enabling quantitative and predictive evaluation of the aqueous mixture nanotoxicity. Individual and binary mixture toxicity tests of ZnO NPs and silver (as AgNO₃) on *Daphnia magna* were conducted and compared to determine whether the presence of Ag ions affects the toxicity of ZnO NPs.

Binary mixture toxicity was evaluated based on the concentration addition (CA) and independent action models. The CA dose-ratio dependent model was found to be the model of best fit for describing the pattern of mixture toxicity. The MIX I and MIX III suspensions (higher ratios of ZnO NPs to AgNO₃) showed a synergism, whereas the MIX II suspension (lower ratio of ZnONPs to AgNO₃) showed an antagonism. The synergistic mixture toxicity at higher ratios of ZnONPs to AgNO₃ was caused by either the physiological or metabolic disturbance induced by the excessive ionic Zn or increased transport and accumulation in *D. magna* via the formation of complex of ionic Ag with ZnO NPs.

Therefore, the toxicity level contributed via their aggregation and physicochemical properties and the dissolved ions played a crucial role in the mixture toxicities of the NPs.

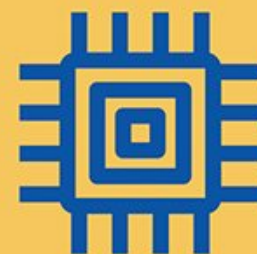


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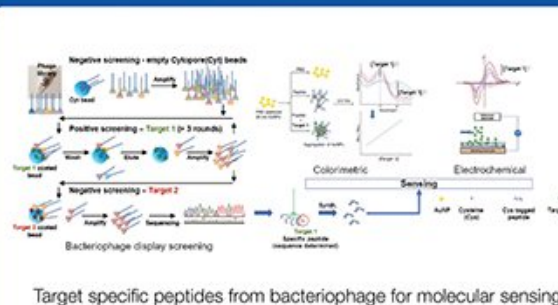
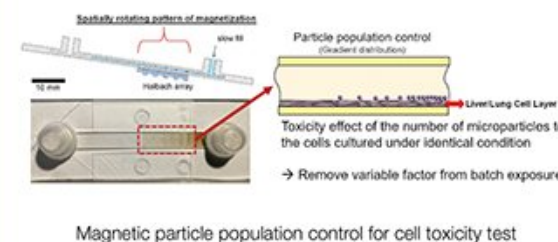


Objectives

The Biosensor group performs various environment-related tasks based on multidisciplinary research. The group mainly conducts projects related to sensing biomarkers necessary for the assessment of eco-toxicity, detecting harmful molecules present in the environment, and controlling particles for the study of cytotoxicity caused by micro-artificial substances. Ultimately, we intend to support toxicity assessment studies through Alternatives to Animal Testing (AAT). Along with our efforts to realize sensor devices which integrate our research results, we also conduct energy-related research for the protection of the environment by means of informatic technologies as well as experimental activities.

R&D Areas

- **Biosensors and Microfluidics**
 - Biomimicking inorganic probe materials
 - Probe materials using gene modified bacteriophages
 - Development of optical, electrical, and electrochemical sensing methods
 - Microfluidic platform for sensing system integration
- **Magnetic Materials**
 - Controlling magnetic particles in various fluidic environments for fine-particle toxicity testing
- **Energy Storage**
 - Heat and gas fluid simulation for optimization of hydrogen energy storage system



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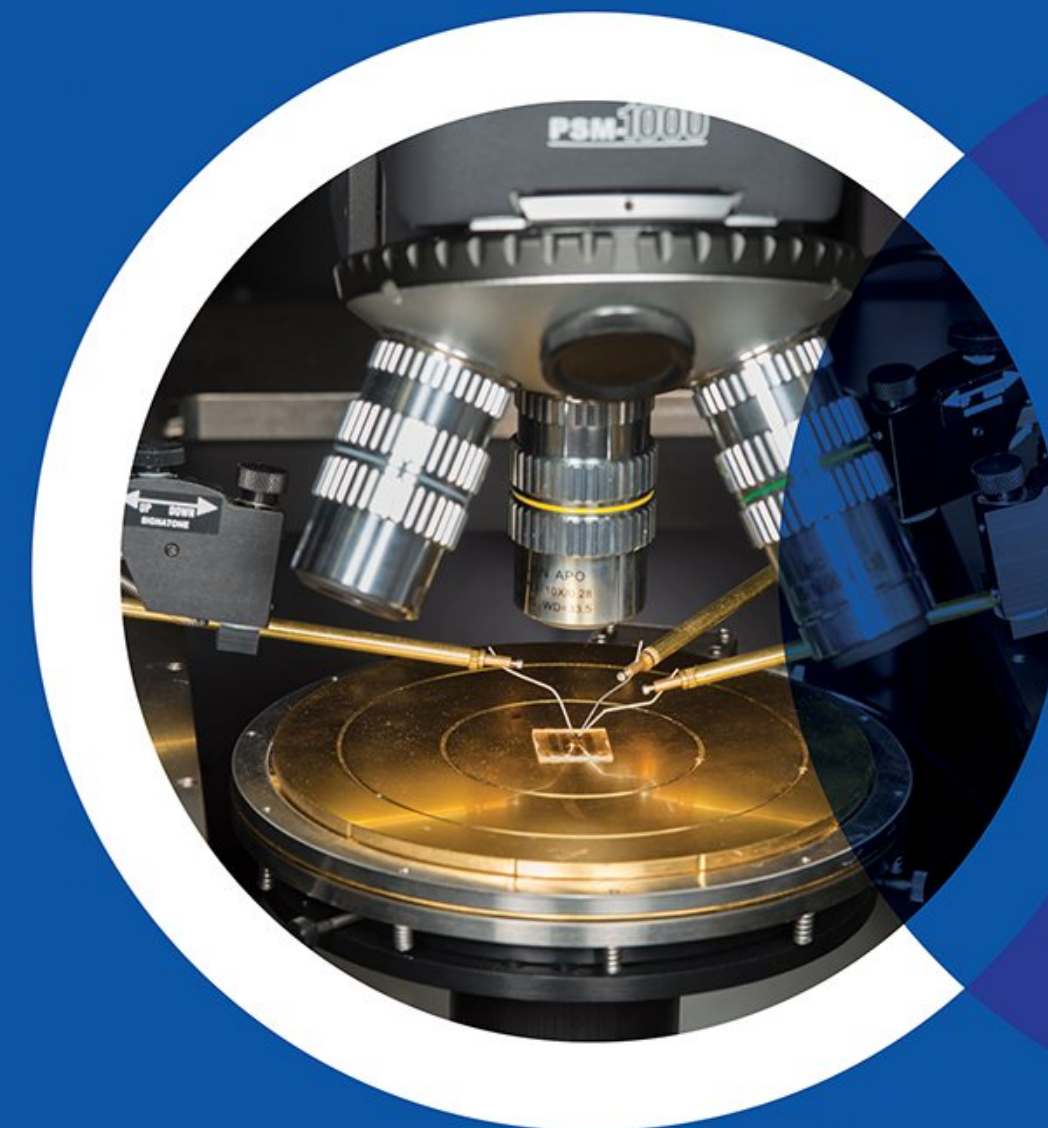
Poster Presentations

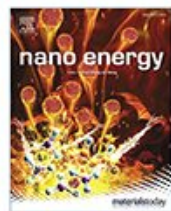
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An “interaction-mediating” strategy towards enhanced solubility and redox properties of organics for aqueous flow batteries

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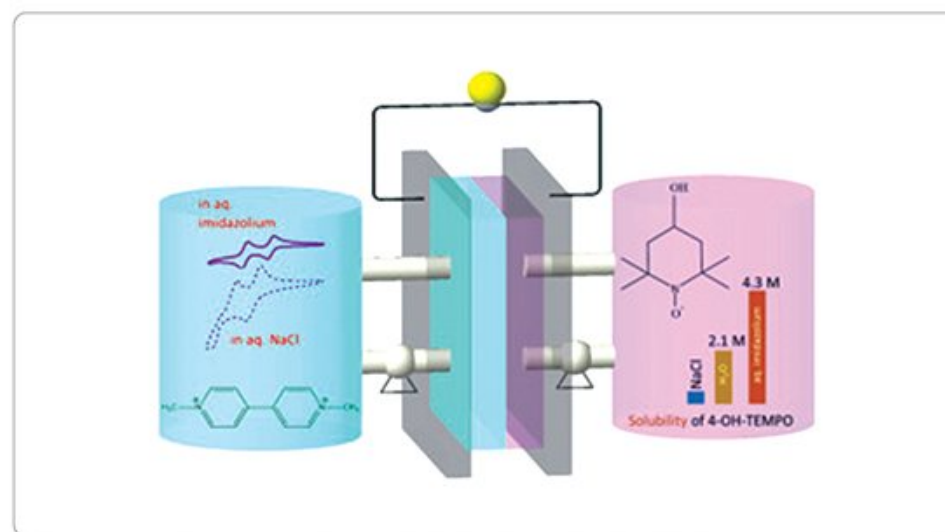
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^e INM-Leibniz Institute for New Materials, 66123, Saarbrücken, Germany

^f Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021, Karlsruhe, Germany

Abstract

Aqueous redox flow batteries using electroactive organic materials are currently attracting significant attention. However, the influence of supporting electrolytes on the aqueous solubility, electrochemical reversibility and chemical stability of the organic components has rarely been investigated. Here, a new electrolyte design strategy towards enhanced solubility and chemical stability of active materials is proposed by using interaction-mediating species. 3 molality aqueous imidazolium chlorides, with high ionic conductivity and water-like flowability, enable a record aqueous solubility of 4.3 M for a commercially available nitroxyl radical and reversible 2e⁻ reaction of unmodified methyl viologen at moderate concentrations. With 0.6 M electrolyte, flow cell shows remarkable chemical stability of the nitroxyl radical, excellent cycling stability over 250 cycles at 80 mA cm⁻², and a peak power density of 121.6 mW cm⁻² at 175 mA cm⁻². Furthermore, nitroxyl radical catholyte with a concentration of 3 M is tested in a flow cell. It maintains an impressive steady energy efficiency of 65% at 30 mA cm⁻². This work paves a new way for the development of high performance aqueous electrolytes based on organic materials.



*Reprinted from An “interaction-mediating” strategy towards enhanced solubility and redox properties of organics for aqueous flow batteries, Volume 69, Zhifeng Huang, Christopher W.M. Kay, Bjorn Kuttich, Daniel Rauber, Tobias Kraus, Hongjiao Li, Sangwon Kim, Ruiyong Chen, Nano Energy, 104464, Copyright (2020), with permission from Elsevier.



SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

Three-dimensional self-assembly using dipolar interaction

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Abstract

Interaction between dipolar forces, such as permanent magnets, generally leads to the formation of one-dimensional chains and rings. We investigated whether it was possible to let dipoles self-assemble into three-dimensional structures by encapsulating them in a shell with a specific shape. We found that the condition for self-assembly of a three-dimensional crystal is satisfied when the energies of dipoles in the parallel and antiparallel states are equal. Our experiments show that the most regular structures are formed using cylinders and cuboids and not by spheroids. This simple design rule will help the self-assembly community to realize three-dimensional crystals from objects in the micrometer range, which opens up the way toward previously unknown metamaterials.

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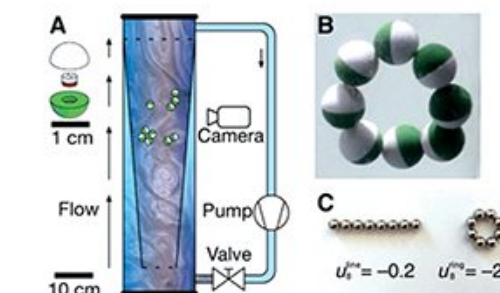


Fig. 1 The self-assembly experiment. (A) 3D printed polymer objects with embedded permanent magnets were inserted in a transparent cylinder with an upward flow. The flow counteracts the drop velocity of the objects, and the flow's turbulence provides a disturbing force. A tapered transparent insert was used to provide a gradient in the flow velocity, which ensured that the objects levitate in front of the video cameras. (B) Spherical objects form linear chains. When eight spheres are inserted in the flow, the most stable configuration is a circle, which has 10% lower energy than a linear chain (C). Photo credit: L. Abelmann (Saarland University and University of Twente).

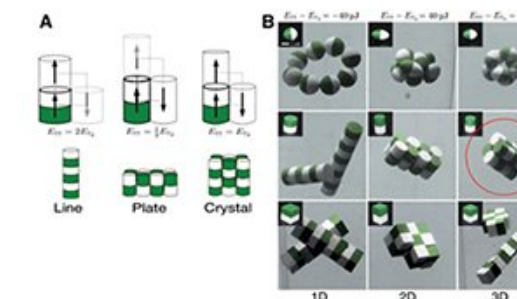


Fig. 2 3D self-assembly of dipoles. (A) Equally spaced dipoles prefer parallel alignment (black arrows). By elongating the shape of the shell around the dipoles, we can favor the antiparallel configuration, so that plates of objects assemble. When the energy of the parallel and antiparallel configuration is exactly equal, we expect 3D crystals. (B) This strategy works best with cylindrical objects. From left to right, we varied the shape so that the energy of the parallel configuration is twice (left), half (center), and exactly equal (right) to that of the antiparallel configuration. The red encircled assembly of cylinders (middle row) is a regular 3D 2 by 2 by 2 cluster. The cylindrical objects in the second row reproduced the plate prediction of (A). The spheroids (top row) and the cubes (bottom row) exhibited line structures in the first column but more complex behavior when their shape was adjusted.



Dr. Yong Oh LEE

Group Leader
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Objectives

The Smart Convergence group is pursuing the improvement of efficiency and effectiveness of model-based prediction methods using artificial intelligence (AI) in various engineering fields. Our research ranges from scientific studies to practical applications, where AI is not widely applied, but has the potential to enhance performance.

R&D Fields

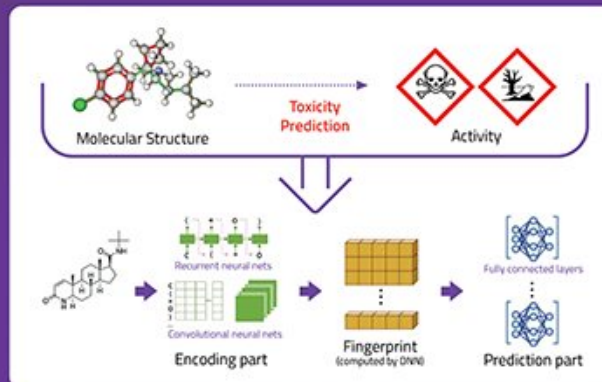
Deep Learning Applications

- Toxicity prediction: QSAR and behavior patterns in Alternatives to Animal Testing (AAT)
- Cell and medical image segmentation
- Motor fault diagnosis and prognosis
- Worker's intensity recognition in collaborative robotics

Data augmentation in data imbalance

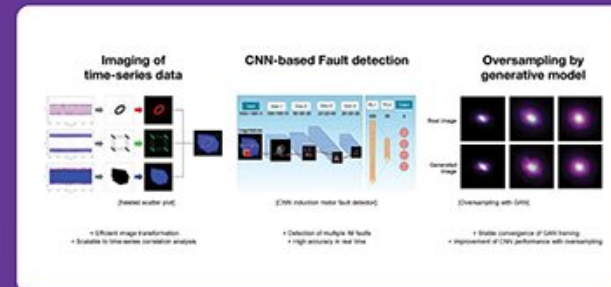
- Generative Adversarial Networks (GANs) for minority class augmentation
- Feature augmentation with interpretable machine learning

1 AI in Bioinformatics



- Computational Toxicology
- Deep learning QSAR model (improved ROC-AUC with balanced sensitivity and specificity)
- Discovery of structure alerts with interpretable feature maps

2 AI in Smart Factory



- Development of fault detection and diagnosis for induction motors using deep learning
- Imaging method for the correlation of time series data (e.g., current, vibration)
- Convolutional Neural Networks (CNN)-based induction fault detection
- Oversampling by generative model for data imbalances

Journals

Yong Oh Lee, and Young Jun Kim. 'The Effect of Resampling on Data-imbalanced Conditions for Prediction towards Nuclear Receptor Profiling Using Deep Learning.' *Molecular informatics* 39.8 (2020): 1900131.
Web of Science Core Collection: SCIE

Sungho Suh, Haebom Lee, Paul Lukowicz, and Yong Oh Lee. 'CEGAN: Classification Enhancement Generative Adversarial Networks for unraveling data imbalance problems.' *Neural Networks* 133 (2021): 69-86.
Web of Science Core Collection: SCIE

Sungho Suh, Joel Jang, Seungjae Won, Mayank Jha, and Yong Oh Lee. 'Supervised Health Stage Prediction Using Convolutional Neural Networks for Bearing Wear.' *Sensors* 20.20 (2020): 5846.
Web of Science Core Collection: SCIE

Books

Yong Oh Lee, and Baekkyoung Sung. 'In Silico Platforms for Predictive Ecotoxicology: From Machine Learning to Deep Learning.' *Chemometrics and Cheminformatics in Aquatic Toxicology*. Wiley, 2021.
* Publication foreseen in May / Aug. 2021.

Oral Presentations

Joel Jang. 'Diagnosis of bearing wear state and prediction of remaining useful lifetime using nested scatter plot.' *PHM Korea 2020*, 23 Jul. 2020, Seoul.

Poster Presentations

Junghyun Kim, Sungho Suh, Yong Oh Lee, and Jongwoon Hwang. 'Enhanced ROI segmentation and text recognition using convolutional encoder and decoder for shipping label inspection.' *IPIU 2020*, 5-7 Feb. 2020, Jeju.

Young Jun Kim, Penny Nymark, Yong Oh Lee, Clemens Wittwehr, and Brigitte Landesmann. 'Application of Adverse Outcome Pathway Framework to COVID-19.' *ISMB 2020*, 13-16 Jul. 2020, Online Meeting, Montreal.

Sangrak Lim, Yong Oh Lee, Young Jun Kim. 'Quantitative evaluation of structural alerts extracted from deep learning QSAR models.' *ISMB 2020*, 13-16 Jul. 2020, Online Meeting, Montreal.

Proceedings

Sangrak Lim, and Yong Oh Lee. 'Predicting Chemical Properties using Self-Attention Multi-task Learning based on SMILES Representation.' *ICPR 2020*, 10-15 Jan. 2021, Online Meeting, Milan.

Sungho Suh, Paul Lukowicz, and Yong Oh Lee. 'Fusion of Global-Local Features for Image Quality Inspection of Shipping Label.' *ICPR 2020*, 10-15 Jan. 2021, Online Meeting, Milan.





CEGAN: Classification Enhancement Generative Adversarial Networks for unraveling data imbalance problems

Sungho Suh ^{a,b}, Haebom Lee ^a, Paul Lukowicz ^{b,c}, Yong Oh Lee ^{a,*}

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^b Department of Computer Science, TU Kaiserslautern, 67663 Kaiserslautern, Germany

^c German Research Center for Artificial Intelligence (DFKI), 67663 Kaiserslautern, Germany

Abstract

The data imbalance problem in classification is a frequent but challenging task. In real-world datasets, numerous class distributions are imbalanced and the classification result under such condition reveals extreme bias in the majority data class. Recently, the potential of GAN as a data augmentation method on minority data has been studied. In this paper, we propose a classification enhancement generative adversarial networks (CEGAN) to enhance the quality of generated synthetic minority data and more importantly, to improve the prediction accuracy in data imbalanced condition.

In addition, we propose an ambiguity reduction method using the generated synthetic minority data for the case of multiple similar classes that are degenerating the classification accuracy. The proposed method is demonstrated with five benchmark datasets. The results indicate that approximating the real data distribution using CEGAN improves the classification performance significantly in data imbalanced conditions compared with various standard data augmentation methods.

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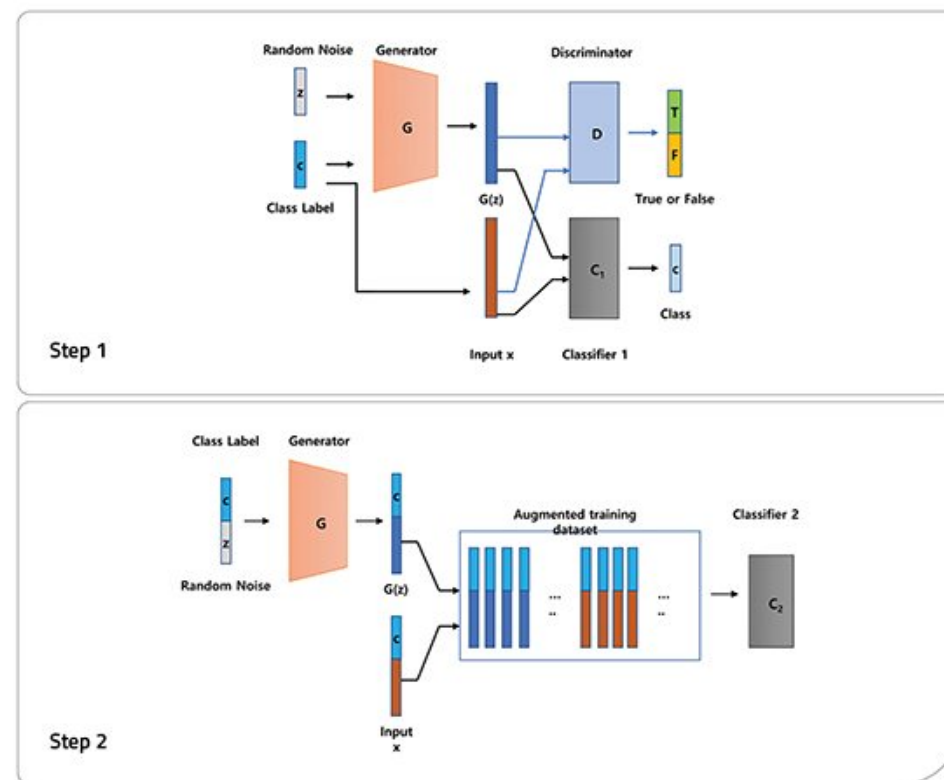


Fig. 2. Overview of training procedure, of CEGAN (Step 1), of the classifier with augmented data (Step 2).

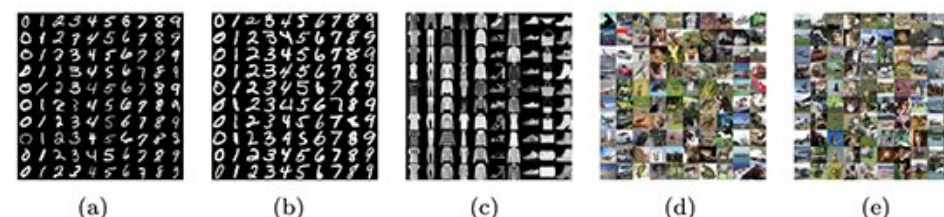


Fig. 3. Example images of each dataset, (a) MNIST, (b) EMNIST, (c) fashion-MNIST, (d) CIFAR-10, (e) CINIC-10.



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Predicting Chemical Properties using Self-Attention Multi-task Learning based on SMILES Representation

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Abstract

In the computational prediction of chemical compound properties, molecular descriptors and fingerprints encoded to low dimensional vectors are used. The selection of proper molecular descriptors and fingerprints is both important and challenging as the performance of such models is highly dependent on descriptors. To overcome this challenge, natural language processing models that utilize simplified molecular input line entry system as input were studied, and several transformer variant models achieved superior results when compared with conventional methods. In this study, we explored the structural differences of the transformer-variant model and proposed a new self-attention based model. The representation learning performance of the self-attention module was evaluated in a multi-task learning environment using imbalanced chemical datasets. The experiment results showed that our model achieved competitive outcomes on several benchmark datasets. The source code of our experiment is available at <https://github.com/arwhirang/samtl> and the dataset is available from the same URL.

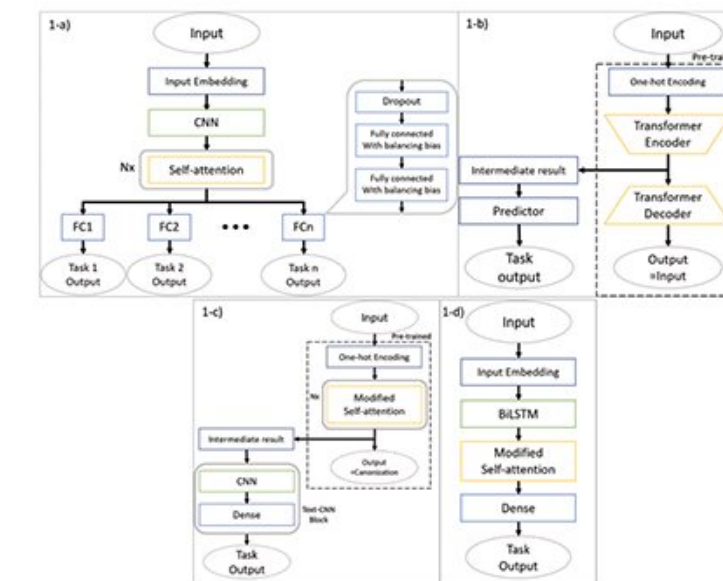


Fig. 1. Model architectures of SA-MTL and existing self-attention based approaches. Simplified overview of our model and existing models. For comparison, the three existing models are depicted with core components only. 1-a) SA-MTL Model: Our SA-MTL consists of three deep learning components. After input embedding, a CNN layer learns the shared underlying factors. The next component is a self-attention module. This self-attention module consists of the encoder part of the transformer model. The last component is the discrete output layer. We represent discrete output layers with FC since each output layer consists of two fully connected layers. The discrete output layers reduce the dimension to match the target tasks. 1-b) Smiles Transformer Model: The Smiles Transformer model uses the intermediate result obtained from the pre-training step. 1-c) Transformer-CNN Model: The Transformer-CNN model also implemented the pre-training step. The model contains text-CNN block for several CNN layers. 1-d) BiLSTM-SA Model: The concept of the BiLSTM-SA model implemented a self-attention module without the multi-task learning scheme. All the three existing studies chose a dense layer as a final predictor, while we adopted the discrete output layer.

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Fusion of Global-Local Features for Image Quality Inspection of Shipping Label

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Abstract

The demands of automated shipping address recognition and verification have increased to handle a large number of packages and to save costs associated with misdelivery. A previous study proposed a deep learning system where the shipping address is recognized and verified based on a camera image capturing the shipping address and barcode area. Because the system performance depends on the input image quality, inspection of input image quality is necessary for image preprocessing.

In this paper, we propose an input image quality verification method combining global and local features. Object detection and scale-invariant feature transform in different feature spaces are developed to extract global and local features from several independent convolutional neural networks.

The conditions of shipping label images are classified by fully connected fusion layers with concatenated global and local features. The experimental results regarding real captured and generated images show that the proposed method achieves better performance than other methods. These results are expected to improve the shipping address recognition and verification system by applying different image preprocessing steps based on the classified conditions.

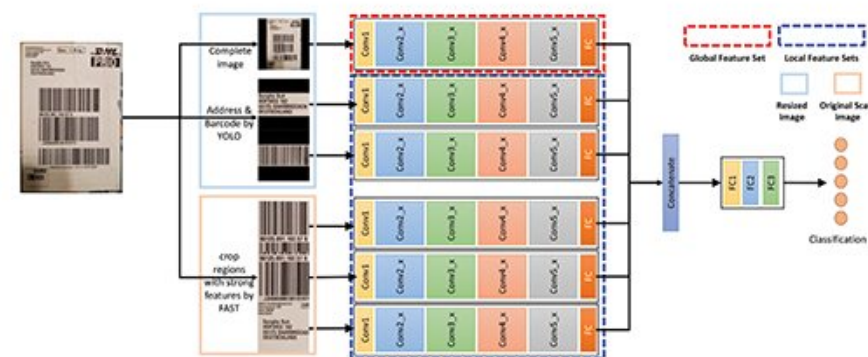


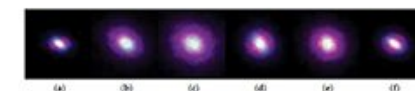
Fig. 4. Overall network architecture of the proposed method

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Relevant Patents (Deep Learning Applications)

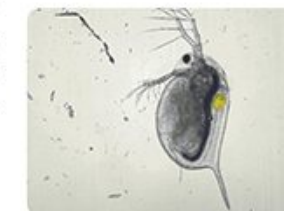
Rotary Machine Fault Detection

For data-driven fault diagnostics and prognostics, a method has been devised that uses Convolutional Neural Networks, after imaging the measured time-series data. Nested Scatter Plot is a image transformation method that provides high accuracy in bearing failure diagnosis and remaining life prediction by representing the correlation of multiple signals.



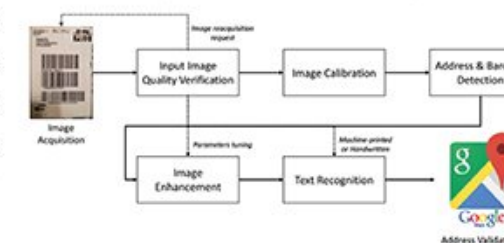
Ecotoxicology Risk Assessment

Changes in behavioral patterns due to toxicity exposure to Daphnia Magna and zebrafish can be detected using animal testing methods for chemical testing (refer to OECD Guidelines for the Testing of Chemicals, Section 2). The application of deep learning-based object segmentation enables the non-invasive, real-time measurement of data such as changes in the heart rate of Daphnia.



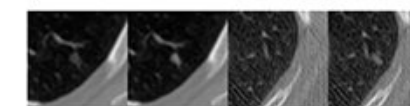
Shipping Label Inspection

The automated shipping address recognition and verification framework, consisting of deep learning based image pre-processings (ROI extraction, angle calibration, image binarization, image quality classification) is a solution for the logistics industry to bypass processes which result in deliveries being made to invalid addresses.



Medical Image Synthesis

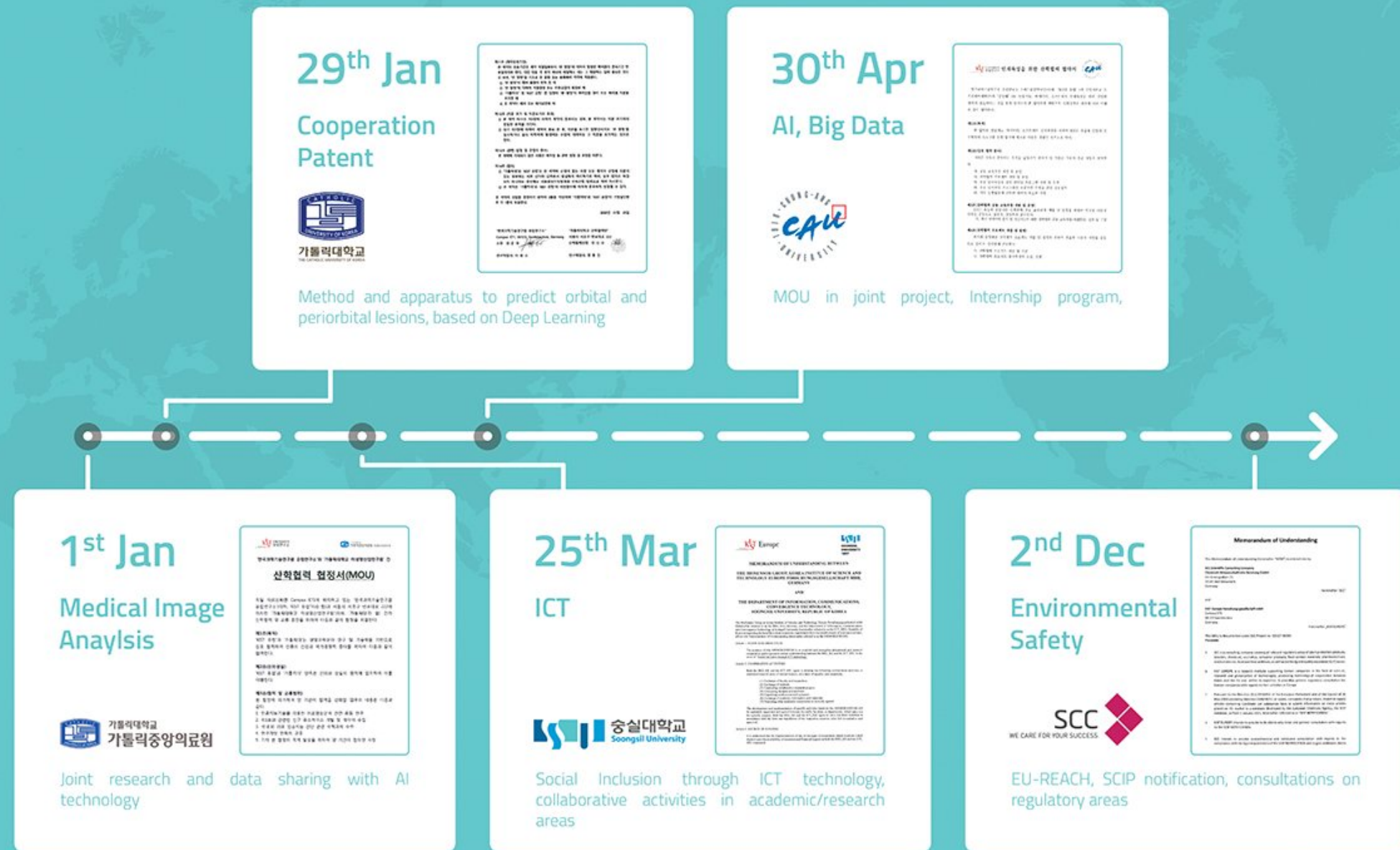
Deep learning has shown excellent performance in medical data analysis, but legal issues related to the protection of personal medical information has been a hurdle for big data collection. A model has been developed which can generate a synthesized lung nodule with adjustable features.



COOPERATION FOR THE FUTURE



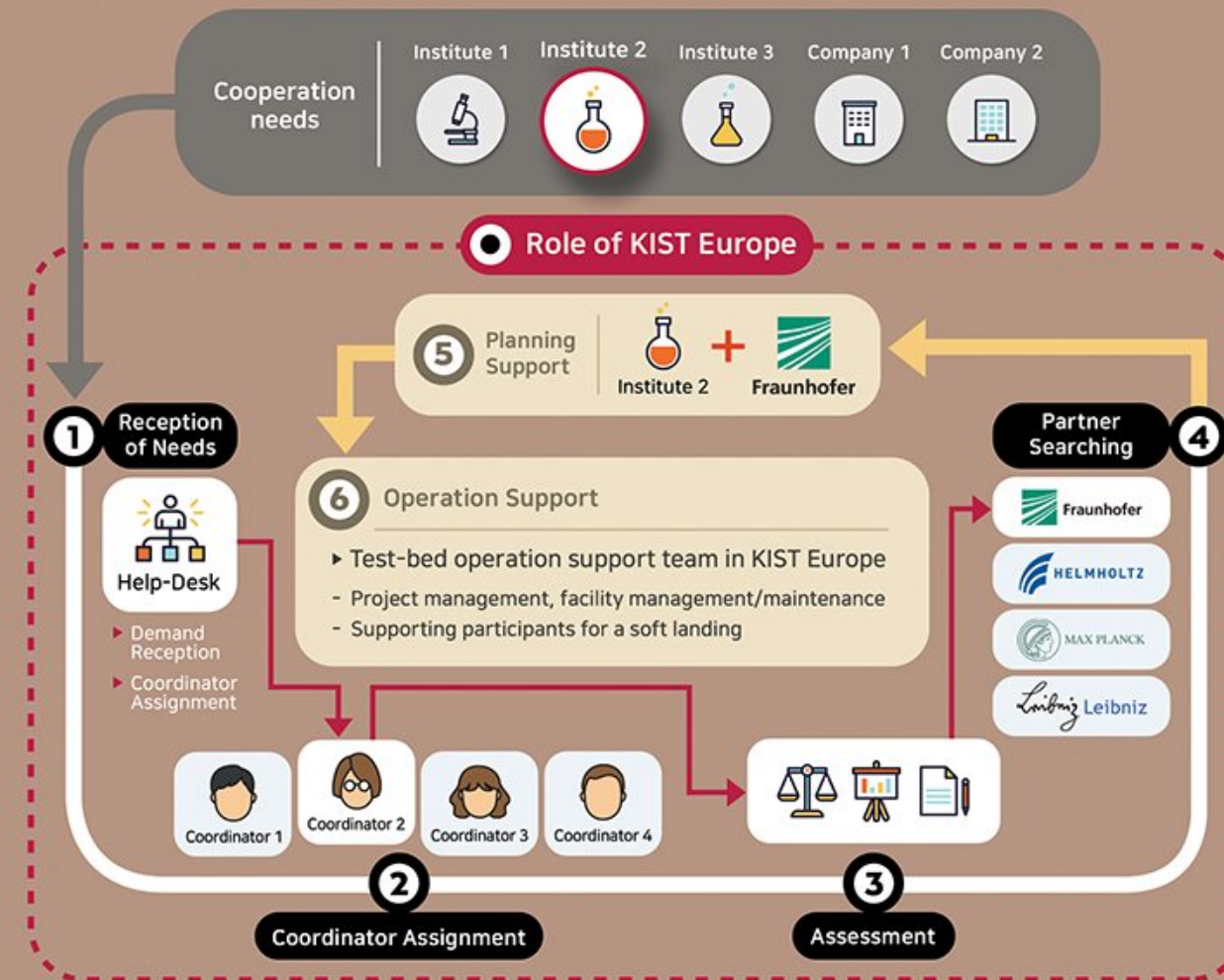
COOPERATION AGREEMENTS



COOPERATION PLATFORM

Open R&D Platform, KIST Europe Korea-EU R&D Cooperation Initiative

Support process for Cooperation Initiative



Definition of Cooperation Initiative

- Platform for on-site feasibility research on topics with high demand in Korea and countries in the EU
- Researchers from both countries can participate in research, with the support of KIST Europe's infrastructure

Category of Cooperation Initiative

- 1 in KIST Europe**
Role of KIST Europe Infra-Sharing
- 2 by KIST Europe**
Role of KIST Europe Partner-Searching
- 3 with KIST Europe**
Role of KIST Europe Joint-Research

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REPRESENTATIVE EVENTS

1 4th K-REACH Infoday

Date/Place 07th Feb 2020 / Bonn, Germany

Topic Consulting on K-REACH and K-BPR regulations to German & European companies

Organizers  Botschaft der Republik Korea Außenstelle Bonn 주독일 대한민국대사관 본분관 

Participants 



2 Kyungnam University Industry-Academic Cooperation Foundation

Date/Place 19th Feb 2020 / Saarbrücken, Germany

Topic Consultation and introduction on the university's industry-academic cooperation foundation in Germany and the Netherlands

Participants : 20



REPRESENTATIVE EVENTS

4 [Webinar] Introduction of SCIP under EU Waste Framework Directive

Date/Place 13th Oct 2020 / Saarbrücken, Germany

Topic Introduction and consultation on SCIP notification to Korean companies

Participants approx. 100 companies



3 Cooperation Talks with Delegation from Korean Embassy in Bonn

Date/Place 19th May 2020 / Saarbrücken, Germany

Topic Introduction on KIST Europe and data sharing of scientific issues

Visitors Science Attaché Mr. Kangwoo Lee
3rd Secretary Mr. Ingang Choi



REPRESENTATIVE EVENTS

5 Global Internship Program on MOUs



Overview

- Experience a long internship by taking part in laboratory activities
 - Signature Research Fields
 - Basic Research Fields



Eligibility

- * Must have a bachelor's or master's degree, or be expected to receive one
- * Must pass a document review
- * Must major in related research areas



Period

- * Runs officially two times a year
- * Generally begins in February & August



LOCATION



How to find KIST Europe

From Frankfurt Airport

Take the fast train (ICE/IC) or local train (RE/RB) from Frankfurt Airport to Saarbrücken Main Station. For more information, see: www.bahn.de (English version available)

Information for Navigation Systems

Stuhlsatzenhausweg 97
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Imprint



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